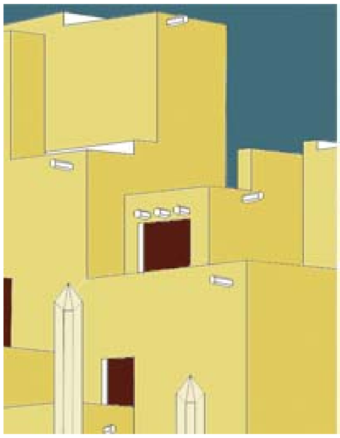
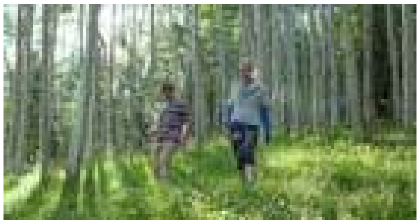


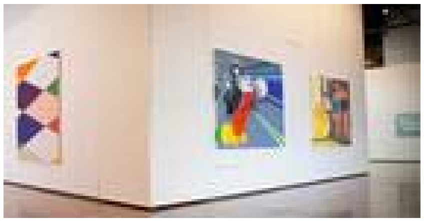
ACCGE-21
OMVPE-18

Santa Fe, New Mexico, USA
2017

Program Book

21st American Conference on Crystal Growth and Epitaxy (ACCGE-21)
and
18th US Workshop on Organometallic Vapor Phase Epitaxy (OMVPE-18)
and
3rd Symposium on 2D Electronic Materials
and
Symposium on Epitaxy of Complex Oxides





July 30 – August 4

Table of Contents

Welcome to Santa Fe, New Mexico

The American Association for Crystal Growth and the conference organizing committees are pleased to extend a warm and friendly welcome to all participants in:

- The 21st American Conference on Crystal Growth and Epitaxy (ACCGE-21)
- The 18th US Workshop on Organometallic Vapor Phase Epitaxy (OMVPE-18)

The jointly held conferences are composed of crosscutting and cutting-edge science and technology. Participants are encouraged to move about this technical landscape to maximize the interaction with their personal interests. Efforts have been made to set up the conference schedule to flow among topical areas and avoid overlapping of similar interest areas, but some conflicts are unavoidable due to the full program and wide range of interest areas of the attendees.

We trust that the outstanding technical program, the beautiful surroundings of Santa Fe, the hospitality of the Eldorado Hotel and Spa and the Hotel St. Francis, and the conference social program will make this a one-of-a-kind conference experience for all attendees, presenters, vendors, sponsors, and guests. It has been a pleasure for the committee to present this event to you and we wish you an excellent, enjoyable, and productive conference.

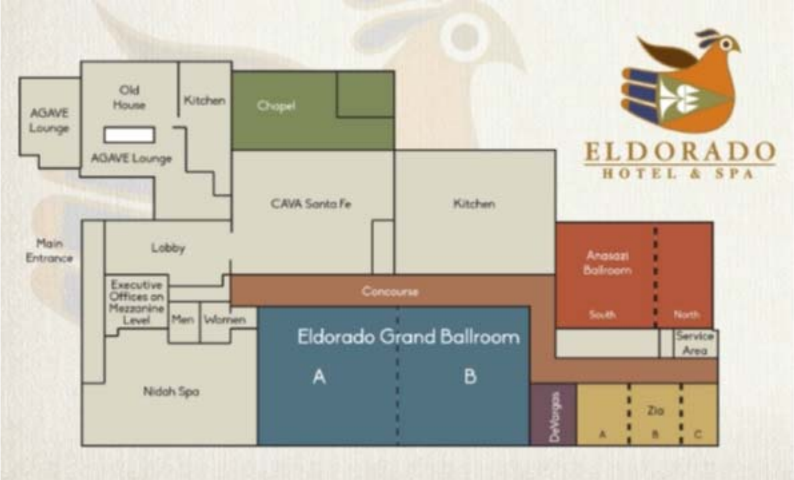
Kevin Zawilski
ACCGE-21 Conference Chair

Carlos Rojo
ACCGE-21 Program Chair

Dan Koleske
OMVPE-18 Conference and Program Co-Chair

Oliver Pitts
OMVPE-18 Conference and Program Co-Chair

Eldorado Floor Plan



St. Francis Floor Plan

Walking Route Between Hotels & Conference

Conference Sponsors and Supporters

At press time, the following companies and organizations have generously given their support to this meeting:

BAE Systems
Coherent Advanced Crystal Group
Crystal Photonics, Inc.
Elsevier BV – Journal of Crystal Growth
EMD Performance Materials
Heraeus
Matheson Tri-Gas, Inc.
Northrop Grumman - Synoptics
ProChem, Inc.
Sandia National Laboratories
The Olsen Foundation/GHO Ventures
Thermcraft, Incorporated

Conference Exhibitors

Visit the exhibit booth in the Eldorado Ballroom

AccuStrata
ADLT (APL Engineered Materials)
Aixtron
Ambrell Induction Heating
American GMG (AGMG)
Applied Ceramics
Dock/Chemicals
EMD Performance Group
Heraeus
Johnson Matthey
k-Space Associates, Inc.
Matheson Tri-Gas, Inc.
ProChem, Inc.
Schunk
SMI (Structured Materials)
STR Software
WEP
Zircar Ceramics, Inc.
Zircar Zirconia

Conference Organizers

ACCGE Conference Chair
Kevin Zawilski, BAE

ACCGE Program Chair
Carlos Rojo, GE

OMVPE Conference Co-Chairs and Program Co-Chairs
Dan Koleske, Sandia National Laboratories
Oliver Pitts, NRC Canada

Secretariat, Website, & Information Management
Shoshana Nash, American Association for Crystal Growth

Treasurer
Luis Zepeda, LLNL

Local Arrangements
Gregory Peake, Sandia National Laboratories
Dan Koleske, Sandia National Laboratories

Corporate Support
Vince Fratello, Quest Integrated
Candace Lynch, INRAD

Government Support
Edith Bourret-Courchesne, LBL
David Bliss, CapeSym
Lynn Boatner, Oak Ridge National Laboratory

Industrial Exhibit
Harry Niedecken, WirlNet Inc.

Publicity
Merry Koschan, University of Tennessee

ACCGE/ OMVPE Proceedings
Tania Paskova, North Carolina State University
Catherine Caneau, retired
Robert Feigelson, Stanford University

Photography Contest
Balaji Ragothamachar, Stonybrook University

AACG Awards

Tom Kuech, University of Wisconsin
Jeffrey Derby, University of Minnesota

Conference Planner
Dori Nielsen, American Association for Crystal Growth

OMVPE Workshop Program Committee (2017)

Andrew Allerman, Sandia National Laboratories
Robert Biefeld, Sandia National Laboratories
Russell Dupuis, Georgia Institute of Technology
John Geisz, National Renewable Energy Laboratory
Dan Koleske, Sandia National Laboratories
Luke Mawst, University of Wisconsin
Oliver Pitts, National Research Council of Canada
Simon Watkins, Simon Fraser University

AACG Organization (2015-2017)

President: Robert Biefeld (Sandia National Laboratories)
Vice President: Joan Redwing (Pennsylvania State University)
Treasurer: Luis Zepeda (Lawrence Livermore National Laboratory)
Secretary: Mariya Zhuravleva (University of Tennessee)
Executive Administrator: Shoshana Nash (AACG)

Executive Committee:

Gordon Banish
Robert Biefeld (Sandia National Laboratories)
Edith Bourret-Courchesne (Lawrence Berkeley National Laboratory)
Antoni Dabkowski (McMaster University)
Jeffrey Derby (University of Minnesota)
James DeYoreo (Lawrence Livermore National Laboratory)
Govindhan Dhanaraj (Aymont Technology, Inc.)
Dirk Ehrentraut (Soraa, Inc.)
Robert Feigelson (Stanford University)
Vincent Fratello (Quest Integrated, Inc.)
Kurt Gaskill (Naval Research Laboratory)
John Geisz (National Renewable Energy Laboratory)
Kenneth Jackson
David Kisailus (University of California Riverside)
Thomas Kuech (University of Wisconsin)
Candace Lynch (Inrad Optics, Inc.)
Irina Mnushkina (Integrated Photonics, Inc.)
Christine Orme (Lawrence Livermore National Laboratory)
Aleksandar Ostrogorsky (Illinois Institute of Technology)
Joan Redwing (Pennsylvania State University)
Juan Carlos Rojo (GE Global Research)
Peter Schunemann (BAE Systems, Inc.)
David Vanderwater
Peter Vekilov (University of Houston)
Christine A. Wang
Simon P. Watkins (Simon Fraser University)
Matt Whittaker (Gooch & Housego)
Andrew Yeckel (University of Minnesota)
Kevin Zawilski (BAE Systems, Inc.)
Luis Zepeda (Lawrence Livermore National Laboratory)
Mariya Zhuravleva (University of Tennessee)

Section Presidents:

WEST
Edith Bourret-Courchesne
Lawrence Berkeley Laboratory

TENNESSEE
Merry Koschan
University of Tennessee

AACGE Sessions

Fundamentals of Crystal Growth
Peter Vekilov, University of Houston

Bulk Crystal Growth
Robert Feigelson, Stanford University
Alex Ostrogorsky, Illinois Institute of Technology

Industrial Crystal Growth Technologies and Equipment
Matt Whittaker, Gooch & Housego

Detector Materials: Scintillators and Semiconductors
Mariya Zhuravleva, University of Tennessee, Knoxville
Gautam Gundiah, APL Engineered Materials, Inc.

Nonlinear Optical and Laser Host Materials
Kevin Stevens, Northrop Grumman-SYNOPTICS

Modeling of Crystal Growth Processes
Jeffrey Derby, University of Minnesota

Biological and Biomimetic Materials
Yu Huang, UCLA
Derk Joester, Northwestern University
Elia Beniash, University of Pittsburgh

Ferroelectric Crystals and Textured Ceramics (NEW)
Jun Luo, TRS Technologies
Rich Meyer, Penn State University

Joint Sessions AACGE / OMVPE

Bulk Growth and Epitaxy for Power Electronics (NEW)
Mike Dudley, Stony Brook University
Balaji Raghothamachar, Stony Brook University

Nanocrystals, Quantum Dots, and Nanowires
Kris Bertness, NIST
Daniel Feezell, University of New Mexico

III/V Nitride and Other WBG Semiconductors
Dirk Ehrentraut, SORAA
Nelson Tansu, Lehigh

Materials for Photovoltaics and Other Energy Technology
John Geisz, NREL

Thin Film Growth, Epitaxy, and Superlattices
Andrey Krysa, University of Sheffield
Toby Garrod, II-VI epiwork

OMVPE Sessions

OMVPE of Compound Semiconductors for Optoelectronics
Sugiyama Masakazu, University of Tokyo

OMVPE of Wide Bandgap Materials for Opto- and Power-Electronics
Yuji Zhao, Arizona State University

OMVPE of Narrow Bandgap Semiconductors
Simon Watkins, Simon Fraser University

Novel OMVPE Techniques and In-Situ Monitoring
Matt Highland, Argonne National Laboratory

Symposia

3rd Symposium on 2D Electronic Materials
Kurt Gaskill, NRL
Joan Redwing, Penn State

Symposium on Epitaxy of Complex Oxides
Ho Nyung Lee, ORNL
Darrell Schlom, Cornell
Lane Martin, University of California, Berkeley

Plenary Speakers

Gerald B. Stringfellow
“Thermodynamic Considerations for Epitaxial Growth of III/V Compounds”
Presentation - Monday, July 31, 2017, 8:30 AM

Gerald B. Stringfellow is a Distinguished Professor in the Department of Materials Science and Engineering and the Department of Electrical and Computer Engineering at the University of Utah. He is the former Dean of the College of Engineering. Before his university career, he was a group manager at Hewlett Packard Laboratories, Palo Alto, California.

He has received numerous awards, most notably, membership in the National Academy of Engineering. These awards include: Frank Prize of IOCG, Fellow of IEEE, Bardeen Award of TMS, the AACG Crystal Growth Award, the von Humboldt US Senior Scientist Award, and the highest award of the University of Utah, the Rosenblatt Prize. He also served as Principal Editor of the Journal of Crystal Growth, and on the editorial boards of many publications.

The research interests of Professor Stringfellow center on the chemistry, epitaxial crystal growth, properties, and device applications of new semiconductor materials, particularly the III/V compounds and alloys. Stringfellow began working on materials for light emitting diodes (LEDs) in 1966 and was among the pioneers of the organometallic vapor phase epitaxial (OMVPE) growth technique, beginning his work in this area in 1975. His work emphasizes the materials science aspects of OMVPE growth. The OMVPE technique is the basic technique now used in the multi-billion-dollar compound semiconductor device industry for light emitting diodes, injection lasers, detectors, and solar cells.

Mercouri G. Kanatzidis
“New Hard Radiation Detection Semiconductor Materials”
Presentation - Monday, July 31, 2017, 9:15 AM

Mercouri G. Kanatzidis is a Professor of Chemistry and of Materials Science and Engineering at Northwestern University in Evanston, Illinois. He also has a senior scientist appointment at Argonne National Laboratory. His interests include the design and synthesis of new materials with emphasis on systems with highly unusual structural/physical characteristics or those capable of energy conversion, energy detection, environmental remediation, and catalysis. After obtaining his B.Sc. degree from Aristotle University in Greece, he received his Ph.D. degree in Chemistry from the University of Iowa and was a postdoctoral research fellow at the University of Michigan and Northwestern University. He holds a Charles E. and Emma H. Morrison Professor Chair at Northwestern University and is the Editor in Chief of the Journal of Solid State Chemistry.

Award Recipients

Criteria for selection for both AACG awards are scientific excellence, clarity of presentation and impact on the field of crystal growth.

Christine A. Wang
American Association of Crystal Growth Award
Presentation - Tuesday, August 1, 2017 8:30 AM

The AACG award is presented for outstanding contributions to the field of crystal growth and epitaxy.

Award Citation: For seminal and innovative contributions to epitaxial crystal growth of III-V compounds semiconductors and the design of high-performance OMVPE reactors.

Bharat Jalan
American Association of Crystal Growth Young Scientist Award
Presentation - Tuesday, August 1, 2017 9:15 AM

The AACG Young Scientist Award is given to an early career scientist working in the fields of crystal growth research, development, practice, theory, modeling, characterization, application or production to recognize his or her outstanding scientific and technical contributions in the field of crystal growth. This award is made based on published papers, patents, conference presentations, products or teaching coming from the candidate's work.

Award Citation: For pioneering work in the development of new growth approaches to synthesize complex oxide heterostructures.

Scope and Purpose of the Conferences

Crystal growth is a broad field that attracts people from a wide variety of disciplines. The purpose of the conference is to bring together scientists and engineers to discuss the entire breadth of activities in crystal growth from bulk to nano, fundamentals to characterization, modeling to equipment design, every type of epitaxy and every type of material from elemental to biological. The conferences feature symposia on important new topics in crystal growth as well as more traditional subjects of enduring interest. Focused and joint sessions have been organized based on the topical distribution of papers and to foster cross-fertilization among fields. While the presentations are the core of the conference schedule, it is the personal interactions with colleagues across the spectrum of crystal growth that give strength to the experience of this meeting and an opportunity to explore fully the issues of importance in the field. The crystal growth community is unique in that the vendor community is intimately integrated with the technical community and the vendor exhibit will give everyone a chance to form and renew commercial and technical relationships. A single registration fee gives attendees access to the ACCGE-21, OMVPE-18, and the topical symposia.

ACCGE-21 will provide a forum for the presentation and discussion of recent research and development activities in all aspects of epitaxial thin film and bulk crystal growth; sessions will integrate fundamentals, experimental and industrial growth processes, characterization and applications. The meeting will focus on a wide range of crystal growth science issues.

The OMVPE-18 Workshop continues a tradition, started at Cornell in 1983, of bringing together specialists in the OMVPE field from industry, academia and government laboratories in an informal atmosphere and scenic surroundings. The workshop is an excellent opportunity to present and discuss new results in the OMVPE field. It also provides a venue for newcomers to the field to familiarize themselves with OMVPE science and technology.

Practical Information

The weather during August in Santa Fe will be warm/hot during the day and cool at night with very low humidity. It is a good idea to bring water along on any tours or walks around the area. Attendees are cautioned that Santa Fe is at a rather high elevation (7200 feet or 2200 m) and that some guests may experience difficulties at first with the altitude. In order to avoid experiencing "mountain sickness" guests are encouraged to limit their physical exertion for the first day or two and to drink plenty of water. For some guests, the consumption of alcoholic beverages may aggravate these effects. If you have issues with high altitude, it would be wise to fly into Albuquerque (5300 feet or 1600 m) and spend the night before driving up to Santa Fe.

It is the responsibility of the conference attendees and their families to have their own health insurance. Costs for medical care while attending the conference cannot be provided by the conference organizing committee, the AACG or its officers.

Proceedings

The Proceedings will be published as a special issue of the *Journal of Crystal Growth*.

Manuscript submission deadline: September 1, 2017

Authors who have a paper accepted for oral or poster presentations at the 21st American Conference on Crystal Growth and Epitaxy/18th US Biennial Workshop on Organometallic Vapor Phase Epitaxy are invited to submit manuscripts for consideration for publication in the conference proceedings. The length of the papers in the Proceedings is limited to four printed pages for regular contributed papers, five printed pages for invited papers and six printed pages for plenary invited papers.

The manuscripts submitted will undergo a peer review process similar to regular publications.

Only work **presented** at the conference and that has not been published, nor is in press, or submitted for publication elsewhere will be considered for inclusion in the Proceedings.

Formatting instructions:

Please follow the formatting recommendations on the website. All manuscripts will be subject to the review process; submissions will be rejected if they do not describe original, unpublished work or are not of high quality. A single printed column (text only) in the Journal of Crystal Growth is approximately 480 words. Please keep the page length limit in mind when preparing your manuscript.

Submission instructions:

Please submit manuscripts using the Elsevier Editorial System which will be located on the AACG website at: www.crystalgrowth.org.

Proceedings Editors,

Tania Paskova, North Carolina State University
Catherine Caneau, retired
Robert Feigelson, Stanford University

Wednesday Afternoon Excursions

Option #1:

Float / Rafting Trip
Wednesday, August 2, 12:00 p.m. - 5:00 p.m.

One of America's most popular adventures, whitewater rafting is becoming a tradition for visitors to Northern New Mexico. The rafting season begins with the snowmelt in spring and generally, lasts through October. The runoff will be lower in August, so the rapids will be less intense and there will be some floating. All levels of rafters, from the novice to the expert, will enjoy this adventure along the Rio Grande. Along the valley floor, experience spectacular scenery, with a full range of whitewater on the "Racecourse" south of Taos.

Due to safety regulations, no one under the age of seven years old or in excess of 230 pounds will be permitted to participate in this event. Waterproof suits and helmets can be provided upon request. If desired, bring extra clothing to change into at the take-out point.

COST: $150 per person includes transportation, guide, bottled water and boxed lunch on board, half-day rafting, rafting guides and all gear, gratuities and tax. Space is limited.

Option #2:

Discover Canyon Road (interactive art tour)
Wednesday, August 2, 2:00pm – 4:00pm

For over a century, artists and art lovers have flocked to Canyon Road, Santa Fe's historic art district. This picturesque area features more than 80 art galleries, unique specialty shops, world-class restaurants, and the historic adobe architecture that gives Santa Fe its legendary southwestern charm. On this interactive gallery tour, join your guide, a local art historian and museum educator, for an insider's look at a small selection of galleries that showcase the breadth and depth of artwork on Canyon Road. Delve into the work on view through activities that encourage deep looking, chat with local artists and gallerists, and discover the history of this charming neighborhood.

COST: $50 per person includes transportation, guide, gratuities and tax. Limit of 24 participants.

Presentation and Poster Instructions

Oral

Each room will have an LCD projector, laser pointer, and microphone. PC laptop computers will be provided by the conference and available for presentations. Please arrive at least 15 minutes before the session begins in order to either load your presentation on the conference laptop or check the connection between your computer and the projector. Note that time lost switching between computers or due to non-functioning computer graphics presentations will be deducted from the speaker's allotted presentation time.

Please direct any presentation questions to the chair for your session.

Time slots:

- Plenary and Prize talks are 45 minutes total (40 min. presentation, 5 min. questions)
- Invited ACCGE talks are 30 minutes total (25 min. presentation, 5 min. questions)
- Contributed ACCGE talks are 15 minutes total (12 min. presentation, 3 min. questions)
- Contributed OMVPE and joint ACCGE/OMVPE talks are 20 minutes total (17 min. presentation, 3 min. questions)

Posters

Posters must fit in a 3' wide x 4' tall space. Push pins will be available in the poster area. Posters sessions are scheduled for Monday and Tuesday afternoons from 5:00 – 7:00pm in the Eldorado Ballroom. Please mount your poster from 2:30 – 5:00 pm on the day of the presentation. Individual poster boards will be identified with poster numbers. Please check the list in the room to determine the number of your poster and mount your poster in the correct space. You or a co-author are expected to be present at your poster during the entire session to answer questions.

Please remove your poster in a timely manner at the end of your poster session.

Schedule Overview

(*) St Francis DeVargas room is located in the St Francis Hotel
(**) Special Q&A session - "What they don't teach you about industrial crystal growth in school"

Technical Program Schedule

Sunday, July 30, 2017

15:00 – 18:00
Registration
CAVA/Lobby

18:00 – 19:00
Welcome Reception
Casa Espana

	Monday 7/31					
Room	Anasazi South	Anasazi North	Chapel Room	Zia	Eldorado (A+B)	St. Francis DeVargas (*)
7:30-8:00	BREAKFAST					
8:00-10:00	INTRO & PLENARY					
10:00-10:30	COFFEE BREAK					
10:30-12:00	FUNDAMENTALS 1	DETECTORS 1	NLO/Laser 1	3rd Symp on 2DEM 1	VENDOR	BIO MAT'LS 1
12:00-13:30	LUNCH					
13:30-15:00	FUNDAMENTALS 2	DETECTORS 2	NLO/Laser 2	3rd Symp on 2DEM 2	VENDOR	BIO MAT'LS 3
15:00-15:30	COFFEE BREAK					
15:30-17:00	FUNDAMENTALS 3	DETECTORS 3	NLO/Laser 3	3rd Symp on 2DEM 3	VENDOR/ POSTER SETUP	BIO MAT'LS 3
17:00-17:30					POSTERS – 1	
17:30-18:00						
18:00-19:00						
19:00-21:00	OMVPE – WBG					

(*) St Francis DeVargas room is located in the St Francis Hotel

Monday, July 31, 2017

8:00 – 10:00
Introduction/Plenary
Anasazi Ballroom

Moderation: Kevin Zawilski, BAE

8:00 – 8:30
Welcome
Kevin Zawilski
Robert Biefeld

8:30 – 9:15
Gerald B. Stringfellow
Invited
"Thermodynamic Considerations for Epitaxial Growth of III/V Compounds"

9:15 – 10:00
Mercouri G. Kanatzidis
Invited
"New Hard Radiation Detection Semiconductor Materials"

10:30 - 12:00
Monday, July 31, 2017
Detector Materials (1 of 5)
Anasazi Ballroom North

Moderation: Gautam Gundiah[1]; Mariya Zhuravleva[2]; [1]APL/US, [2]TN/Us

10:30 - 11:00
THE ELIMINATION OF SUZUKI PHASE PRECIPITATES FROM SINGLE CRYSTALS OF DIVALENT-ION-DOPED ALKALI HALIDES: IMPROVED SCINTILLATORS FOR RADIATION DETECTION
Lynn Boatner[1]; Eleanor Comer[2]; Gomez Wright[2]; Joanne Ramey[2]; Richard Riedel[2]; Gerald Jellison[2]; James Kolopus[2]; [1]ORNL, TN/Us, [2]Oak Ridge National Laboratory, TN/Us

11:00 - 11:15
STRUCTURE AND THERMAL EXPANSION OF CSCAI3:EU AND CSSRBR3:EU SCINTILLATORS
Matthew Loyd[1]; Adam Lindsey[2]; Maulik Patel[1]; Charles Melcher[3]; Mariya Zhuravleva[1]; [1]University of Tennessee, TN/Us, [2]Scintillation Materials Research Center, TN/Us, [3]University of Tennessee-Knoxville, TN/Us

11:15 - 11:30
GROWTH AND LUMINESCENCT PROPERTIES OF $\mathrm{CS_2HFI_6}$-BASED SINGLE CRYSTAL SCINTILLATORS
Shohei Kodama[1]; Shunsuke Kurosawa[2]; Akihiro Yamaji[3]; Jan Pejchal[4]; Robert Kral[5]; Yuji Ohashi[6]; Kei Kamada[6]; Yuui Yokota[7]; Martin Nikl[8]; Akira Yoshikawa[3]; [1]Institute for Materials Research, Jp, [2]Department of Physics, Yamagata University, Jp, [3]Institute for Materials Research, Tohoku University, Jp, [4]Institute of Physics CAS, , [5]Institute of Physics of the Czech Academy of Sciences, Cz, [6]NICHe, Tohoku University, Jp, [7]Tohoku University, Jp, [8]Institute of Physics, Czech Academy of Sciences, Cz

11:30 - 11:45
CRYSTAL GROWTH OF CESIUM HAFNIUM CHLORIDE SCINTILLATORS
Stephanie Lam[1]; Arnold Burger[2]; Shariar Motakef[1]; [1]CapeSym Inc., MA/Us, [2]Fisk University, TN/Us

11:45 - 12:00

EFFECTS OF CA/SR RATIO CONTROL ON OPTICAL AND SCINTILLATION PROPERTIES OF EU-DOPED LI(CA,SR)ALF$_6$ SINGLE CRYSTALS
Yuui Yokota[1]; Chieko Tanaka[1]; Shunsuke Kurosawa[2]; Akihiro Yamaji[3]; Yuji Ohashi[4]; Kei Kamada[4]; Martin Nikl[5]; Akira Yoshikawa[3]; [1]Tohoku University, Jp, [2]Department of Physics, Yamagata University, Jp, [3]Institute for Materials Research, Tohoku University, Jp, [4]NICHe, Tohoku University, Jp, [5]Institute of Physics, Czech Academy of Sciences, Cz

10:30 - 12:00
Monday, July 31, 2017
Fundamentals of Crystal Growth (1 of 9)
Anasazi Ballroom South

Moderation: Peter. Vekilov, U of Houston/US

10:30 - 11:00
WHAT DETERMINES A NUCLEATION PATHWAY?
Yuki Kimura, Institute of Low Temperature Science, Hokkaido University., Jp

11:00 - 11:30
CLASSICAL OR MULTI-STEP NUCLEATION
Dominique Maes[1]; James Lutsko[2]; Sander Stroobants[1]; Mike Sleutel[1]; Sudha Chinnu[1]; Marco Potenza[3]; Peter Vekilov[4]; [1]Vrije Universiteit Brussel, Be, [2]Universite Libre de Bruxelles, Be, [3]University of Milano, It, [4], Us

11:30 - 12:00
LA MER BURST NUCLEATION AND GROWTH: ASSUMPTIONS, MODELS, AND DATA
Baron Peters, University of California - Santa Barbara, Us

10:30 – 11:30
Monday, July 31, 2017
Nonlinear Optical and Laser Host Materials (1 of 3)
Chapel Room

Moderation: Kevin Stevens, Northrop Grumman-SYNOPTICS//US

10:30 - 11:00
SOME CURRENT DEVELOPMENTS IN HYDROTHERMAL CRYSTAL GROWTH OF BORATES FOR UV NONLINEAR OPTICS
Joseph Kolis; Colin McMillen; Rylan Terry; Henry Giesber; Clemson University, SC/Us

11:00 - 11:15
SYNTHESIS, GROWTH AND CHARACTERIZATION OF NOVEL NONLINEAR OPTICAL MATERIAL: 4-FLUOROBENZYL TRIPHENYLPHOSPHONIUMCHLORIDE
Arul Haribabu[1]; K Sugandhi[1]; S Bharathi[2]; A Jeya Rajendran[2]; K Eswara Moorthi[2]; M P Kannan[2]; [1]Department of Science and Humanities, Kumaraguru College of Technology (Autonomous), In, [2]Advanced Materials Research Laboratory, Department of Chemistry, Loyola College, In

11:15 - 11:30
MEASUREMENTS OF D COEFFICIENTS OF SOME CUBIC CRYSTALS AT INFRARED WAVELENGTHS
Joel Murray[1]; Jean Wei[1]; Shekhar Guha[2]; [1]UES, Inc., OH/Us, [2]Air Force Research Laboratory, OH/Us

10:30 - 12:00
Monday, July 31, 2017
Biological and Biomimetic Materials (1 of 3)

St Francis De Vargas

Moderation: Derk Joester[1]; Elia Beniash[2]; Yu Huang[3]; [1] Northwestern U/US, [2]University of Pittsburgh/US, [3]UCLA/US

10:30 - 11:00
ASSEMBLY OF VIRUS NANOREACTORS
Trevor Douglas, Indiana University, Us

11:00 - 11:30
BIO-INSPIRED CRYSTAL GROWTH OF TRANSITION METAL OXIDES IN CONFINEMENT
Lara Estroff, Cornell University, NY/Us

11:30 - 11:45
NOVEL BIO-INSPIRED SEMICONDUCTOR/AMINO ACID COMPOSITE SINGLE CRYSTALS: FROM CRYSTAL GROWTH TO BAND GAP ENGINEERING
Iryna Polishchuk[1]; Boaz Pokroy[2]; [1]Technion, Il, [2]Technion Institute of Technology, Il

11:45 - 12:00
DESIGN AND SYNTHESIS OF FUNCTIONALIZED SELF-ASSEMBLED MONOLAYERS (SAMS) AS IN VITRO MODEL OF THE ORGANIC INTERFACES IN THE SITE-SELECTIVE MINERALIZATION PROCESS IN THE CHITON TOOTH.
Linus Stegbauer[1]; Derk Joester[2]; [1]Northwestern University, MSE, Us, [2]Northwestern University, IL/Us

10:30 - 12:00
Monday, July 31, 2017

3rd Symposium on 2D Electronic Materials (1 of 6)
Zia Ballroom

Moderation: Kurt Gaskill[1]; JoanM. Redwing[2]; [1]NRL/US, [2]PennState/US

10:30 - 11:00
TEMPLATED CVD OF LARGE-AREA WS_2 WITH OHMIC GRAPHENE EDGE CONTACTS
Michael Fuhrer, Monash University, VIC/Au

11:00 - 11:20
OPTIMIZING TRANSITION METAL DISULFIDE METALORGANIC CHEMICAL VAPOR DEPOSITION PROCESSES USING NON-DISPERSIVE INFRARED GAS ANALYZERS
James Maslar[1]; Berc Kalanyan[2]; Brent Sperling[1]; William Kimes[1]; Ravindra Kanjolia[3]; [1]NIST, Us, [2]National Institute of Standards and Technology, Us, [3]EMD Performance Materials, MA/Us

11:20 - 11:40
OPTIMIZATION OF MOVPE OF 2D MOS_2
M Heuken[1]; M Marx[2]; Y -R Lin[2]; H Kalisch[2]; A Vescan[2]; A Grundmann[2]; [1], , [2]RWTH Aachen University, De

11:40 - 12:00
EPITAXIAL GROWTH OF MOLYBDENUM DISULFIDE ON GALLIUM NITRIDE
Robert Burke[1]; Kehao Zhang[2]; Dmitry Ruzmetov[1]; Andrew Herzing[3]; Glen Birdwell[1]; Mahesh Neupane[1]; Terrance O'regan[1]; Barbara Nichols[1]; Matt Chin[1]; Alex Mazzoni[1]; Albert Davydov[3]; Joshua Robinson[2]; Madan Dubey[1]; Tony Ivanov[1]; [1]US Army Research Laboratory, MD/Us, [2]The Pennsylvania State University, PA/Us, [3]National Institute of Standards and Technology, MD/Us

13:30 - 15:00

Monday, July 31, 2017
Detector Materials (2 of 5)
Anasazi Ballroom North

Moderation: Gautam Gundiah[1]; Mariya Zhuravleva[2]; [1]APL/US, [2]TN/Us

13:30 - 13:45
PHASE EQUILIBRIA AND SEGREGATION IN BRIDGMAN GROWTH OF CS_2LIYCL_6
Frank Ruta[1]; Robert Feigelson[1]; Stacy Swider[2]; Stephanie Lam[2]; [1]Stanford University, CA/Us, [2]CapeSym Inc., MA/Us

13:45 - 14:15
HIGH-THROUGHPUT GROWTH OF SRI_2(EU) AND CLYC SCINTILLATORS BY THE EFG METHOD
Stacy Swider[1]; George Calvert[2]; Matthew Overholt[1]; Frank Ruta[2]; Robert Feigelson[2]; [1]CapeSym Inc., MA/Us, [2]Stanford University, MA/Us

14:15 - 14:45
PULSED NEUTRON IMAGING STUDIES OF IN SITU GROWTH OF NEUTRON AND GAMMA DETECTOR MATERIALS
John Z Larese; Christopher Crain; Nicholas Strange; University of Tennessee, TN/Us

14:45 - 15:00
SIMULTANEOUS GROWTH OF 38 MM DIAMETER $KCAI_3$:EU SCINTILLATOR
Matthew Loyd[1]; Luis Stand[2]; Charles Melcher[3]; Mariya Zhuravleva[1]; [1]University of Tennessee, TN/Us, [2]Scintillation Materials Research Center, University of Tennessee, TN/Us, [3]University of Tennessee-Knoxville, TN/Us

13:30 - 15:00
Monday, July 31, 2017
Fundamentals of Crystal Growth (2 of 9)

Moderation: Peter. Vekilov, U of Houston/US
Anasazi Ballroom South

13:30 - 14:00
IMPACT OF ADDITIVES ON THE CRYSTALLIZATION OF PHARMACEUTICAL SUBSTANCES
Lynne Taylor, Purdue University, IN/Us

14:00 - 14:30
NUCLEATION OF CRYSTALS OF HARD POLYHEDRA
Julia Dshemuchadse; Samanthule Nola; Richmond Newman; Sharon Glotzer; University of Michigan, MI/Us

14:30 - 15:00
SMALL-VOLUME NUCLEATION
Stéphane Veesler; N Candoni; R Grossier; R Morin; CINaM-CNRS, Fr

13:30 - 15:00
Monday, July 31, 2017
Nonlinear Optical and Laser Host Materials (2 of 3)
Chapel Room

Moderation: Kevin Stevens, Northrop Grumman-SYNOPTICS /US

13:30 - 14:00

ADVANCES IN NONLINEAR OPTICAL CRYSTALS FOR THE MID-INFRARED
Peter Schunemann, BAE Systems, NH/Us

14:00 - 14:30
THERMO-OPTIC AND STRESS-OPTIC PROPERTIES OF CADMIUM SILICON PHOSPHIDE
David Zelmon[1]; William Poston[2]; John Kunkel[2]; [1]Air Force Research Laboratory, Us, [2]US Air Force Research Laboratory, OH/Us

14:30 - 14:45
ADVANCES SINGLE CRYSTAL $CDSIP_2$ FOR HIGH ENERGY MID-INFRARED GENERATION
Kevin Zawilski[1]; Peter Schunemann[1]; F Kenneth Hopkins[2]; [1]BAE Systems, NH/Us, [2]Air Force Research Laboratory, AFRL/RX, OH/Us

14:45 - 15:00
OPTICAL ABSORPTION BANDS IN CDSIP2 CRYSTALS
Elizabeth Scherrer[1]; Brant Kananen[1]; Nancy Giles[1]; Larry Halliburton[2]; F Kenneth Hopkins[3]; Peter Schunemann[4]; Kevin Zawilski[4]; [1]Air Force Institute of Technology, Us, [2]West Virginia University, WV/Us, [3]Air Force Research Laboratory, AFRL/RX, OH/Us, [4]BAE Systems, NH/Us

13:30 - 15:00
Monday, July 31, 2017
Biological and Biomimetic Materials (2 of 3)
St Francis De Vargas

Moderation: Derk Joester[1]; Elia Beniash[2]; Yu Huang[3]; [1] Northwestern U/US, [2]University of Pittsburgh/US, [3]UCLA/US

13:30 - 14:00
ANTIMALARIALS INHIBIT HEMATIN CRYSTALLIZATION BY UNIQUE DRUG-SURFACE SITE INTERACTIONS
Peter Vekilov, , Us

14:00 - 14:30
THE SECONDARY AND QUATERNARY STRUCTURE OF AMELOGENIN ON HYDROXYAPATITE
Wendy Shaw[1]; Rajith Arachchige[1]; Sarah Burton[1]; Junxia Lu[2]; Yimin Xu[1]; Jinhui Tao[1]; Barbara Tarasevich[1]; Garry Buchko[1]; [1]Pacific Northwest National Laboratory, WA/Us, [2]Shanghai Tech, Cn

14:30 - 14:45
SPECIFIC AND NON-SPECIFIC INTERACTIONS WITH GROWING CALCITE CRYSTALS -LIVE IMAGING AFM STUDIES
Amir Berman; Bidisha Tah; Ben-Gurion University, Il

14:45 - 15:00
QUANTIFYING CRYSTALLIZATION KINETICS OF AMORPHOUS CALCIUM CARBONATE USING DROPLET MICROFLUIDICS
Jack Cavanaugh; Michael Whittaker; Derk Joester; Northwestern University, IL/Us

13:30 - 15:00
Monday, July 31, 2017
3rd Symposium on 2D Electronic Materials (2 of 6)
Zia Ballroom

Moderation: Kurt Gaskill[1]; JoanM. Redwing[2]; [1]NRL/US, [2]PennState/US

13:30 - 14:00

STUDIES OF LOCAL ELECTRONIC PROPERTIES IN GRAPHENE AND 2D MATERIALS
Olga Kazakova, NPL, Gb

14:00 - 14:20
INFLUENCE OF SUBSTRATE ON THE GROWTH AND PROPERTIES OF THIN 3R NBS2 FILMS GROWN BY CHEMICAL VAPOR DEPOSITION.
Azimkhan Kozhakhmetov[1]; Tanushree Choudhury[2]; Zakaria Al Balushi[1]; Yixuan Chen[3]; Ying Liu[3]; Joan Redwing[2]; [1]Dept. of Materials Science and Eng., The Pennsylvania State University, PA/Us, [2]The Pennsylvania State University, PA/Us, [3]Department of Physics, The Pennsylvania State University, PA/Us

14:20 - 14:40
GROUP IV CHALCOGENIDES: EMERGING 2D AND LAYERED SEMICONDUCTORS
Peter Sutter[1]; Yuan Huang[2]; Hannu-Pekka Komsa[3]; Arkady Krasheninnikov[4]; Eli Sutter[5]; [1]University of Nebraska-Lincoln, NE/Us, [2]Brookhaven National Laboratory, Us, [3]Aalto University, Fi, [4]Helmholz-Zentrum Dresden-Rossendorf, De, [5],

14:40 - 15:00
VAPOR PHASE EPITAXY OF HEXAGONAL BORON NITRIDE ON SAPPHIRE
Anthony Rice[1]; Andrew Allerman[2]; Mary Crawford[2]; Thomas Beechem[2]; Taisuke Ohta[2]; Douglas Medlin[2]; Catalin Spataru[2]; Jeffrey Figiel[2]; Michael Smith[2]; [1]Sandia National Laboratories, NM/Us, [2]Sandia National Laboratories, Us

15:30 – 16:45
Monday, July 31, 2017
Detector Materials (3 of 5)
Anasazi Ballroom North

Moderation: Gautam Gundiah[1]; Mariya Zhuravleva[2]; [1] APL/US, [2]TN/Us

15:30 - 15:45
MITIGATION OF SECOND-PHASE PARTICLES IN SINGLE CRYSTALS VIA POST-GROWTH TREATMENT: TEMPERATURE GRADIENT ZONE MELTING AND ANNEALING
Nathan Morgan[1]; Kerry Wang[2]; Jeffrey Derby[1]; [1]University of Minnesota, MN/Us, [2]University of Minnesota - Twin Cities, MN/Us

15:45 - 16:00
MODELING AND EXPERIMENTAL ANALYSIS OF ZINC DISTRIBUTION AND DISLOCATION DENSITY EVOLUTION IN CZT BRIDGMAN CRYSTAL GROWTH
Alex Galyukov[1]; Vladimir Artemyev[2]; Andrey Smirnov[2]; Vasif Mamedov[2]; Vladimir Kalaev[2]; Zhou Changhe[3]; Chao Xu[3]; Shiwen Sun[3]; [1]STR US, Inc., VA/Us, [2]STR Group, Inc. – Soft-Impact, Ltd., Ru, [3]Shanghai Institute of Technical Physics, Chinese Academy of Sciences, Cn

16:00 - 16:15
TOWARDS OPTIMIZATION OF ACRT SCHEDULES APPLIED TO THE GRADIENT FREEZE GROWTH OF CADMIUM ZINC TELLURIDE
Mia Divecha[1]; Jedidiah McCoy[2]; Kelvin Lynn[2]; Jeffrey Derby[3]; [1]University of Minnesota, Us, [2]Washington Stat University, WA/Us, [3]University of Minnesota, MN/Us

16:15 - 16:30
ALTERNATIVE CRYSTAL GROWTH TECHNIQUES FOR THALLIUM BROMIDE SEMICONDUCTOR RADIATION DETECTORS
AMLAN Datta[1]; Piotr Becla[1]; Kris Becla[1]; Shariar Motakef[2]; [1]CapeSym, Inc., MA/Us, [2]CapeSym Inc., MA/Us

16:30 - 16:45
ANISOTROPIC AND TEMPERATURE-DEPENDENT THERMAL CONDUCTIVITY OF LEAD IODIDE

Arne Croell[1]; Justus Tonn[2]; Ekkehard Post[3]; Harald Böttner[4]; Andreas Danilewsky[2]; [1]University of Alabama in Huntsville, AL/Us, [2]University of Freiburg, De, [3]Netzsch Gerätebau GmbH, De, [4]Fraunhofer IPM (retired), De

15:30 - 17:00
Monday, July 31, 2017
Fundamentals of Crystal Growth (3 of 9)
Anasazi Ballroom South

Moderation: Peter Vekilov, U of Houston/US

15:30 - 16:00
CURRENT STATUS & FUTURE CHALLENGES IN CRYSTAL GROWTH PREDICTION
Michael Doherty, University of California Santa Barbara, CA/Us

16:00 - 16:30
EXPERIMENT AND PREDICTION OF SURFACE TEMPLATED POLYMORPHS AND SOLVATES
Alastair Florence, CMAC, Technology Innovation Centre, University of Strathclyde, Gb

16:30 - 17:00
UNRAVELING COMPLEXITY IN THE CRYSTALLIZATION OF PHARMACEUTICAL SOLIDS
Susan Reutzel-Edens, Eli Lilly and Company, Us

15:30 – 16:30
Monday, July 31, 2017
Nonlinear Optical and Laser Host Materials (3 of 3)
Chapel Room

Moderation: Kevin Stevens, Northrop Grumman-SYNOPTICS/US

15:30 - 15:45
GROWTH AND PROCESSING OF ORIENTATION-PATTERNED SEMICONDUCTOR WAVEGUIDES FOR MID-IR FREQUENCY CONVERSION
Peter Schunemann[1]; Daniel Magarrell[2]; Paul Moffitt[2]; Peter Ketteridge[2]; Bradley Deshano[3]; Rita Peterson[4]; [1]BAE Systems, NH/Us, [2]BAE Systems, Inc., NH/Us, [3]Air Force Research Laboratory (AFRL/RYDH), OH/Us, [4]Air Force Research Laboratory, OH/Us

15:45 - 16:00
HETEROEPITAXY OF ORIENTATION-PATTERNED NONLINEAR OPTICAL MATERIALS
Vladimir Tassev[1]; Shiva Vangala[2]; Rita Peterson[1]; Michael Snure[1]; [1]Air Force Research Laboratory, OH/Us, [2]Azimuth Corporation, OH/Us

16:00 - 16:15
TUNABLE3-5 AND 7-12 µM PICOSECOND OPTICAL PARAMETRIC AMPLIFIER BASED ON LIINSE2 MID-INFRARED CRYSTAL
Xutang Tao, State Key Laboratory of Crystal Materials, Cn

16:15 - 16:30
GROWTH OF CHROMIUM DOPED FORSTERITE CR:MG_2SIO_4 LASER CRYSTALS FROM NON-STOICHIOMETRIC MELTS AND THE PROLONGED HIGH-TEMPERATURE OXIDIZING ANNEALING OF THE CRYSTALS AS THE TOOLS FOR CHANGE THE OXIDATION STATES OF CHROMIUM IN THE CRYSTALS
Viktoriia Sanina[1]; Kirill Subbotin[2]; Denis Lis[1]; Evgenii Zharikov[1]; [1]A.M.Prokhorov General Physics Institute of Russian Academy of Sciences, Ru, [2]A.M.Prokhorov General Physics Institute Russian Academy of Sciences, Ru

15:30 - 17:00
Monday, July 31, 2017
Biological and Biomimetic Materials (3 of 3)
St Francis De Vargas

Moderation: Derk Joester[1]; Elia Beniash[2]; Yu Huang[3]; [1] Northwestern U/US, [2]University of Pittsburgh/US, [3]UCLA/US

15:30 - 16:00
WHAT YOUR MOTHER NEVER TOLD YOU ABOUT APATITE...AND HOW TO EXPLOIT IT
Jill Pasteris, Washington University in St. Louis, MO/Us

16:00 - 16:30
TOOTH ENAMEL FORMATION: THE ESSENTIAL ROLE OF AMELOGENIN PHOSPHORYLATION
Henry Margolis[1]; Nah-Young Shin[2]; Hajime Yamazaki[2]; Seth Margolis[3]; Megan Pugach[1]; James Simmer[4]; Elia Beniash[5]; [1]The Forsyth Institute, MA/Us, [2]Harvard School of Dental Medicine, MA/Us, [3]The Johns Hopkins University School of Medicine, MD/Us, [4]University of Michigan School of Dentistry, MI/Us, [5]University of Pittsburgh School of Dental Medicine, PA/Us

16:30 - 17:00
REGULATION OF COCCOLITH CALCITE FORMATION
Andre Scheffel[1]; Sanja Sviben[1]; Assaf Gal[1]; Damien Faivre[2]; [1]Max-Planck Institute of Molecular Plant Physiology, De, [2]Max-Planck Institute of Colloids and Interfaces, De

15:30 - 17:20
Monday, July 31, 2017
3rd Symposium on 2D Electronic Materials (3 of 6)
Zia Ballroom

Moderation: Kurt Gaskill[1]; JoanM. Redwing[2]; [1]NRL/US, [2]PennState/US

15:30 - 16:00
REMOTE EPITAXY THROUGH GRAPHENE SAVES WAFER COST VIA 2DLT
Jeehwan Kim, MIT,

16:00 - 16:30
TWO-DIMENSIONAL GALLIUM NITRIDE REALIZED VIA GRAPHENE ENCAPSULATION
Zakaria Al Balushi[1]; Joshua Robinson[2]; Joan Redwing[2]; [1]Dept. of Materials Science and Eng., The Pennsylvania State University, PA/Us, [2]The Pennsylvania State University, PA/Us

16:30 - 17:00
THE GROWTH AND ELECTRONIC PROPERTIES OF ULTRA-THIN EPITAXIAL TOPOLOGICAL DIRAC SEMIMETAL NA_3BI FILMS
Mark Edmonds, Monash University, Au

17:00 - 17:20
THE EFFECTS OF COMPOSITION, GROWTH CONDITIONS AND DOPING ON VERTICAL BRIDGMAN GROWTH OF THE TOPOLOGICAL INSULATOR BI2TE2SE
David Snyder[1]; Randal Cavalero[1]; Robert Lavelle[1]; Ron Redwing[2]; [1]Penn State Applied Research Laboratory, PA/Us, [2]Penn State MatSE, Us

17:00 - 19:00
Monday, July 31, 2017
Poster Session (1 of 2) & Vendor Reception

Eldorado Grand Ballroom

P1-1

GROWTH AND MAGNETIC PROPERTIES OF PRCO2 SINGLE CRYSTALS

Yong Liu; Arjun Pathak; Yaroslav Mudryk; Qisheng Lin; Vitalij Pecharsky; Thomas Lograsso; Ames Laboratory, IA/Us

P1-2

GROWTH, MICROSTRUCTURE AND MECHANICAL PROPERTIES OF IRIDIUM FIBER CRYSTAL BY ALLOY-MICRO-PULLING-DOWN METHOD

Yuui Yokota[1]; Takayuki Nihei[2]; Yuji Ohashi[3]; Shunsuke Kurosawa[4]; Kei Kamada[3]; Akira Yoshikawa[2]; [1]Tohoku University, Jp, [2]Institute for Materials Research, Tohoku University, Jp, [3]NICHe, Tohoku University, Jp, [4]Department of Physics, Yamagata University, Jp

P1-3

GROWTH AND INTERNAL STRUCTURE OF CO-CR-MO ALLOY FIBER CRYSTALS BY ALLOY-MICRO-PULLING-DOWN METHOD

Takayuki Nihei[1]; Yuui Yokota[2]; Akihiro Yamaji[1]; Yuji Ohashi[3]; Shunsuke Kurosawa[4]; Kei Kamada[3]; Akira Yoshikawa[1]; [1]Institute for Materials Research, Tohoku University, Jp, [2]Tohoku University, Jp, [3]NICHe, Tohoku University, Jp, [4]Department of Physics, Yamagata University, Jp

P1-4

GROWTH AND PIEZOELECTRIC PROPERTIES OF $CA_3TA(GA_{1-X}SC_X)_3SI_2O_{14}$ BULK SINGLE CRYSTALS

Yu Igarashi[1]; Yuui Yokota[2]; Yuji Ohashi[3]; Kenji Inoue[4]; Akihiro Yamaji[5]; Yasuhiro Shoji[5]; Kei Kamada[3]; Shunsuke Kurosawa[6]; Akira Yoshikawa[5]; [1], , [2]Tohoku University, Jp, [3]NICHe, Tohoku University, Jp, [4]Piezo Studio Inc., Jp, [5]Institute for Materials Research, Tohoku University, Jp, [6]Department of Physics, Yamagata University, Jp

P1-5

STUDIES ON GROWTH ASPECTS, PROPERTIES AND EFFECTS OF H^+ ION IMPLANTATION ON ORGANIC SINGLE CRYSTAL: L-HISTIDINIUM SEMISUCCINATE (LHS)

H Arul[1]; D Rajan Babu[2]; R Ezhil Vizhi[2]; [1]Department of Science and Humanities, Kumaraguru College of Technology (Autonomous),, In, [2]Advanced Materials Research Centre, Department of Physics, School of Advanced Sciences, VIT University, In

P1-6

SYNTHESIS, GROWTH AND CHARACTERIZATION OF METAL ORGANIC SODIUM HYDROGEN OXALATE MONOHYDRATE SINGLE CRYSTAL

D S Ajisha[1]; R Ezhil Vizhi[1]; D Rajan Babu[2]; H Arul[3]; [1]VIT University, In, [2]Advanced Materials Research Centre, Department of Physics, School of Advanced Sciences, VIT University, In, [3]Department of Science and Humanities, Kumaraguru College of Technology (Autonomous),, In

P1-7

GROWTH OF DETECTOR GRADE CADMIUM ZINC TELLURIDE VIA IMPLEMENTATION OF CRUCIBLE ROTATION IN MODIFIED VERTICAL BRIDGMAN METHOD

Jedidiah McCoy[1]; Saketh Kakkireni[2]; Santosh Swain[2]; Mia Divecha[3]; Jeffrey Derby[4]; Kelvin Lynn[1]; [1]Washington Stat University, WA/Us, [2]Washington State University, WA/Us, [3]University of Minnesota, Us, [4]University of Minnesota, MN/Us

P1-8

MELT GROWTH OF ZINC ALUMINATE SPINEL SINGLE CRYSTAL BY THE MICRO-PULLING DOWN METHOD UNDER ATMOSPHERIC PRESSURE

Akria Yoshikawa[1]; Kei Kamada[2]; Yasuhiro Shoji[3]; Vladimir Kochurikhin[4]; Shunsuke Kurosawa[5]; Akihiro Yamaji[3]; Yuji Ohashi[2]; Yuui Yokota[6]; [1]IMR, Tohoku Univeristy, Jp, [2]NICHe, Tohoku University, Jp, [3]Institute for Materials Research, Tohoku University, Jp, [4]General Physics Institute, Russian Academy of Sciences, Ru, [5]Department of Physics, Yamagata University, Jp, [6]Tohoku University, Jp

P1-9

REVISITING CAPILLARITY AND ITS IMPACT ON SHAPE EVOLUTION DURING CZOCHRALSKI CRYSTAL GROWTH

Simon Brandon; Oleg Weinstein; Technion, Il

P1-10

CRYSTAL GROWTH AND CHARACTERIZATION OF UNDOPED AND DY-DOPED TLPB$_2$BR$_5$ FOR NUCLEAR DETECTION AND IR LASERS

U Hommerich[1]; EiEi Brown[1]; Daniel Hart[2]; M Swain[1]; H Chen[3]; S Trivedi[3]; [1]Hampton University, Us, [2]Hampton University, VA/Us, [3]Brimrose Technology Corporation, MD/Us

P1-11

ZONE-REFINEMENT PURIFICATION, FILTERING METHOD AND GROWTH DIFFICULTIES OF EUROPIUM DOPED STRONTIUM IODIDE (SRI$_2$:EU^{2+}) SCINTILLATOR SINGLE CRYSTAL FOR RADIATION DETECTION APPLICATIONS

A Raja[1]; D Joseph Daniel[2]; P Ramasamy[1]; S G Singh[3]; S Sen[3]; S C Gadkari[3]; [1]SSN College of Engineering, In, [2]Kyungpook National University, Kr, [3]Bhabha Atomic Research Centre, In

P1-12

PALLADIUM OXIDE THIN FILMS FOR OXIDIZING GASES DETECTION

Alexander Samoylov[1]; Valentin Ievlev[1]; Stanislav Ryabtsev[1]; Alexey Shaposhnik[2]; Alexey Sinelnikov[1]; [1]Voronezh State University, Ru, [2]Voronezh State Agricultural University, Ru

P1-13

BORON CODOPING OF CZOCHRALSKI GROWN LUTETIUM ALUMINUM GARNET AND THE EFFECT ON SCINTILLATION PROPERTIES

Camera Foster[1]; Merry Koschan[2]; Chuck Melcher[2]; Yuntao Wu[2]; [1], TN/Us, [2]University of Tennessee, Us

P1-14

CRYSTAL GROWTH OF KCAI3:EU AND KSR2I5:EU SCINTILLATORS USING THE MICRO-PULLING-DOWN METHOD

Mariya Zhuravleva[1]; Robert Kral[2]; Matthew Loyd[1]; Chuck Melcher[3]; Shunsuke Kurosawa[4]; Akira Yoshikawa[5]; [1]University of Tennessee, TN/Us, [2]Institute of Physics of the Czech Academy of Sciences, Cz, [3]University of Tennessee, Us, [4]Department of Physics, Yamagata University, Jp, [5]Institute for Materials Research, Tohoku University, Jp

P1-15

SPATIAL DISTRIBUTION OF EU IN BABRCL:EU SINGLE CRYSTAL ASSESSED BY LASER INDUCTED BREAKDOWN SPECTROSCOPY (LIBS)

Tetiana Shalapska[1]; Didier Perrodin[2]; Jhanis Gonzalez[2]; Dayana Oropeza[2]; Xianglei Mao[2]; Vassilia Zobra[2]; Gregory Bizarri[2]; Edith Bourret-Courchesne[2]; [1]Lawrence Berkeley National Laboratory, Us, [2]Lawrence Berkeley National Laboratory, CA/Us

P1-16

CZOCHRALSKI GROWTH AND SCINTILLATION PROPERTIES OF CE DOPED GADOLINIUM SCANDIUM ALUMINIUM GARNET SINGLE CRYSTALS

Kei Kamada[1]; Vladimir Kochurikhin[2]; Shunsuke Kurosawa[3]; Yuji Ohashi[1]; Yuui Yokota[4]; Akira Yoshikawa[5]; [1]NICHe, Tohoku University, Jp, [2]General Physics Institute, Russian Academy of Sciences, Ru, [3]Department of Physics, Yamagata University, Jp, [4]Tohoku University, Jp, [5]Institute for Materials Research, Tohoku University, Jp

P1-17

BULK GROWTH OF THE CSPBBR$_3$ PEROVSKITE, STRUCTURE AND OPTICAL PROPERTIES

Didier Perrodin[1]; Roberto Reis[1]; Tetiana Shalapska[2]; Stephen Derenzo[1]; Edith Bourret[1]; Gregory Bizarri[1]; [1]Lawrence Berkeley National Laboratory, CA/Us, [2]Lawrence Berkeley National Laboratory, Us

P1-18

LI^+, NA^+ AND K^+ CO-DOPING EFFECTS ON SCINTILLATION PROPERTIES OF CE:$GD_3GA_3AL_2O_{12}$ SINGLE CRYSTALS
Masao Yoshino[1]; Kei Kamada[2]; Vladimir Kochurikhin[3]; Mikhail Ivanov[3]; Martin Nikl[4]; Satoshi Okumura[5]; Seiichi Yamamoto[5]; Jung Yeol Yeom[6]; Yasuhiro Shoji[7]; Shunsuke Kurosawa[8]; Yuui Yokota[9]; Yuji Ohashi[2]; Akira Yoshikawa[7]; [1]C&A Corporation, Jp, [2]NICHe, Tohoku University, Jp, [3]General Physics Institute, Russian Academy of Sciences, Ru, [4]Institute of Physics, Czech Academy of Sciences, Cz, [5]Graduate School of Medicine Department of Radiological and Medical Laboratory Sciences, Nagoya University, Jp, [6]Korea University, Kr, [7]Institute for Materials Research, Tohoku University, Jp, [8]Department of Physics, Yamagata University, Jp, [9]Tohoku University, Jp

P1-19
BRIDGEMAN GROWTH AND CHARACTERIZATION OF PYN-PMN-PT FERROELECTRIC SINGLE CRYSTALS
Samuel Taylor[1]; Jun Luo[2]; Wes Hackenberger[2]; Shujun Zhang[3]; Thomas Shrout[4]; Fei Li[4]; [1]TRS Technologies Inc., PA/Us, [2]TRS Technologies, Inc., Us, [3]University of Wollongong, Au, [4]Pennsylvania State University, PA/Us

P1-20
SURFACE FREE ENERGY AND THE MORPHOLOGY OF FLUORITE CRYSTALS
Takaomi Suzuki; Ayano Tsukagoshi; Faculty of Engineering, Shinshu University, Jp

P1-21
APPLICATION OF ULTRASOUND FOR CONTROL OF THE SUGAR CRYSTALLIZATION PROCESS
Zdenek Bubnik; Vladimir Pour; Andrea Hinkova; Svatopluk Henke; Evzen Sarka; University of Chemistry and Technology, Prague, Cz

P1-22
GROWTH AND SCINTILLATION PROPERTIES OF CE:$LACL_3$/$AECL_2$ (AE=MG, CA, SR, BA) EUTECTICS FOR X-RAY IMAGING APPLICATIONS
Akria Yoshikawa[1]; Kei Kamada[2]; Yuki Furuya[3]; Shunsuke Kurosawa[4]; Akihiro Yamaji[5]; Yasuhiro Shoji[5]; Yuji Ohashi[2]; Yuui Yokota[6]; [1]IMR, Tohoku Universiry, Jp, [2]NICHe, Tohoku University, Jp, [3]Institute for Materials Research (IMR), Jp, [4]Department of Physics, Yamagata University, Jp, [5]Institute for Materials Research, Tohoku University, Jp, [6]Tohoku University, Jp

P1-23
HIGH-QUALITY N-TYPE GAN GROWN BY HVPE: SI VS O DOPING AND THERMAL CONDUCTIVITY
Tania Paskova[1]; Plamen Paskov[2]; Michael Slomski[2]; Jacob Leach[3]; John Muth[2]; [1]North Carolina State University, , [2]North Carolina State University, Us, [3]Kyma Technology, Us

P1-24
SCALING AND SCINTILLATION PERFORMANCE OF TL2LIYCL6:CE
Ivan Khodyuk[1]; Stacy Swider[2]; Shariar Motakef[2]; [1]CapeSym, Us, [2]CapeSym Inc., MA/Us

P1-25
EFFECT OF (Incomplete Title)
Farit Urakaev, Sobolev Institute of Geology and Mineralogy of the Siberian Branch of the Russian Academy of Sciences, Ru

P1-26
INVESTIGATION OF ACTIVATORS FOR SCINTILLATION IN LANTHANUM IODIDE
Mariya Zhuravleva[1]; Robyn Collette[2]; Daniel Rutstrom[1]; Matthew Loyd[3]; Luis Stand[4]; Chuck Melcher[5]; [1]Department of Materials Science and Engineering University of Tennessee Knoxville, TN/Us, [2], Us, [3]University of Tennessee, TN/Us, [4]Scintillation Materials Research Center, University of Tennessee, TN/Us, [5]University of Tennessee, Us

P1-27
EFFECT OF MASK ORIENTATION AND GROWTH PARAMETERS ON THE EPITAXIAL LATERAL OVERGROWTH OF GAN ON FREE-STANDING NONPOLAR SUBSTRATES

Saadat Mishkat-Ul-Masabih[1]; Andrew Aragon[2]; Morteza Monavarian[3]; Daniel Feezell[4]; [1]University of New Mexico, Us, [2]University of New Mexico, Center for High Technology Materials, Us, [3]University of New Mexico, NM/Us, [4]University of New Mexico, Center for High Technology Materials, Us

19:00 - 21:00
Monday, July 31, 2017
OMVPE of Wide Bandgap Materials for Opto- and Power-Electronics
Anasazi Ballroom South

19:00 - 19:20
GAN EPITAXY ON GLASS USING A (111) SILICON SEED LAYER FORMED BY ALUMINUM-INDUCED CRYSTALLIZATION
Mel Hainey Jr.[1]; Zakaria Al Balushi[2]; Ke Wang[3]; Nathan Martin[2]; Anushka Bansal[2]; Joan Redwing[4]; [1]Penn State University, Materials Research Institute, Us, [2]Dept. of Materials Science and Eng., The Pennsylvania State University, PA/Us, [3]Penn State University, Materials Characterization Laboratory, Us, [4]The Pennsylvania State University, PA/Us

19:20 - 19:40
STRESS ENGINEERED ALGAN/GAN POWER ELECTRONIC DEVICE STRUCTURES
Isra Mahaboob[1]; Kasey Hogan[2]; Emma Rocco[3]; Fatemeh Shahedipour-Sandvik[2]; [1]Colleges of Nanoscale Science and Engineering , SUNY Albany, NY/Us, [2]Colleges of Nanoscale Science and Engineering, Us, [3]Colleges of Nanoscale Science and Engineering, NY/Us

19:40 - 20:00
INFLUENCE OF THE SUBSTRATE ORIENTATION ON STRUCTURAL AND ELECTRICAL PROPERTIES OF HOMOEPITAXIAL β-GA$_2$O$_3$ THIN FILMS GROWN BY MOVPE
Guenter Wagner; Martin Albrecht; Michele Baldini; Andreas Fiedler; Zbigniew Galazka; Klaus Irmscher; Robert Schewski; Institute for Crystal Growth, De

20:00 - 20:20
GROWTH OF GAN ON 2D BN BY MOCVD FOR FLEXIBLE ELECTRONICS
Michael Snure[1]; Nicholas Glavin[2]; Kelson Chabak[2]; Qing Paduano[2]; [1]Air Force Reseach Laboratory , OH/Us, [2]Air Force Reseach Laboratory, OH/Us

20:20 - 20:40
GAN P-I-P-I-N SEPARATE ABSORPTION AND MULTIPLICATION ULTRAVIOLET AVALANCHE PHOTODIODES BY METALORGANIC CHEMICAL VAPOR DEPOSITION
Mi-Hee Ji[1]; Jeomoh Kim[2]; Theeradetch Detchprohm[1]; Shyh-Chiang Shen[1]; Russell Dupuis[1]; [1]Georgia Institute of Technology, GA/Us, [2]LG Electronics, Kr

20:40 - 21:00
UV AIR-GAP/AL$_X$GA$_{1-X}$N DISTRIBUTED BRAGG REFLECTORS FABRICATED USING CONDUCTIVITY-SELECTIVE ELECTROCHEMICAL ETCHING
YOUNGJAE Park[1]; Theeradetch Detchprohm[1]; Oliver Moreno[1]; Karan Mehta[1]; Yuh-Shiuan Liu[1]; Shuo Wang[2]; Shyh-Chiang Shen[1]; P Douglas Yoder[1]; Fernando Ponce[2]; Russell Dupuis[1]; [1]Georgia Institute of Technology, GA/Us, [2]Arizona State University, AZ/Us

	Tuesday 8/1					
Room	Anasazi South	Anasazi North	Chapel Room	Zia	Eldorado (A+B)	St. Francis DeVargas (*)
7:30-8:00	BREAKFAST					
8:00-10:00	AWARDS PLENARY					
10:00-10:30	COFFEE BREAK					
10:30-12:00	FUNDAMENTALS 4	DETECTORS 4	Symp Epi Com. Oxide 1	3rd Symp on 2DEM 4	VENDOR	BULK & EPI POWER ELEC 1
12:00-13:30	LUNCH					
13:30-15:00	FUNDAMENTALS 5	DETECTORS 5	Symp Epi Com. Oxide 2	3rd Symp on 2DEM 5	VENDOR	
15:00-15:30	COFFEE BREAK					
15:30-17:00	FUNDAMENTALS 6	INDUSTRIAL 1	Symp Epi Com. Oxide 3	3rd Symp on 2DEM 6	VENDOR/ POSTER SETUP	
17:00-17:30					POSTERS – 2	
17:30-18:00						
18:00-19:00						
19:00-21:00	OMVPE – Comp. Semic					

(*) St Francis DeVargas room is located in the St Francis Hotel

Tuesday, August 1, 2017

8:00 – 10:00
Awards Session
Anasazi Ballroom

Moderation: Tom Kuech and Jeff Derby

8:30 – 9:15
Christine A. Wang
American Association for Crystal Growth Award
“Science and Technology of OMVPE for Advanced III-V Semiconductor Materials and Devices”

9:15 – 10:00
Bharat Jalan
American Association for Crystal Growth Young Scientist Award
“Band-Engineered Complex Oxide Interfaces: Role of Defects and Growth Approaches”

10:30 - 12:00
Tuesday, August 1, 2017
Detector Materials (4 of 5)
Anasazi Ballroom North

Moderation: Gautam Gundiah[1]; Mariya Zhuravleva[2]; [1] APL/US, [2]TN/Us

10:30 - 11:00
CONTROLLING SCINTILLATOR PROPERTIES VIA CODOPING: AN OVERVIEW
Chuck Melcher[1]; Merry Koschan[2]; Mariya Zhuravleva[3]; Adam Lindsey[2]; Yuntao Wu[1]; Harold Rothfuss[2]; Fang Meng[2]; Sam Donnald[2]; Kan Yang[2]; Jason Hayward[2]; Lars Eriksson[2]; [1]University of Tennessee, Us, [2]Scintillation Materials Research Center, TN/Us, [3]University of Tennessee, TN/Us

11:00 - 11:15
INFLUENCE OF CODOPING, NON-STOICHIOMETRY AND GA ADMIXTURE ON LUAG:CE SCINTILLATION PROPERTIES
Jan Pejchal[1]; Vladimir Babin[2]; Alena Beitlerova[2]; Romana Kucerkova[2]; Petr Prusa[2]; Dalibor Panek[3]; Tomas Parkman[4]; Kei Kamada[5]; Akira Yoshikawa[6]; [1]Institute of Physics CAS, , [2]Institute of Physics CAS, Cz, [3]faculty of Biomedical Engineering, Czech Technical University, Cz, [4]Faculty of Biomedical Engineering, Czech Technical University, Cz, [5]NICHe, Tohoku University, Jp, [6]Institute for Materials Research, Tohoku University, Jp

11:15 - 11:30
CRYSTAL GROWTH AND TEMPERATURE DEPENDENCE OF LIGHT OUTPUT OF CE-DOPED (GD, LA, Y)$_2$SI$_2$O$_7$ SINGLE CRYSTALS
Takahiko Horiai[1]; Shunsuke Kurosawa[2]; Rikito Murakami[3]; Yasuhiro Shoji[4]; Jan Pejchal[5]; Akihiro Yamaji[4]; Yuji Ohashi[6]; Kei Kamada[6]; Yuui Yokota[7]; Tomohiro Ishizu[8]; Yasuo Ohishi[8]; Taisuke Nakaya[8]; Akira Yoshikawa[4]; [1], , [2]Department of Physics, Yamagata University, Jp, [3]C&A Corporation, Jp, [4]Institute for Materials Research, Tohoku University, Jp, [5]Institute of Physics CAS, , [6]NICHe, Tohoku University, Jp, [7]Tohoku University, Jp, [8]Hamamatsu Photonics K. K., Jp

11:30 - 11:45
GROWTH AND SCINTILLATION PROPERTIES OF DIRECTIONALLY SOLIDIFIED CE:LABR3/AEBR2 (AE=MG, CA, SR, BA) EUTECTIC SYSTEM
Akria Yoshikawa[1]; Yuki Furuya[2]; Kei Kamada[3]; Hiroyuki Chiba[2]; Shunsuke Kurosawa[4]; Akihiro Yamaji[5]; Yasuhiro Shoji[5]; Yuji Ohashi[3]; Yuui Yokota[6]; [1]IMR, Tohoku University, Jp, [2]Institute for Materials Research (IMR), Jp, [3]NICHe, Tohoku University, Jp, [4]Department of Physics, Yamagata University, Jp, [5]Institute for Materials Research, Tohoku University, Jp, [6]Tohoku University, Jp

11:45 - 12:00
CRYSTAL GROWTH AND SCINTILLATION PROPERTIES OF ND-DOPED (GD, LA)$_2$SI$_2$O$_7$ CRYSTAL AS INFRA-RED SCINTILLATOR
Shunsuke Kurosawa[1]; Toetsu Shishido[2]; Takahiko Horiai[2]; Shohei Kodama[3]; Takamasa Sugawara[3]; Kunio Yubuta[2]; Akihiro Yamaji[3]; Yuji Ohashi[4]; Yuui Yokota[5]; Kei Kamada[4]; Akira Yoshikawa[3]; [1]Department of Physics, Yamagata University, Jp, [2]Institute for Materials Research,Tohoku University, Jp, [3]Institute for Materials Research, Tohoku University, Jp, [4]NICHe, Tohoku University, Jp, [5]Tohoku University, Jp

10:30 - 12:00
Tuesday, August 1, 2017
Fundamentals of Crystal Growth (4 of 9)
Anasazi Ballroom South

Moderation: Peter Vekilov, U of Houston/US

10:30 - 11:00
IN-SITU ATOMIC FORCE MICROSCOPY STUDIES OF POLYMER MICELLE-CALCITE INTERACTIONS
Lara Estroff; Coit Hendley; Cornell University, NY/Us

11:00 - 11:30
NUCLEATION AND GROWTH OF CRYSTALLINE CARBONATES FROM AMORPHOUS PRECURSORS
Derk Joester, Northwestern University, IL/Us

11:30 - 12:00
GUINIER-PRESTON ZONES WITHIN A BIOGENIC SINGLE CRYSTAL: A BIOLOGICAL PRESTRESSING STRATEGY
Boaz Pokroy, Technion Institute of Technology, Il

10:30 - 12:00
Tuesday, August 1, 2017
Symposium on Epitaxy of Complex Oxides (1 of 11)
Chapel Room

Moderation: Ho Nyung Lee[1]; Darrel Schlom[2]; Lane Martin[3]; [1]ONRL/US, [2]Cornell/US, [3]Berkeley/US

10:30 - 11:00
ENGINEERING CORRELATED DIRAC ELECTRONS IN SRIRO$_3$/SRTIO$_3$ SUPERLATTICE
HIDENORI Takagi[1]; Daigorou Hirai[2]; Naoka Hiraoka[2]; Jobu Matsuno[3]; [1]Max Planck Institute for Solid State Research, De, [2]Department of Physics, University of Tokyo, Jp, [3]RIKEN, Jp

11:00 - 11:30
EPITAXIAL GROWTH OF LOW VALENCE TRANSITION-METAL OXIDES EXHIBITING NOVEL ELECTRONIC STATES
Akira Ohtomo, Tokyo Institute of Technologuy, Jp

11:30 - 12:00
WHAT TO DO WHEN YOUR IDEAL SINGLE CRYSTAL SUBSTRATE IS NOT AVAILABLE: HOW COMBINATORIAL SUBSTRATE EPITAXY OPENS NEW DOORS TO EPITAXIAL SYNTHESIS.
Paul Salvador[1]; Gregory Rohrer[2]; John Kitchin[2]; Wilfrid Prellier[3]; [1]Carnegie Mellon University, Us, [2]Carnegie Mellon University, PA/Us, [3]Laboratoire CRISMAT, CNRS UMR 6508, ENSICAEN, Universite de Basse-Normandie, Fr

10:30 - 12:00
Tuesday, August 1, 2017
Bulk Growth & Epitaxy for Power Elect. (1 of 3)
St Francis De Vargas

Moderation: Michael Dudley; Balaji Raghothamachar; Stony Brook/US

10:30 - 11:00
EPIGROWTH CHALLENGES FOR HIGH-VOLTAGE SIC POWER DEVICES
James Cooper, Sonrisa Research, Inc., Us

11:00 - 11:30
IMPACT OF TRANSITION METAL IMPURITIES ON NITRIDE DEVICES
Darshana Wickramaratne, Materials Department, UC Santa Barbara, Us

11:30 - 12:00
GROWTH OF GA$_2$O$_3$ FOR DEVICE PRODUCTION
Serdal Okur[1]; Nick Sbrockey[2]; Tom Salagaj[2]; Gary Tompa[3]; Yao Yao[4]; Robert Davis[4]; Lisa Porter[4]; Luke Lyle[4]; [1]Structured Materials Industries, Inc., Us, [2]Structured Materials Industries, NJ/Us, [3]Structured Materials Industries, Inc., NJ/Us, [4]Carnegie Mellon University, Us

10:30 - 12:00
Tuesday, August 1, 2017

3rd Symposium on 2D Electronic Materials (4 of 6)
Zia Ballroom

Moderation: Kurt Gaskill[1]; JoanM. Redwing[2]; [1]NRL/US, [2]PennState/US

10:30 - 11:00
NUCLEATION AND GROWTH OF WSE$_2$: ENABLING LARGE GRAIN TRANSITION METAL DICHALCOGENIDES
Christopher Hinkle, University of Texas at Dallas, TX/Us

11:00 - 11:20
NUCLEATION AND GROWTH KINETICS OF MONOLAYER TUNGSTEN DISELENIDE (WSE$_2$) FILMS ON SAPPHIRE
Xiaotian Zhang; Tanushree Choudhury; Bhakti Jariwala; Fu Zhang; Nasim Alem; Joshua Robinson; Joan Redwing; The Pennsylvania State University, PA/Us

11:20 - 11:40
ATOMIC LAYER AND METALORGANIC CHEMICAL VAPOR DEPOSITION OF MOS$_2$ AND WS$_2$ FROM BIS(TERT-BUTYLIMIDO)-BIS(DIALKYLAMIDO) COMPOUNDS
Berc Kalanyan[1]; James Maslar[2]; William Kimes[3]; Brent Sperling[3]; Ravindra Kanjolia[4]; [1]National Institute of Standards and Technology, Us, [2]NIST, Us, [3]National Institute of Standards and Technology, MD/Us, [4]EMD Performance Materials, Us

11:40 - 12:00
EFFECT OF SAPPHIRE SUBSTRATE ORIENTATION ON NUCLEATION AND GROWTH OF TRANSITION METAL DICHALCOGENIDES
Tanushree Choudhury; Xiaotian Zhang; Joan Redwing; The Pennsylvania State University, PA/Us

13:30 - 15:00
Tuesday, August 1, 2017

Detector Materials (5 of 5)
Anasazi Ballroom North

Moderation: Gautam Gundiah[1]; Mariya Zhuravleva[2]; [1] APL/US, [2]TN/Us

13:30 - 13:45
FLOATING-ZONE CRYSTAL GROWTH AND CHARACTERIZATION OF THE SCINTILLATOR $MG_4TA_2O_9$
Dongsheng Yuan[1]; Didier Perrodin[2]; Tetiana Shalapska[3]; Edith Bourret[2]; Gregory Bizarri[2]; [1]Lawrence Berkeley National Lab, Us, [2]Lawrence Berkeley National Laboratory, CA/Us, [3]Lawrence Berkeley National Laboratory, Us

13:45 - 14:00
HYDROTHERMAL GROWTH AND CHARACTERIZATION OF UO2 SINGLE CRYSTALS GROWN ON NON-NATIVE SUBSTRATES
Martin Kimani[1]; James Mann[2]; Karl Rickert[3]; James Petrosky[4]; David Turner[2]; [1]KBRWyle Aerospace Group, CA/Us, [2]Air Force Research Laboratory, OH/Us, [3]Oak Ridge Institute for Science and Education, TN/Us, [4]Air Force Institute of Technology, OH/Us

14:00 - 14:15
GROWTH AND OPTICAL PROPERTIES OF CR-DOPED BETA-GA_2O_3 CRYSTALS AS RED AND INFRARED SCINTILLATOR BY THE FLOATING ZONE METHOD
Shunsuke Kurosawa[1]; Toetsu Shishido[2]; Akihiro Yamaji[2]; Takahiko Horiai[3]; Shohei Kodama[2]; Takamasa Sugawara[2]; Akiko Nomura[2]; Kunio Yubuta[2]; Yuji Ohashi[4]; Yuui Yokota[5]; Kei Kamada[4]; Akira Yoshikawa[2]; Akimasa Ohnishi[6]; Mamoru Kitaura[6]; [1]Department of Physics, Yamagata University, Jp, [2]Institute for Materials Research, Tohoku University, Jp, [3], , [4]NICHe, Tohoku University, Jp, [5]Tohoku University, Jp, [6]Faculty of Science, Yamagata University, Jp

14:15 - 14:30
HYDROTHERMAL GROWTH OF THO2, UXTH1-XO2 AND UO2 SINGLE CRYSTALS FOR NEUTRON DETECTION
James Mann[1]; Martin Kimani[2]; Christina Dugan[3]; Christopher Young[4]; Karl Rickert[5]; James Petrosky[4]; [1]Air Force Research Laboratory, OH/Us, [2]KBRWyle Aerospace Group, CA/Us, [3]Air Force Institute of Technology, Us, [4]Air Force Institute of Technology, OH/Us, [5]Oak Ridge Institute for Science and Education, TN/Us

14:30 - 14:45
SOLUTION GROWTH AND SCINTILLATION PROPERTIES OF 9-PHENYLCARBAZOLE
Edgar Van Loef; Gary Markosyan; Urmila Shirwadkar; Mickel McClish; Kanai Shah; RMD, MA/Us

14:45 - 15:00
RECENTLY DEVELOPED UNIDIRECTIONAL ORGANIC SINGLE CRYSTAL CYLINDERS FOR SCINTILLATOR APPLICATION
Krishnasamy Sankaranarayanan, Alagappa University, In

13:30 - 15:00
Tuesday, August 1, 2017
Fundamentals of Crystal Growth (5 of 9)
Anasazi Ballroom South

Moderation: Peter Vekilov, U of Houston/US

13:30 - 14:00
IN-SITU OBSERVATION OF ICE CRYSTAL SURFACES AT THE MOLECULAR LEVEL BY ADVANCED OPTICAL MICROSCOPY
Gen Sazaki; Ken-ichiro Murata; Masahiro Inomata; Jialu Chen; Ken Nagashima; Yoshinori Furukawa; Institute of Low Temperature Science, Hokkaido University, Jp

14:00 - 14:30
FORMATION AND PROPOGATION OF MACROSTEPS IN THE PRESENCE OF IMPURITIES
James Lutsko[1]; Mike Sleutel[2]; Alexander Van Driessche[3]; [1]Universite Libre de Bruxelles, Be, [2]Vrije Universiteit Brussel, Be, [3]Univ. Grenoble Alpes, Fr

14:30 - 14:45
NUCLEATION AND GROWTH OF TWO-DIMENSIONAL ISLANDS OF COLLOIDAL CRYSTALS
Jun Nozawa[1]; Satoshi Uda[2]; Suxia Guo[1]; Junpei Okada[2]; Haruhiko Koizumi[1]; [1]Institute for Materials Research, Tohoku University, Jp, [2]Tohoku University, Jp

14:45 - 15:00
HERRING'S SCALING LAW OF DIFFUSION REVISITED
Marek Petrik, Philipps University, De

13:30 - 15:00
Tuesday, August 1, 2017
Symposium on Epitaxy of Complex Oxides (2 of 11)
Chapel Room

Moderation: Ho Nyung Lee[1]; Darrel Schlom[2]; Lane Martin[3]; [1]ONRL/US, [2]Cornell/US, [3]Berkeley/US

13:30 - 14:00
NEW STRAIN STATES IN EPITAXIAL COMPLEX OXIDES
Judith Macmanus-Driscoll[1]; Ady Suwardi[1]; Haiyan Wang[2]; Aiping Chen[3]; Quanxi Jia[4]; [1]University of Cambridge, Gb, [2]Purdue University, Us, [3]CINT, Los Alamos, NM/Us, [4]Univ. at Buffalo, SUNY, Department of Materials Design and Innovation, NY/Us

14:00 - 14:30
DOPANT SITE STRUCTURE ANALYSIS IN PEROVSKITES
Mikk Lippmaa, Institute for Solid State Physics, University of Tokyo, Jp

14:30 - 15:00
PROBING INTERFACIAL SUPERCONDUCTIVITY IN FE-BASED SUPERCONDUCTORS BY IN-SITU ARPES
Hong Ding, Institute of Physics, Chinese Academy of Sciences, Cn

13:30 - 15:00
Tuesday, August 1, 2017
3rd Symposium on 2D Electronic Materials (5 of 6)
Zia Ballroom

Moderation: Kurt Gaskill[1]; JoanM. Redwing[2]; [1]NRL/US, [2]PennState/US

13:30 - 14:00
GROWTH-MICROSTRUCTURE-(ELECTRONIC)PROPERTY CORRELATIONS IN 2D MATERIALS.
Srinivasan Raghavan, Indian Institute of Science, In

14:00 - 14:20
GROWTH OF LARGE-AREA, SINGLE-CRYSTAL GRAPHENE AND GRAPHENE BILAYERS FOR ELECTRONIC DEVICES
Yufeng Hao, Nanjing University,

14:20 - 14:40
SYNTHESIS AND CHARACTERIZATION OF GRAPHENE BASED THERMOACOUSTIC DEVICES

Nick Sbrockey[1]; Tom Salagaj[1]; Thottam Kalkur[2]; Gary Tompa[3]; [1]Structured Materials Industries, NJ/Us, [2]University of Colorado at Colorado Springs, Us, [3]Structured Materials Industries, Inc., NJ/Us

14:40 - 15:00
MECHANISMS OF HYDROGEN INTERCALATION IN EPITAXIAL GRAPHENE
Kevin Daniels[1]; Anthony Boyd[2]; Anindya Nath[3]; Rachael Myers-Ward[2]; Kurt Gaskill[4]; [1]U.S. Naval Research Laboratory, Us, [2]US Naval Research Laboratory, DC/Us, [3]George Mason University, VA/Us, [4],

15:30 - 17:00
Tuesday, August 1, 2017
Industrial Crystal Growth Technologies and Equipment (1 of 2)
Anasazi Ballroom North

Moderation: Matt Whittaker, Gooch & Housego/US

15:30 - 16:00
ADVANCES IN SINGLE-CRYSTAL FIBERS AND THIN RODS GROWN BY LASER HEATED PEDESTAL GROWTH
Gisele Maxwell, shasta crystals inc., Us

16:00 - 16:15
MARKET TREND IN THE SAPPHIRE INDUSTRY AND A DISCUSSION FOR DEVELOPMENT DIRECTION
Jongkwan Park; Matthew Jensen; Ryan Loquist; Clark Blockburger; Matthew Montgomery; Rubicon Technology, IL/Us

16:15 - 16:30
SINGLE CRYSTAL GROWTH OF SUBMILLIMETRE DIAMETER SAPPHIRE TUBE BY THE MICRO-PULLING DOWN METHOD FOR ULTRASOUND-FACILITATED DRUG DELIVERY SYSTEM
Kei Kamada[1]; Vladimir Kochurikhin[2]; Gushchina Liudmila[2]; Mikhail Ivanov[2]; Yasuhiro Shoji[3]; Shunsuke Kurosawa[4]; Yuji Ohashi[1]; Yuui Yokota[5]; Akira Yoshikawa[3]; [1]NICHe, Tohoku University, Jp, [2]General Physics Institute, Russian Academy of Sciences, Ru, [3]Institute for Materials Research, Tohoku University, Jp, [4]Department of Physics, Yamagata University, Jp, [5]Tohoku University, Jp

16:30 - 16:45
UNIDIRECTIONAL SOLIDIFICATION OF IR/IR-RH FIBER CRYSTALS FOR THERMOCOUPLE BY ALLOY-MICRO-PULLING DOWN METHOD
Rikito Murakami[1]; Yuui Yokota[2]; Kei Kamada[3]; Yasuhiro Shoji[4]; Shunsuke Kurosawa[5]; Yuji Ohashi[3]; Akihiro Yamaji[4]; Akira Yoshikawa[4]; [1]C&A Corporation, Jp, [2]Tohoku University, Jp, [3]NICHe, Tohoku University, Jp, [4]Institute for Materials Research, Tohoku University, Jp, [5]Department of Physics, Yamagata University, Jp

16:45 - 17:00
CRYSTALLIZATION OF ALPHA-LACTOSE MONOHYDRATE (α-LM) FROM AQUEOUS SOLUTION USING DIFFERENT ORGANIC SOLVENTS
P Parimaladevi; K Vinodhini; Srinivasan Karuppannan; Bharathiar University, In

15:30 – 16:30
Tuesday, August 1, 2017
Fundamentals of Crystal Growth (6 of 9)
Anasazi Ballroom South

Moderation: Peter Vekilov, U of Houston/US

15:30 - 16:00

COLLOIDAL NANOSTRUCTURES: IN-SITU ELECTRON MICROSCOPY OF PLASMON-MEDIATED SYNTHESIS, CHEMISTRY AND SELF-ASSEMBLY
Eli Sutter, ,

16:00 - 16:30
STEP MORPHOLOGY OF 2D ISLANDS ON THE (110) FACE OF LYSOZYME CRSYTALS GROWN IN SPACE
Katsuo Tsukamoto[1]; Hitoshi Miura[2]; Hironori Hondoh[3]; [1]Osaka University, Jp, [2]Nagoya City University, Jp, [3]Hiroshima University, Jp

15:30 - 17:30
Tuesday, August 1, 2017
Symposium on Epitaxy of Complex Oxides (3 of 11)
Chapel Room

Moderation: Ho Nyung Lee[1]; Darrel Schlom[2]; Lane Martin[3]; [1]ONRL/US, [2]Cornell/US, [3]Berkeley/US

15:30 - 16:00
ADVANCED PULSED LASER DEPOSITION
Gertjan Koster, University of Twente, Nl

16:00 - 16:30
SYNTHESIS OF FREESTANDING SINGLE-CRYSTAL OXIDE THIN FILMS AND HETEROSTRUCTURES
Yasuyuki Hikita, SLAC National Accelerator Laboratory, Us

16:30 - 16:45
NON-EQUILIBRIUM SYNTHESIS OF HIGHLY POROUS SINGLE-CRYSTALLINE OXIDE NANOSTRUCTURES
Dongkyu Lee[1]; Xiang Gao[1]; Lisah Fan[1]; Erjia Guo[1]; Thomas Farmer[1]; William Heller[1]; Michael Fitzsimmons[1]; Matthew Chisholm[2]; Ho Nyung Lee[1]; [1]Oak Ridge National Laboratory, TN/Us, [2]Oak Ridge National Laboratory, Us

16:45 - 17:00
TUNING FUNCTIONAL PROPERTIES IN OXIDE NANOCOMPOSITES
Aiping Chen[1]; Erik Enriquez[1]; Haiyan Wang[2]; Judith Macmanus-Driscoll[3]; Quanxi Jia[4]; [1]CINT, Los Alamos, NM/Us, [2]Purdue University, Us, [3]University of Cambridge, Gb, [4]Univ. at Buffalo, SUNY, Department of Materials Design and Innovation, NY/Us

17:00 - 17:30
CATION STOICHIOMETRY CONTROL FOR HIGH-QUALITY EPITAXY OF COMPLEX OXIDES BY PULSED LASER DEPOSITION
Tsuyoshi Ohnishi, National Institute for Materials Science,

15:30 - 17:20
Tuesday, August 1, 2017
3rd Symposium on 2D Electronic Materials (6 of 6)
Zia Ballroom

Moderation: Kurt Gaskill[1]; JoanM. Redwing[2]; [1]NRL/US, [2]PennState/US

15:30 - 16:00
GRAPHENE QUANTUM RESISTANCE STANDARD
Alexander Tzalenchuk, National Physical Laboratory, Gb

16:00 - 16:30
POLYMER ASSISTED SUBLIMATION GROWTH OF EPITAXIAL GRAPHENE FOR QUANTUM RESISTANCE METROLOGY

Mattias Kruskopf[1]; Davood Momeni Pakdehi[1]; Klaus Pierz[1]; Stefan Wundrack[1]; Rainer Stosch[1]; Thorsten Dziomba[1]; Martin Götz[1]; Jens Baringhaus[1]; Johannes Aprojanz[2]; Christoph Tegenkamp[2]; Jakob Lidzba[3]; Thomas Seyller[3]; Frank Hohls[1]; Franz Ahlers[1]; Hans Schumacher[1]; [1]Physikalisch-Technische Bundesanstalt, De, [2]Institute of Solid State Physics of Leibniz Universität Hannover, De, [3]Institute of Physics of Technische Universität Chemnitz, De

16:30 - 16:50
IMPACT OF QUASI-FREE STANDING GRAPHENE EPITAXIAL GRAPHENE ON TERAHERTZ OPTOELECTRONICS
D Gaskill[1]; Kevin Daniels[2]; M Jadidi[3]; A Shuskov[3]; A Boyd[1]; A Nath[4]; R L Myers-Ward[1]; T Murphy[3]; H D Drew[3]; [1]Naval Research Laboratory, DC/Us, [2]U.S. Naval Research Laboratory, Us, [3]University of Maryland, MD/Us, [4]George Mason University, VA/Us

16:50 - 17:20
FORMATION OF GRAPHENE NANORIBBONS AND SHEETS BY DIFFUSION OF CARBON IN LIQUID METALS INDUCED BY ELECTROCHARGING ASSISTED PROCESS
Lourdes Salamanca-Riba[1]; Xiaoxiao Ge[2]; Liangbing Hu[2]; Oded Rabin[2]; Manfred Wuttig[2]; Balu Balachandran[3]; Daniel Cole[4]; [1]University of Maryland, Us, [2]University of Maryland, MD/Us, [3]Argonne National Laboratory, IL/Us, [4]Army Research Laboratory, MD/Us

17:00 - 19:00
Tuesday, August 1, 2017
Poster Session (2 of 2)
Eldorado Grand Ballroom

P2-1
SUBMILLIMETER-SIZED NATAO3 SINGLE CRYSTALS GROWN VIA COOLING OF NA_2MOO_4 FLUX
Sayaka Suzuki[1]; Haruka Saito[2]; Tetsuya Yamada[3]; Katsuya Teshima[3]; [1]Faculty of Engineering, Shinshu University, Jp, [2]Graduate School of Science and Technology, Shinshu University, Jp, [3]Center for Energy and Environmental Science, Shinshu University, Jp

P2-2
GROWTH ANGLE - A MICROSCOPIC VIEW
Konstantin Mazuruk[1]; Martin Volz[2]; Arnold Croll[1]; [1]University of Alabama in Huntsville, AL/Us, [2]NASA Marshall Space Flight Center, AL/Us

P2-3
POTASSIUM-COBALT SULFIDE CRYSTAL GROWTH ASSISTED BY LOW FREQUENCY VIBRATIONS
Andrey Sadovskiy[1]; Ivan Ermochenkov[2]; Evgeniya Dubovenko[2]; Marina Zykova[2]; Ekaterina Sukhanova[2]; Igor Avetissov[2]; [1]IPG, Ru, [2]Dmitry Mendeleev Univeristy of Chemical Technology of Russia, Ru

P2-4
INVESTIGATION OF ENHANCED ROOM TEMPERATURE FERROMAGNETISM IN CO DOPED SNO_2 NANOPARTICLES
Rajan Renu[1]; R Ezhil Vizhi[1]; D Rajan Babu[2]; H Arul[3]; [1]VIT University, In, [2]Advanced Materials Research Centre, Department of Physics, School of Advanced Sciences, VIT University, In, [3]Kumaraguru Institute of Technology, In

P2-5
CALCIUM CARBONATE IN THE SUGAR TECHNOLOGY
Evzen Sarka; Zdenek Bubnik; University of Chemistry and Technology, Prague, Cz

P2-6
ANALYSIS OF VERTICAL GRADIENT FREEZE (VGF) PROCESS SCALE-UP FOR THE GROWTH OF CADMIUM ZINC TELLURIDE (CZT) SINGLE-CRYSTAL, LARGE-AREA SUBSTRATES

John Roerig[1]; Nathan Morgan[1]; Kelly Jones[2]; Scott Johnson[2]; Jeffrey Derby[1]; [1]University of Minnesota, MN/Us, [2]Raytheon Vision Systems, CA/Us

P2-7

POCESSING OF CONCENTRATED SOLAR RADIATION PV MODULES ON THE BASIS OF ALGAAS-GAAS HETEROSTRUCTURES

Ia Trapaidze[1]; Gela Goderdzishvili[1]; Lia Trapaidze[2]; Rafiel Chikovani[1]; [1]Dep. of Physics, Georgian Technical University, Ge, [2]Dep. orf Physics, Tbilisi State Univeristy, Ge

P2-8

AXIAL VIBRATION CONTROL TECHNIQUE FOR CRYSTAL GROWTH FROM LIQIUD

Andrey Sadovskiy[1]; Vladimir Kostikov[2]; Ekaterina Sukhanova[3]; Igor Avetissov[3]; [1]IPG, Ru, [2]Dmitry Mendeleev University of Chemical Technology of Russia, Ru, [3]Dmitry Mendeleev Univeristy of Chemical Technology of Russia, Ru

P2-9

MONTE CARLO STUDY OF THE GROWTH KINETICS DURING MBE OF GAAS ON THE SUBSTRATES WITH DIFFERENT ORIENTATIONS

Maxim Solodovnik; Sergey Balakirev; Oleg Ageev; Ilya Mikhaylin; Mikhail Eremenko; Southern Federal University, Ru

P2-10

MODELING THE DEFECT STRUCTURE OF GROWING CRYSTAL USING THE VLASOV MODEL FOR SOLIDS

Vitalyi Igorevich Talanin; Igor Evgenievich Talanin; Vladislav Igorevich Lashko; Department of Computer Science & Software Engineering, Institute of Economics & Information Technology, Ua

P2-11

GROWTH OF ZNO NANOROD ARRAYS ON PATTERNED SUBSTRATES

Jan Grym; Ondřej Černohorský; Roman Yatskiv; Šárka Chlupová; Antonín Schenk; Nikola Bašinová; David Roesel; Jan Vaniš; Stanislav Tiagulskyi; Institute of Photonics and Electronics of the CAS, Cz

P2-12

KINETIC MONTE CARLO MODEL OF DROPLET EPITAXY FOR IN/GAAS(001) NANOSTRUCTURES: EXPERIMENTS AND THEORY

Sergey Balakirev; Maxim Solodovnik; Oleg Ageev; Mikhail Eremenko; Ilya Mikhaylin; Southern Federal University, Ru

P2-13

SYNTHESIS OF WATER SOLUBLE, LUMINESCENT LFNH NANOCRYSTALS FOR BIOLOGICAL APPLICATIONS

Mahendra Khandpekar[1]; Tarannum Attar[2]; [1]Birla College of Arts, Science & Commerce, In, [2]G M Momins College of ASC, In

P2-14

HOT-PRESSED PRODUCTION AND LASER PROPERTIES OF FE^{2+}:ZNS AND FE^{2+}:ZNSE

Roman Avetisov[1]; Stanislav Balabanov[2]; Konstantin Firsov[3]; Evgenii Gavrishchuk[2]; Andrey Gladilin[3]; Vladimir Ikonnikov[2]; Viktor Kalinushkin[3]; Igor Kononov[3]; Oleg Uvarov[3]; Marina Zykova[1]; Elena Mozhevitina[1]; Dmitry Savin[2]; Natalia Timofeeva[2]; Igor Avetissov[1]; [1]Dmitry Mendeleev Univeristy of Chemical Technology of Russia, Ru, [2]G.G. Devyatykh Institute of Chemistry of High-Purity Substances of the RAS, Ru, [3]Prokhorov General Physics Institute, Russian Academy of Sciences, Ru

P2-15

GROWTH OF SCHEELITE-LIKE DISORDERED DOUBLE MOLYBDATE AND TUNGSTATE SINGLE CRYSTALS FROM STOICHIOMETRIC AND NON-STOICHIOMETRIC MELTS

Kirill Subbotin[1]; Denis Lis[2]; Valerii Voronov[1]; Anatolii Titov[1]; Valerii Senin[3]; Viktoriia Sanina[2]; Evgenii Zharikov[2]; [1]A.M.Prokhorov General Physics Institute Russian Academy of Sciences, Ru, [2]A.M.Prokhorov General Physics

Institute of Russian Academy of Sciences, Ru, [3]Vernadsky Institute of Geochemistry and Analytical Chemistry RAS, Ru

P2-16

INFLUENCE OF RAW MATERIALS' PURITY ON GROWTH AND PROPERTIES OF β-BBO CRYSTALS

Andrey Sadovskiy[1]; Marina Zykova[2]; Elena Mozhevitina[2]; Andrew Khomyakov[2]; Alexander Ostrovskiy[3]; Roman Avetisov[2]; Alexander Yurkin[3]; Igor Avetissov[2]; [1]IPG, Ru, [2]Dmitry Mendeleev Univeristy of Chemical Technology of Russia, Ru, [3]Crystals of Sybiria Ltd., Ru

P2-17

GROWTH AND CHARACTERIZATION OF PHTHALIC ACID CRYSTALS IN PRESENCE OF HEXAMETHYLENETETRAMINE

Subbiah Meenakshisundaram; C Balakrishnan; S Sivaraman; R Markkandan; RM Sockalingam; Annamalai university, In

P2-18

GROWTH AND CHARACTERIZATION OF DIAQUATETRAKIS (1H-IMIDAZOLE-KN3)- MAGNESIUM DICHLORIDE SINGLE CRYSTAL

H Arul[1]; Nagaradona Suneetha[2]; D Rajan Babu[3]; R Ezhil Vizhi[3]; [1]Department of Science and Humanities, Kumaraguru College of Technology (Autonomous),, In, [2]VIT University, In, [3]Advanced Materials Research Centre, Department of Physics, School of Advanced Sciences, VIT University, In

P2-19

CYCLOHEXYLAMMONIUM CINNAMATE SINGLE CRYSTAL FOR NONLINEAR OPTICAL APPLICATIONS

R Gomathi[1]; S Madeswaran[1]; D Rajan Babu[1]; H Arul[2]; [1]Advanced Materials Research Centre, Department of Physics, School of Advanced Sciences, VIT University, In, [2]Department of Science and Humanities, Kumaraguru College of Technology (Autonomous),, In

P2-20

PECULIARITIES OF BULK BAY$_2$F$_8$ SINGLE CRYSTALS GROWTH FOR OBTAINING LUMINESCENCE IN THE UV REGION.

Anastasiia Uvarova[1]; Aleksandr Pushkar[2]; [1], Ru, [2]Doctor Web, Ru

P2-21

SINGLE-CRYSTAL FIBER OF TETRAPHENYLPHOSPHONIUM BROMIDE FOR STIMULATED RAMAN SCATTERING

YAN Ren[1]; GUANG QIANG Wang[2]; XU TANG Tao[2]; [1]INSTITUTE OF CRYSTAL MATERIALS, Cn, [2]INSTITUTE OF CRYSTAL MATERIALS SHANDONG UNIVERSITY, Cn

P2-22

MULTIFRACTAL SPECTRUM INVARIANCE OF SPATIAL NANOFORMS ON THE SURFACE OF ZNXCD1-XTE-SI HETEROSTRUCTURES SYNTHESIZED BY VARIOUS TECHNOLOGIES.

Vladimir Kuznetsov[1]; Pavel Moskvin[2]; Vlad Rudnitskiy[2]; [1]Saint-Petersburg State Electrotechnical University, Ru, [2]Zhytomyr state technology University, Ua

P2-23

OPTIMIZATION OF THE INTERFACIAL MISFIT ARRAY GROWTH MODE OF GASB EPILAYERS ON GAAS SUBSTRATE

Djalal Benyahia[1]; Łukasz Kubiszyn[2]; Krystian Michalczewski[1]; Artur Kębłowski[2]; Piotr Martyniuk[1]; Józef Piotrowski[2]; Antoni Rogalski[1]; [1]Military University of technology, Pl, [2]Vigo System S.A., Pl

P2-24

EX-SITU PROFILING OF TIO$_2$ FILM GROWTH USING SYNCHROTRON RADIATION

Kyle Kulinski[1]; Daniel Steckhahn[2]; Brandon Gunn[2]; Chris Tassone[3]; Andrew Ichimura[1]; [1]San Francisco State University, Us, [2]San Francisco State University, CA/Us, [3]Stanford Synchrotron Radiation Lightsource, CA/Us

P2-25
ELECTRICAL CHARACTERIZATION OF ALD DEPOSITED PBTIO3 THIN FILMS
Nick Sbrockey[1]; Gary Tompa[2]; Aaron Welsh[3]; Jung Yang[3]; Susan Trolier-Mckinstry[3]; Ronald Polcawich[4]; Daniel Potrepka[4]; [1]Structured Materials Industries, NJ/Us, [2]Structured Materials Industries, Inc., NJ/Us, [3]Penn State University, Us, [4]U.S. Army Research Laboratory, Us

P2-26
ANALYSIS OF THE FLOATING SILICON METHOD (FSM) FOR THE HORIZONTAL GROWTH OF CRYSTALLINE SILICON RIBBONS
Kerry Wang[1]; Jeffrey Derby[2]; [1]University of Minnesota - Twin Cities, MN/Us, [2]University of Minnesota, MN/Us

P2-27
GROWTH OF VERY THIN AL_2O_3 LAYER BY ATOMIC LAYER DEPOSITION AND ITS MODULATION OF ELECTRICAL PROPERTIES IN METAL/INP CONTACTS
Hogyoung Kim; Byung Joon Choi; Seoul National University of Science and Technology, Kr

19:00 - 21:00
Tuesday, August 1, 2017
OMVPE of Compound Semiconductors
Anasazi Ballroom South

Moderation: Masakazu Sugiyama, University of Tokyo/JP

19:00 - 19:20
III-V NANO-RIDGE GROWTH ON (001) SI FOR OPTOELECTRONICS
Bernardette Kunert[1]; Yves Mols[1]; Yuting Shi[2]; Dries Van Thourhout[2]; Marianna Pantouvaki[1]; Joris Van Campenhout[1]; Robert Langer[2]; [1]Imec, Be, [2]INTEC Department Ghent University, Be

19:20 - 19:40
DEGRADATION BEHAVIOR OF LASER DIODES WITH HIGHLY STRAINED INGAAS QWS WITH EMISSION WAVELENGTH BETWEEN 1120 NM AND 1180 NM
Frank Bugge; Gunnar Blume; David Feise; Nils Werner; Katrin Paschke; Markus Weyers; Ferdinand-Braun-Institut, De

19:40 - 20:00
EXTREMELY RAPID GAAS GROWTH BY MOVPE FOR LOW-COST PV APPLICATIONS
Akinori Ubukata[1]; Hassanet Sodabanlu[2]; Kentaroh Watanabe[2]; Syuichi Koseki[1]; Yoshiki Yano[1]; Toshiya Tabuchi[1]; Takeyoshi Sugaya[3]; Koh Matsumoto[1]; Yoshiaki Nakano[2]; Masakazu Sugiyama[2]; [1]Taiyo Nippon Sanso, Jp, [2]The university of Tokyo, Jp, [3]National Institute of advanced industrial science and technology, Jp

20:00 - 20:20
SETUP FOR IN-SITU ELECTRON MICROSCOPIC STUDIES OF SEMICONDUCTOR GROWTH
Kerstin Volz, Philipps-University Marburg, De

20:20 - 20:40
PHOTOLUMINESCENCE EXCITATION SPECTROSCOPY OF ANTIMONY DONORS IN ZINC OXIDE
Simon Watkins[1]; Faezeh Mohammadbeigi[2]; Senthil Kumar[1]; Katrina Stirling[1]; [1]Department of Physics, Simon Fraser University, BC/Ca, [2]Department of Physics, SimonFraser University, BC/Ca

20:40 - 21:00
SPATIO-TIME-RESOLVED CATHODOLUMINESCENCE STUDY OF THICK III-POLAR AND N-POLAR INGAN
Zakaria Al Balushi[1]; Joan Redwing[2]; [1]Dept. of Materials Science and Eng., The Pennsylvania State University, PA/Us, [2]The Pennsylvania State University, PA/Us

08:00 - 10:00
Thin Film Growth, Epitaxy, and Superlattices (1 of 2)
Anasazi Ballroom North

Moderation: Andrey Krysa[1]; Toby Garrod[2]; [1]U of Sheffield/GB, [2]II-VI/US

08:00 - 08:30
GROWTH, STABILITY, AND APPLICATIONS OF GAAS$_{1\text{-}X}$BI$_X$ MATERIALS THROUGH THE LENS OF MICROSTRUCTURAL DEVELOPMENT
Susan Babcock[1]; Thomas Kuech[2]; Luke Mawst[3]; Dane Morgan[2]; Weixin Chen[4]; Kamran Forghani[1]; Yingxin Guan[2]; Honghyuk Kim[1]; Guangfu Luo[2]; Adam Wood[1]; [1]University of Wisconsin-Madison, WI/Us, [2]University of Wisconsin Madison, Us, [3]University of Wisconsin-madison, WI/Us, [4]Department of Materials Science and Engineering, University of Wisconsin-Madison, WI/Us

08:30 - 09:00
EPITAXIAL GROWTH OF III-V QUANTUM DOT LASERS ON SILICON SUBSTRATES FOR SILICON PHOTONICS
Huiyun Liu, University College London, Gb

09:00 - 09:20
INTERFACE ANALYSIS FOR STRAINED LAYER SUPERLATTICES BY ATOM PROBE TOMOGRAPHY
Ayushi Rajeev[1]; Weixin Chen[2]; Jeremy Kirch[3]; Susan Babcock[3]; Luke Mawst[4]; Thomas Kuech[5]; Tom Earles[6]; [1]University of Wisconsin Madison, WI/Us, [2]Department of Materials Science and Engineering, University of Wisconsin-Madison, WI/Us, [3]University of Wisconsin-Madison, WI/Us, [4]University of Wisconsin-madison, WI/Us, [5]University of Wisconsin Madison, Us, [6]Intraband LLC, WI/Us

09:20 - 09:40
SUBSTRATE EVALUATION FOR HIGH QUALITY BORON PHOSPHIDE GROWTH
Yu Yang[1]; Xuejing Wang[2]; Jianqiu Guo[3]; Balaji Raghothamachar[3]; Michael Dudley[3]; Balabalaji Padavala[4]; Clint Frye[4]; James Edgar[4]; [1]Stony Brook University, , [2]Purdue University, Us, [3]Stony Brook University, NY/Us, [4]Kansas State University, Us

09:40 - 10:00
GROWTH, TRANSFER, AND CHARACTERIZATION OF GE AND SIGE NANOMEMBRANES ON III-V SUBSTRATES
Abhishek Bhat[1]; Xiaorui Cui[1]; Yingxin Guan[2]; Shelley Scott[1]; Thomas Kuech[2]; Max Lagally[1]; [1]University of Wisconsin-Madison, Us, [2]University of Wisconsin Madison, Us

	Wednesday 8/2				
Room	Anasazi South	Anasazi North	Chapel Room	Zia	Eldorado (A+B)
7:30-8:00	BREAKFAST				
8:00-10:00	FUNDAMENTALS 7	THIN FILMS 1	Symp Epi Com. Oxide 4	FERRO & TEXTURE CERAMICS 1	VENDOR
10:00-10:30	COFFEE BREAK				
10:30-12:00	FUNDAMENTALS 8	THIN FILMS 2	Symp Epi Com. Oxide 5	BULK 1	VENDOR
12:00-13:30	EXCURSIONS				
13:30-15:00					
15:00-15:30					
15:30-17:00					
17:00-17:30					
17:30-18:00					
18:00-19:00					
19:00-21:00					RECEPTION/ BANQUET

Wednesday, August 2, 2017

08:00 - 10:00
Wednesday, August, 2, 2017
Fundamentals of Crystal Growth (7 of 9)
Anasazi Ballroom South

Moderation: Peter Vekilov, U of Houston/US

08:00 - 08:30
THE SYNERGY OF MODELING AND NOVEL EXPERIMENTS FOR MELT CRYSTAL GROWTH RESEARCH
Jeffrey Derby, University of Minnesota, MN/Us

08:30 - 09:00
STRUCTURE OF SOLID-LIQUID GROWTH INTERFACES: GAN-GA AND SI/GE-IN
Elias Vlieg[1]; Aryan De Jong[1]; Vedran Vonk[2]; [1]Radboud University, Institute for Molecules and Materials, Nl, [2]DESY, De

09:00 - 09:30
GROWTH OF MOLECULAR SYSTEMS
Frank Schreiber, Tuebingen University, De

09:30 - 09:45
DISLOCATION AIDED ORIENTATION ALIGNMENT DURING INITIAL STAGES OF CRYSTAL GROWTH
Amit Samanta; Andrew Lange; Tammy Olson; Selim Elhadj; Lawrence Livermore National Laboratory, CA/Us

09:45 - 10:00
TWINNING DURING CZOCHRALSKI GROWTH OF HEAVILY-DOPED, DISLOCATION-FREE SINGLE CRYSTAL SILICON
Joel Kearns, NASA John H. Glenn Research Center, OH/Us

08:00 - 10:00
Wednesday, August, 2, 2017
Symposium on Epitaxy of Complex Oxides (4 of 11)
Chapel Room

Moderation: Ho Nyung Lee[1]; Darrel Schlom[2]; Lane Martin[3]; [1]ONRL/US, [2]Cornell/US, [3]Berkeley/US

08:00 - 08:15
HIGH MOBILITY BASNO3 FILMS GROWN BY MOLECULAR BEAM EPITAXY AND FIELD EFFECT TRANSISTOR
Jisung Park[1]; Hanjong Paik[2]; Debdeep Jena[3]; Darrell Schlom[2]; [1]Department of Material Science and Engineering, Cornell University, Us, [2]School of Electrical and Computer Engineering, Cornell University,, NY/Us, [3]Department of Material Science and Engineering, Cornell University, NY/Us

08:15 - 08:30
ADSORPTION-CONTROLLED GROWTH OF LA-DOPED $BASNO_3$BY MOLECULAR-BEAM EPITAXY
Hanjong Paik[1]; Zhen Chen[2]; Edward Lochocki[3]; Ariel Seidner[4]; Amit Verma[5]; Nicholas Tanen[4]; Jisung Park[4]; Masaki Uchida[6]; ShunLi Shang[7]; Bi-Cheng Zhou[7]; Zi-Kui Liu[7]; Debdeep Jena[8]; Kyle Shen[3]; David Muller[9]; Darrell Schlom[9]; [1]School of Electrical and Computer Engineering, Cornell University,, NY/Us, [2]Applied and Engineering Physics, Cornell University, NY/Us, [3]Department of Physics, Cornell University, Us, [4]Department of Material Science and Engineering, Cornell University, Us, [5]School of Electrical and Computer Engineering, Cornell University, Us, [6]Department of Applied Physics and Quantum-Phase Electronics Center (QPEC), University of

Tokyo, Jp, [7]Department of Materials Science and Engineering, The Pennsylvania State University, Us, [8]Department of Material Science and Engineering, Cornell University, NY/Us, [9]Cornell University, Us

08:30 - 09:00
NOVEL RADICAL-BASED MOLECULAR BEAM EPITAXY APPROACH FOR METAL OXIDE FILMS CONTAINING ELEMENTS OF LOW OXIDATION POTENTIAL
Bharat Jalan, University of Minnesota, MN/Us

09:00 - 09:30
SYNTHESIS STRATEGIES FOR CONTROLLING THE IN-PHASE OCTAHEDRAL ROTATION AXIS IN PBNM-TYPE PEROVSKITES
Steven May, Drexel University, PA/Us

09:30 - 10:00
PUSHING THE ENVELOPE ON UNDERSTANDING AND SUPPRESSING ATOM AND ION DIFFUSION ACROSS COMPLEX OXIDE INTERFACES
Scott Chambers; Steven Spurgeon; Yingge Du; Peter Sushko; Pacific Northwest National Laboratory, WA/Us

08:00 - 10:00
Wednesday, August, 2, 2017
Ferroelectric crystals and textured ceramics (1 of 3)
Zia Ballroom

Moderation: Jun Luo[1]; RichardJ. Meyer[2]; [1]TRS/US, [2]Penn State/US

08:00 - 08:30
RECENT DEVELOPMENTS AND UNDERSTANDING OF HIGH-PERFORMANCE PIEZO-/FERROELECTRIC SINGLE CRYSTALS OF COMPLEX PEROVSKITE
Zuo-Guang Ye, Simon Fraser University, BC/Ca

08:30 - 09:00
CRYSTAL GROWTH AND DOMAIN MEMORY EFFECT OF PMN-PT NEAR MPB
Qiang Li; CHAO Xu; Department of Chemistry, Tsinghua University, Cn

09:00 - 09:15
GROWTH, SIMULATION AND PROPERTIES CHARACTERIZATION OF LARGE SIZE $PB(IN_{1/2}NB_{1/2})O_3$-$PB(MG_{1/3}NB_{2/3})O_3$-$PBTIO_3$SINGLE CRYSTAL BY MODIFIED BRIDGEMAN METHOD
Kexin Song[1]; Zhuo Xu[2]; Zhenrong Li[1]; Fei Li[3]; Shiji Fan[1]; Sanhong Wang[1]; Haisheng Guo[1]; Ming Ma[1]; Yao Liu[1]; [1]Xian Jiaotong university, Cn, [2]Xian Jiaotong University, Cn, [3]Material Research Lab, Pennsylvania State University, Us

09:15 - 09:30
HIGH CURIE-TEMPERATURE (T_C) PIEZO-/FERROELECTRIC SINGLE CRYSTALS WITH BISMUTH-BASED COMPLEX PEROVSKITES: GROWTH, STRUCTURES AND PROPERTIES
Zuo-Guang Ye; Zenghui Liu; Hua Wu; Alisa Paterson; Simon Fraser University, BC/Ca

09:30 - 09:45
LEAD-FREE CRYSTAL GROWTH: FROM KTN TO KNN
Hao Tian; Peng Tan; Harbin Institute of Technology, Cn

09:45 - 10:00
COMPOSITION DESIGN AND PIEZOELECTRIC PROPERTY OF PURE KXNA1-XNBO3 SINGLE CRYSTAL FABRICATED BY SEED-FREE SOLID-STATE CRYSTAL GROWTH
Minhong Jiang; Chongyan Hao; Zhengfei Gu; Guilin University of Electronic Technology, Cn

10:30 - 12:00
Wednesday, August, 2, 2017
Thin Film Growth, Epitaxy, and Superlattices (2 of 2)
Anasazi Ballroom North

Moderation: Andrey Krysa[1]; Toby Garrod[2]; [1]U of Sheffield/GB, [2]II-VI/US

10:30 - 11:00
HIGH-INDEX-CONTRAST PHOTONIC CRYSTAL (HC-PC) QUANTUM CASCADE LASERS FABRICATED BY OMVPE
Luke Mawst[1]; Chris Sigler[2]; Colin Boyle[2]; Jeremy Kirch[3]; Don Lindberg Iii[4]; Tom Earles[4]; Dan Botez[2]; [1]University of Wisconsin-madison, WI/Us, [2]Department of Electrical and Computer Engineering, University of Wisconsin-Madison, WI/Us, [3]University of Wisconsin-Madison, WI/Us, [4]Intraband LLC, WI/Us

11:00 - 11:20
TUNING PHASE-SEPARATION AND ATOMIC-ORDERING IN ALGAINP FOR METAMORPHIC DEVICES
Kunal Mukherjee[1]; Eugene Fitzgerald[2]; [1]University of California Santa Barbara, CA/Us, [2]Massachusetts Institute of Technology, MA/Us

11:20 - 11:40
DOMAIN EPITAXY IN ANATASE TIO_2-SAPPHIRE THIN FILM HETEROSTRUCTURE: A NOVEL EPITAXIAL MATCH DERIVED FROM SOLUTION PHASE SYNTHESIS
Marissa Martinez[1]; Andrew Ichimura[2]; Christopher Tassone[3]; [1]University of Colorado, CO/Us, [2]San Francisco State University, Us, [3]Stanford Synchrotron Radiation Lightsource, CA/Us

11:40 - 12:00
IN-SITU SURFACE X-RAY SCATTERING INVESTIGATION INTO HYBRID OXIDE MOLECULAR BEAM EPITAXY GROWTH MECHANISMS FOR PEROVSKITE MATERIALS
Tassie Andersen[1]; Say Young Cook[2]; Hawoong Hong[3]; Laurence Marks[2]; Dillon Fong[4]; [1], Us, [2]Northwestern University, IL/Us, [3]Argonne National Laboratory, IL/Us, [4]Argonne National Laboratory, Us

10:30 – 11:45
Wednesday, August, 2, 2017
Fundamental of Crystal Growth (8 of 9)
Anasazi Ballroom South

Moderation: Peter. Vekilov, U of Houston/US

10:30 - 11:00
THE GROWTH AND DECOMPOSITION OF METASTABLE SEMICONDUCTING ALLOYS
Thomas Kuech[1]; Yingxin Guan[1]; Susan Babcock[2]; Luke Mawst[3]; Dane Morgan[1]; Guangfu Luo[1]; [1]University of Wisconsin Madison, Us, [2]University of Wisconsin-Madison, WI/Us, [3]University of Wisconsin-madison, WI/Us

11:00 - 11:30
THERMODYNAMICS OF DEPOSITION-FLUX DEPENDENT INTRINSIC FILM STRESS
Marcel J Rost[1]; Amirmehdi Saedi[2]; [1]Leiden Institute of Physics, Nl, [2]Leiden Institute of Chemistry, Nl

11:30 - 11:45
STRESS-DIRECTED COMPOSITIONAL PATTERNING OF COMPOUND SEMICONDUCTORS AND STRESS MAPPING BY 2D MICRO-RAMAN IMAGING
Brian Rummel; Michael Rimada; Sang Han; University of New Mexico, NM/Us

10:30 - 12:00

Wednesday, August, 2, 2017
Symposium on Epitaxy of Complex Oxides (5 of 11)
Chapel Room

Moderation: Ho Nyung Lee[1]; Darrel Schlom[2]; Lane Martin[3]; [1]ONRL/US, [2]Cornell/US, [3]Berkeley/US

10:30 - 11:00
OPTOELECTRONIC PROPERTIES OF EPITAXIALLY STRAINED COMPLEX OXIDES FROM FIRST PRINCIPLES
Sebastian Reyes-Lillo[1]; Jeffrey Neaton[2]; [1]LBNL, CA/Us, [2]Molecular Foundry, LBNL, CA/Us

11:00 - 11:15
ELASTIC STRAIN ENGINEERING OF PBTIO3 THIN FILMS GROWN BY REACTIVE MOLECULAR-BEAM EPITAXY
Eric Langenberg[1]; Eva Smith[2]; Hari Nair[3]; Neus Domingo[4]; Gustau Catalan[4]; Darrell Schlom[1]; [1]Cornell University, Us, [2]Department of Material Science and Engineering, Cornell University, Us, [3]Cornell University, NY/Us, [4]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC, Barcelona Institute of Science and Technology, Campus Universitat Autònoma de Barcelona, Es

11:15 - 11:30
STRAIN CONTROL OF CATIONIC DISTRIBUTION IN $BI_4TI_3O_{12}$-$BIFEO_3$ COMPOSITE FILMS
Changhee Sohn[1]; Dongkyu Lee[2]; Xiang Gao[2]; Ho Nyung Lee[2]; [1]Oak Ridge National Laboratory, Us, [2]Oak Ridge National Laboratory, TN/Us

11:30 - 12:00
SHARPENED VO2 PHASE TRANSITION VIA CONTROLLED RELEASE OF EPITAXIAL STRAIN
Chang-Beom Eom, University of Wisconsin-Madison, Us

10:30 - 12:00
Wednesday, August, 2, 2017
Bulk Crystal Growth (1 of 5)
Zia Ballroom

Moderation: Robert Feigelson[1]; Aleksandar Ostrogorsky[2]; [1]Stanford/US, [2] IIT/US

10:30 - 11:00
IN SITU DIAGNOSTICS OF SCINTILLATOR CRYSTAL GROWTH PROVIDED BY ENERGY-RESOLVED NEUTRON IMAGING
Anton Tremsin[1]; Didier Perrodin[2]; Adrian Losko[3]; Sven Vogel[3]; Mark Bourke[3]; Jeffrey Peterson[4]; Jeffrey Derby[4]; Takenao Shinohara[5]; Gregory Bizarri[2]; Edith Bourret[2]; [1]University of California, CA/Us, [2]Lawrence Berkeley National Laboratory, CA/Us, [3]Los Alamos National Laboratory, NM/Us, [4]University of Minnesota, MN/Us, [5]Japan Atomic Energy Agency, Jp

11:00 - 11:15
FINITE-ELEMENT MODELING OF SCINTILLATOR CRYSTAL GROWTH WITHIN A BRIDGMAN FURNACE IMAGED VIA NEUTRON SCATTERING
Chang Zhang[1]; Jeffrey Peterson[1]; Jan Seebeck[1]; Anton Tremsin[2]; Didier Perrodin[3]; Gregory Bizarri[3]; Edith Bourret[3]; Sven Vogel[4]; Jeffrey Derby[1]; [1]University of Minnesota, MN/Us, [2]University of California, CA/Us, [3]Lawrence Berkeley National Laboratory, CA/Us, [4]Los Alamos National Laboratory, NM/Us

11:15 - 11:30
PREPARATION AND CHARACTERIZATION OF TERNARY CESIUM HAFNIUM CHLORIDE SINGLE CRYSTALS
Robert Kral[1]; Petra Zemenova[2]; Ales Bystricky[2]; Vitezslav Jary[2]; Vladimir Babin[2]; Antonin Cihlar[2]; Karel Nitsch[2]; Pavel Veverka[2]; Martina Kohoutkova[3]; Shohei Kodama[4]; Shunsuke Kurosawa[5]; Yuui Yokota[6]; Akira Yoshikawa[4];

Martin Nikl[2]; [1]Institute of Physics of the Czech Academy of Sciences, Cz, [2]Institute of Physics, Czech Academy of Sciences, Cz, [3]University of Chemistry and Technology Prague, Cz, [4]Institute for Materials Research, Tohoku University, Jp, [5]Department of Physics, Yamagata University, Jp, [6]Tohoku University,

11:30 - 12:00
SOLUTION GROWTH OF BULK ORGANIC CRYSTALS
Natalia Zaitseva[1]; Leslie Carman[2]; Andrew Glenn[2]; Andrew Mabe[2]; Stephen Payne[2]; [1]Lawrence Livermore National Laboratory, Us, [2]Lawrence Livermore National Laboratory, CA/Us

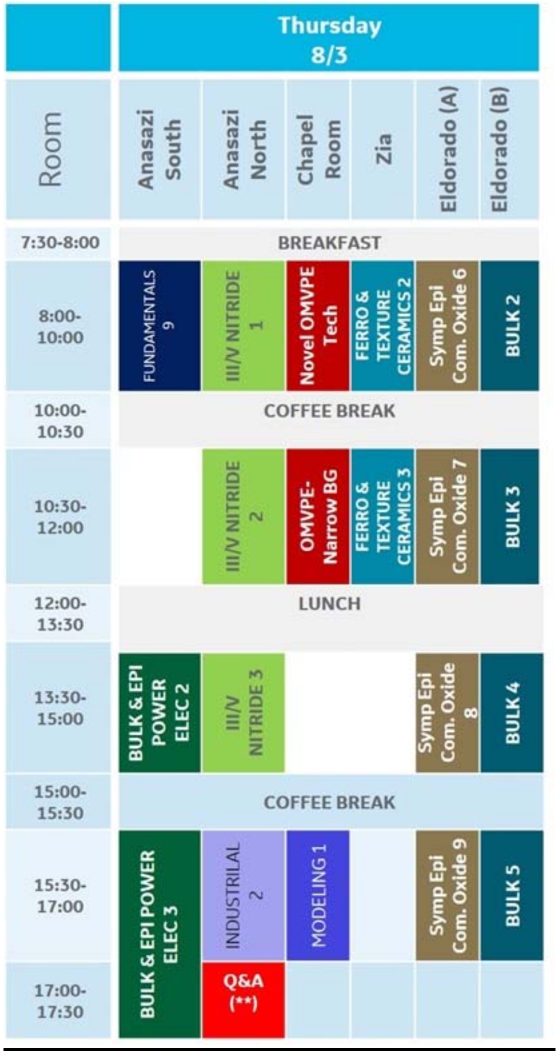
12:00-5:00
Group Excursions

6:00-7:00
Banquet Reception
Eldorado A & B

7:00-9:00
Banquet
Tickets are required.

Tickets are included with purchase of REGULAR REGISTRATION. Additional banquet tickets are available for purchase at Registration.

A limited number of donated tickets are available for students. Please sign up at registration before Wednesday morning and check back Wednesday at noon to see if you have received a ticket.



	Thursday 8/3					
Room	Anasazi South	Anasazi North	Chapel Room	Zia	Eldorado (A)	Eldorado (B)
7:30-8:00	BREAKFAST					
8:00-10:00	FUNDAMENTALS 9	III/V NITRIDE 1	Novel OMVPE Tech	FERRO & TEXTURE CERAMICS 2	Symp Epi Com. Oxide 6	BULK 2
10:00-10:30	COFFEE BREAK					
10:30-12:00		III/V NITRIDE 2	OMVPE-Narrow BG	FERRO & TEXTURE CERAMICS 3	Symp Epi Com. Oxide 7	BULK 3
12:00-13:30	LUNCH					
13:30-15:00	BULK & EPI POWER ELEC 2	III/V NITRIDE 3			Symp Epi Com. Oxide 8	BULK 4
15:00-15:30	COFFEE BREAK					
15:30-17:00	BULK & EPI POWER ELEC 3	INDUSTRILAL 2	MODELING 1		Symp Epi Com. Oxide 9	BULK 5
17:00-17:30		Q&A (**)				

Thursday, August 3, 2017

08:00 – 9:30
III/V Nitride and Other WBG Semiconductors (1 of 3)
Anasazi Ballroom North

Moderation: Dirk Ehrentraut[1]; Nelson Tansu[2]; [1]SOORA, [2]Lehigh

08:00 - 08:30
THICK HVPE GAN FILMS WITH DRAMATICALLY IMPROVED PROPERTIES
Jaime Freitas[1]; James Culbertson[2]; Nadeemullah Mahadik[1]; Shuang Wu[3]; Balaji Raghothamachar[4]; Michael Dudley[4]; Tomasz Socacki[5]; Michal Bockowski[5]; [1]Naval Research Laboratory, DC/Us, [2]Naval Research LAboratory, DC/Us, [3]Dept. of Mat. Sc., Stony Brook University, NY/Us, [4]Stony Brook University, NY/Us, [5]UNIPRESS, Institute of High Pressure, Pl

08:30 - 08:50
SINGLE-CRYSTAL-LIKE III-NITRIDE THIN FILMS DIRECTLY GROWN ON METAL TAPE
Jae-Hyun Ryou[1]; Shahab Shervin[2]; Kamrul Alam[2]; Kaveh Shervin[2]; Seung-Hwan Kim[2]; Tae Hoon Chung[3]; Jie Chen[2]; Wiejie Wang[2]; Sara Pouladi[2]; Rebecca Forrest[2]; Jiming Bao[2]; [1]University of Houston, TX/Us, [2]University of Houston, Us, [3]KOPTI, Kr

08:50 - 09:10
STRAIN RELAXATION PROPERTIES OF OMVPE-GROWN ALINN SEMICONDUCTORS
Wei Sun[1]; Renbo Song[2]; Jonathan Wierer, Jr.[2]; Nelson Tansu[2]; [1]Lehigh University, Us, [2]Lehigh University, PA/Us

09:10 - 09:30
THREADING DISLOCATION REDUCTION IN GAN ON SI(111) BY USING THREE DIMENSIONAL ISLAND GROWTH
Shane Chang, National Chiao Tung University , Tw

08:00 – 9:15
Thursday, August 3, 2017
Fundamentals of Crystal Growth (9 of 9)
Anasazi Ballroom South

Moderation: Peter Vekilov, U of Houston/US

08:00 - 08:15
ON ALLEVIATING MORPHOLOGICAL INSTABILITIES IN THE TRAVELING HEATER METHOD (THM) VIA THE ACCELERATED CRUCIBLE ROTATION TECHNIQUE (ACRT)
Jeffrey Peterson; Jeffrey Derby; University of Minnesota, MN/Us

08:15 - 08:30
GROWTH TEMPERATURE OPTIMIZATION OF GAAS-BASED $IN_{0.83}GA_{0.17}AS$ PHOTODETECTOR STRUCTURES ON $IN_{X}AL_{1-X}AS$ BUFFERS
Xingyou Chen; Yi Gu; Yonggang Zhang; Yingjie Ma; Suping Xi; Ben Du; Jian Zhang; Yanhui Shi; Wanyan Ji; Yi Zhu; Shanghai Institute of Microsystem and Information Technology (SIMIT), Chinese Academy of Sciences (CAS), Cn

08:30 - 08:45
INFLUENCE OF OXYGEN DIFFUSION ON DISLOCATION DENSITY IN SI SINGLE CRYSTAL
Satoshi Nakano[1]; Wataru Fukushima[2]; Hirofumi Harada[1]; Yoshiji Miyamura[1]; Koichi Kakimoto[1]; [1]Research Institute for Applied Mechanics, Kyushu University, Jp, [2]Kyushu University, Jp

08:45 - 09:00

GA(NASSB) CLOSE TO 1 EV GROWN WITH DTBAA

Eduard Sterzer[1]; Nattermann Lukas[2]; Oliver Maßmeyer[2]; Benjamin Ringler[2]; Carsten Von Hänisch[3]; Wolfgang Stolz[2]; Kerstin Volz[2]; [1]Material Sciences Center, De, [2]Philipps-Universität Marburg, Material Sciences Center and Faculty of Physics, De, [3]Philipps-Universität Marburg, Faculty of Chemistry, De

09:00 - 09:15

REVISITING THE TWINNING MECHANISM IN DIRECTIONAL SOLIDIFICATION OF MULTI-CRYSTALLINE SILICON SHEET

Chung-Wen Lan; H K Lin; Dept. of Chem. Eng., National Taiwan University, Tw

08:00 - 09:40
Thursday, August 3, 2017
Novel OMVPE Techniques and In-Situ Monitoring
Chapel Room

Moderation: Matt Highland, Argonne National Laboratory/US

08:00 - 08:20

IN SITU COHERENT X-RAY SCATTERING STUDIES DURING OMVPE OF GAN

Guangxu Ju[1]; Dongwei Xu[1]; Matt Highland[2]; Andrew Ulvestad[3]; Carol Thompson[4]; Jeffrey Eastman[5]; Peter Zapol[3]; Angel Yanguas-Gil[3]; Paul Fuoss[5]; Gregory Stephenson[1]; [1]Argonne National Laboratory, IL/Us, [2]Argonne National Lab, IL/Us, [3]Materials Science Div., Argonne National Lab, IL/Us, [4]Department Of Physics, Northern Illinois University, Us, [5]Materials Science Division, Argonne National Lab, IL/Us

08:20 - 08:40

BROADBAND IN SITU OPTICAL MONITORING FOR OMVPE GROWTH

George Atanasoff[1]; Christopher Metting[2]; [1]AccuStrata, Inc., MD/Us, [2]AccuStrata, MD/Us

08:40 - 09:00

CHARACTERIZING AMPOULE PERFORMANCE FOR LOW VAPOR PRESSURE PRECURSOR DELIVERY

James Maslar[1]; William Kimes[1]; Brent Sperling[1]; William Kimmerle[2]; Kyle Kimmerle[2]; [1]NIST, Us, [2]NSI, Us

09:00 - 09:20

HIGH TEMPERATURE OMVPE REACTOR WITH REDUCED PREMATURE REACTION AND IMPROVED HEATING EFFICIENCY

Kuang-Hui Li[1]; Hamad Alotaibi[2]; Xiaohang Li[2]; [1]KAUST, Sa, [2]King Abdullah University of Science and Technology (KAUST), Sa

09:20 - 09:40

EPITAXIAL GROWTH OF GA_2O_3 BY MOCVD USING OXYGEN: EXPERIMENTAL STUDY AND MODEL VERIFICATION

Maxim Bogdanov[1]; Anna Lobanova[2]; Roman Talalaev[1]; Alex Galyukov[3]; Fikadu Alema[4]; Brian Hertog[4]; Andrei Osinsky[4]; [1]STR Group, Inc. – Soft-Impact, Ltd., Ru, [2]STR, Ru, [3]STR US, Inc., VA/Us, [4]Agnitron Technology, Inc., MN/Us

08:00 - 10:00
Thursday, August 3, 2017
Ferroelectric crystals and textured ceramics (2 of 3)
Zia Ballroom

Moderation: Jun Luo[1]; RichardJ. Meyer[2]; [1]TRS/US, [2]Penn State/US

08:00 - 08:30

TRACKING FERROELECTRIC DOMAIN GROWTH USING LASER SCATTERING TOMOGRAPHY

Robert Feigelson; Howard Lee; Robert Demattei; Stanford University, CA/Us

08:30 - 09:00
MANUFACTURING AND UNIFORMITY OF GRAIN TEXTURED PIEZOELECTRIC CERAMICS
Mark Fanton[1]; Richard Meyer[2]; Elizabeth Kupp[2]; Beecher Watson[2]; Yunfei Chang[2]; Gary Messing[2]; [1]Penn State University, Us, [2]Penn State University, PA/Us

09:00 - 09:15
PROCESSING-ELECTROMECHANICAL PROPERTY RELATIONSHIPS IN TEXTURED PMNT
Richard Meyer[1]; Mark Fanton[2]; Gary Messing[1]; Elizabeth Kupp[1]; Yunfei Change[1]; Beecher Watson[1]; [1]Penn State University, PA/Us, [2]Penn State University, Us

09:15 - 09:30
SHEAR PIEZOELECTRIC PROPERTIES OF RELAXOR-PBTIO3 SINGLE CRYSTALS
Ming Ma[1]; Fei Li[2]; Kexin Song[3]; Yangbin Liu[2]; Zhenrong Li[3]; Shiji Fan[3]; Sanhong Wang[3]; Zhuo Xu[4]; [1]Xi'an Jiaotong University, Cn, [2]Electronic Materials Research Laboratory, Key Laboratory of the Ministry of Education and International Center for Dielectric Research,Xi'an Jiaotong University, Cn, [3]Xian Jiaotong university, Cn, [4]Xian Jiaotong University, Cn

09:30 - 10:00
ELECTRO-OPTIC AND NONLINEAR-OPTICAL PROPERTIES OF PB(MG$_{1/3}$NB$_{2/3}$)O$_3$-PBTIO$_3$SINGLE CRYSTAL
Zhuo Xu; Xin Liu; Xiaotian Fu; Ye Zhao; Weigang Zhao; Yongyong Zhuang; Xiaoyong Wei; Peng Luan; Xian Jiaotong University, Cn

08:15 - 10:00
Thursday, August 3, 2017
Bulk Crystal Growth (2 of 5)
Eldorado Grand Ballroom (B)

Moderation: Aleksandar Ostrogorsky, IIT/US

08:15 - 08:45
PROGRESS IN CZOCHRALSKI CRYSTAL GROWTH OF DISLOCATION FREE SILICON, AND POTENTIAL OF CONTINUOUS CZOCHRALSKI FOR NEXT GENERATION SILICON
Joel Kearns, NASA John H. Glenn Research Center, OH/Us

08:45 - 09:00
TOWARDS GRAPHITE-FREE HOT ZONE FOR DIRECTIONAL SOLIDIFICATION OF SILICON
Natasha Dropka[1]; Iryna Buchovska[2]; Iris Herrmann-Geppert[2]; Frank Kießling[2]; Ulrich Degenhardt[3]; [1]Leibniz Institute for Crystal Growth (IKZ) , De, [2]Leibniz Institute for Crystal Growth (IKZ), De, [3]FCT Ingenieurkeramik GmbH, De

09:00 - 09:15
NUMERICAL SIMULATION OF THE THERMAL AND FLOW FIELDS FOR A CZOCHRALSKI SILICON GROWTH WITH THE SYMMETRIC OR ASYMMETRIC CUSP-SHAPED MAGNETIC FIELD
Thi Hoai Thu Nguyen[1]; Jyh Chen Chen[2]; Chieh Hu[2]; Chun Hung Chen[2]; [1]Department of Mechanical Engineering, National Central University, Tw, [2]National Central University, Tw

09:15 - 09:30
INFLUENCE OF CONTAINMENT ON THE GROWTH OF GERMANIUM-SILICON IN MICROGRAVITY
Martin Volz[1]; Konstantin Mazuruk[2]; Arne Croell[2]; Tina Sorgenfrei[3]; [1]NASA Marshall Space Flight Center, AL/Us, [2]University of Alabama in Huntsville, AL/Us, [3]University of Freiburg, De

09:30 - 09:45
DONOR IMPURITY INCORPORATION DURING LAYER GROWTH OF ZN II-VI SEMICONDUCTORS

Douglas Barlow, Santa Fe College, FL/Us

09:45 - 10:00
AXIAL INFLECTION POINT TEMPERATURE PROFILES FOR THE ENGINEERING OF CONVEX CRYSTAL GROWTH INTERFACES IN BRIDGMAN SYSTEMS
Jeffrey Peterson; Jeffrey Derby; University of Minnesota, MN/Us

08:45 - 10:00
Thursday, August 3, 2017
Symposium on Epitaxy of Complex Oxides (6 of 11)
Eldorado Grand Ballroom (A)

Moderation: Ho Nyung Lee[1]; Darrel Schlom[2]; Lane Martin[3]; [1]ONRL/US, [2]Cornell/US, [3]Berkeley/US

08:45 - 09:00
STRAIN TUNING OF ELECTRONIC GROUND STATE IN CA_2RUO_4 EPITAXIAL THIN FILMS
Hari Nair[1]; Jacob Ruf[2]; Yang Liu[3]; Benjamin Grisafe[4]; Nikhil Shukla[4]; Celesta Chang[5]; Qiang Han[6]; Andrew Millis[6]; David Muller[7]; Suman Datta[4]; Kyle Shen[2]; Darrell Schlom[7]; [1]Cornell University, NY/Us, [2]Department of Physics, Cornell University, Us, [3]Department of Physics, Zhejiang University, Cn, [4]Department of Electrical Engineering, University of Notre Dame, Us, [5]Applied and Engineering Physics, Cornell University, Us, [6]Department of Physics, Columbia University, Us, [7]Cornell University, Us

09:00 - 09:30
SUBSTRATE 'THERMINATION' AND THE ROLE OF SURFACE RECONSTRUCTION FOR THE EPITAXY OF PEROVSKITE OXIDES
Wolfgang Braun; Maren Jäger; Jochen Mannhart; Max Planck Institute for Solid State Research, De

09:30 - 10:00
MAGNETISM AT INTERFACES IN COMPLEX OXIDES GROWN USING MOLECULAR BEAM EPITAXY
Anand Bhattacharya, Argonne National Laboratory, Us

10:00-11:40
Thursday, August 3, 2017
III/V Nitride and Other WBG Semiconductors (2 of 3)
Anasazi Ballroom North

Moderation: Dirk Ehrentraut[1]; Nelson Tansu[2]; [1]SOORA, [2]Lehigh

10:30 - 11:00
BASIC AMMONOTHERMAL GROWTH OF BULK GAN IN MOLYBDENUM CAPSULES
Siddha Pimputkar[1]; James Speck[2]; Shuji Nakamura[2]; [1]Lehigh University, PA/Us, [2]University of California, Santa Barbara, CA/Us

11:00 - 11:20
THE SODIUM FLUX TECHNIQUE FOR BULK GALLIUM NITRIDE
Paul Von Dollen[1]; Mohammed Abo Alreesh[1]; Siddha Pimputkar[2]; Hamad Albrithen[3]; Shuji Nakamura[4]; James Speck[4]; [1]University of California, Santa Barbara, Us, [2]Lehigh University, PA/Us, [3]King Adbulaziz City for Science and Technology, Sa, [4]University of California, Santa Barbara, CA/Us

11:20 - 11:40
IN-SITU GROWTH MODE CONTROL OF ALN ON SIC SUBSTRATE BY SUBLIMATION CLOSED SPACE TECHNIQUE
Daichi Dojima[1]; Koji Ashida[2]; Tadaaki Kaneko[2]; [1]Kwansei Gakuin University , Jp, [2]Kwansei Gakuin University, Jp

10:30 - 11:50
Thursday, August 3, 2017
OMVPE of Narrow Bandgap Semiconductors
Chapel Room

Moderation: Simon Watkins, Simon Fraser University/CA

10:30 - 10:50
IMF GROWTH OF GASB ON V-GROOVED SI WITH ASPECT RATIO TRAPPING
Billy Lai[1]; Qiang Li[2]; Kei Lau[2]; [1]The Hong Kong University of Science and Technology, Hk, [2]Hong Kong University of Science and Technology, Hk

10:50 - 11:10
OMVPE GROWTH OF STRAIN-COMPENSATED GAAS$_{1\text{-}Y}$P$_{Y}$/GAAS$_{1\text{-}X}$BI$_{X}$ QUANTUM WELL ACTIVE REGION LASERS
Honghyuk Kim[1]; Yingxin Guan[2]; Thomas Kuech[2]; Luke Mawst[3]; [1]University of Wisconsin-Madison, WI/Us, [2]University of Wisconsin Madison, Us, [3]University of Wisconsin-madison, WI/Us

11:10 - 11:30
THERMODYNAMIC STABILITY ANALYSIS OF BI-CONTAINING III-V QUATERNARY ALLOYS AND THE EPITAXIAL STRAIN EFFECTS
Yingxin Guan; Guangfu Luo; Dane Morgan; Thomas Kuech; University of Wisconsin Madison, Us

11:30 - 11:50
GROWTH AND CHARACTERIZATION OF IN$_{X}$GA$_{1\text{-}X}$SB METAMORPHIC BUFFER LAYERS BY METAL-ORGANIC VAPOR PHASE EPITAXY ON THE GASB SUBSTRATE
Yingxin Guan[1]; Aaron Tan[2]; Susan Babcock[3]; Luke Mawst[4]; Thomas Kuech[1]; [1]University of Wisconsin Madison, Us, [2]University of Wisconsin Madison, WI/Us, [3]University of Wisconsin-Madison, WI/Us, [4]University of Wisconsin-madison, WI/Us

10:30 - 12:00
Thursday, August 3, 2017
Symposium on Epitaxy of Complex Oxides (7 of 11)
Eldorado Grand Ballroom (A)

Moderation: Ho Nyung Lee[1]; Darrel Schlom[2]; Lane Martin[3]; [1]ONRL/US, [2]Cornell/US, [3]Berkeley/US

10:30 - 11:00
HIGH PRESSURE OXYGEN SPUTTER DEPOSITION OF PEROVSKITE OXIDE METALS AND SEMICONDUCTORS
Chris Leighton[1]; Jeff Walter[1]; Koustav Ganguly[1]; Palak Ambwani[1]; Shameek Bose[1]; Peng Xu[1]; Abhinav Prakash[1]; Greg Haugstad[1]; Jaume Gazquez[2]; Neven Biskup[3]; Maria Varela[3]; Jong Seok Jeong[1]; Andre Mkhoyan[1]; Bharat Jalan[1]; [1]University of Minnesota, MN/Us, [2]Universidad Complutense de Madrid, Es, [3]Universidad de Complutense de Madrid, Es

11:00 - 11:15
GROWTH OF HIGH QUALITY EPITAXIAL LAALO3 ON SRTIO3 ON (001) SI VIA MOLECULAR-BEAM EPITAXY
Zhe Wang[1]; Darrell Schlom[2]; [1]Cornell University, NY/Us, [2]Cornell University, Us

11:15 - 11:30
GROWTH OF DEFECT MITIGATING, METASTABLE (SRTIO$_{3}$)$_{N}$(BATIO$_{3}$)$_{M}$SRO SUPERLATTICES
Natalie Dawley[1]; Megan Holtz[2]; Gerhard Olsen[2]; Xifeng Lu[3]; Nathan Orloff[3]; Che-Hui Lee[2]; Jingshu Zhang[2]; James Booth[3]; Craig Fennie[2]; David Muller[2]; Darrell Schlom[2]; [1]Cornell University, NY/Us, [2]Cornell University, Us, [3]NIST, Us

11:30 - 12:00
EPITAXIAL GROWTH OF EXTREME-MOBILITY OXIDES
Jon-Paul Maria, North Carolina State University, NC/Us

10:30 - 12:00
Thursday, August 3, 2017
Bulk Crystal Growth (3 of 5)
Eldorado Grand Ballroom (B)

Moderation: Robert Feigelson[1]; Aleksandar Ostrogorsky[2]; [1]Stanford/US, [2] IIT/US

10:30 - 11:00
TWO-INCH, HIGH TRANSPARENCY ALUMINUM NITRIDE SINGLE CRYSTAL GROWTH FOR COMMERCIAL APPLICATIONS
Leo Schowalter; Robert Bondokov; Jianfeng Chen; Murugesu Yoganathan; Takashi Suzuki; Shailaja Rao; Toru Kimura; Keisuke Yamaoka; Crystal IS, Inc., Us

11:00 - 11:15
SUBLIMATION GROWTH AND CHARACTERIZATION OF ERBIUM NITRIDE CRYSTALS
Hayder Alatabi; Balabalaji Padavala; James Edgar; Kansas State University, Us

11:15 - 11:30
FROM X-RAYS TO NEUTRONS (AND BEYOND): CASE STUDIES OF COMPLEX VANADATES GROWN FROM MICRONS TO CENTIMETERS (AND BEYOND)
Colin McMillen[1]; Vasile Garlea[2]; Michael McGuire[2]; Liurukara Sanjeewa[3]; Joseph Kolis[1]; [1]Clemson University, SC/Us, [2]Oak Ridge National Laboratory, Us, [3]Clemson University, Us

11:30 - 11:45
POSSIBLE PRESENCE OF AL-GA COMPLEX IN THE $CA_3TA(GA,AL)_3SI_2O_{14}$ MELT AND ITS PARTITIONING DURING GROWTH FROM THE MELT
Satoshi Uda; Shuhei Sakano; Chihiro Koyama; Junpei Okada; Tohoku University, Jp

11:45 - 12:00
GROWTH OF CORUNDUM CRYSTALS FOR CALIBRATION STANDARDS USED IN DETERMINING GEOGRAPHICAL ORIGIN OF NATURAL RUBIES AND SAPPHIRES
Zachary Cole[1]; Jennifer Stone-Sundberg[2]; Randy Equall[1]; Tim Thomas[3]; John Emmett[4]; [1]FLIR - Scientific Materials, Us, [2]Crystal Solutions, OR/Us, [3]PDX Photonics, OR/Us, [4]Crystal Chemistry, WA/Us

10:30 - 10:45
Thursday, August 3, 2017
Ferroelectric crystals and textured ceramics (3 of 3)
Zia Ballroom

Moderation: Jun Luo[1]; RichardJ. Meyer[2]; [1]TRS/US, [2]Penn State/US

10:30 - 10:45
PROPERTY MODIFICATION OF RELAXOR-PT CRYSTALS BY ACCEPTOR AND DONOR DOPANTS
Jun Luo[1]; Sam Taylor[1]; Fei Li[2]; Shujun Zhang[3]; Tom Shrout[2]; Wes Hackenberger[1]; [1]TRS Technologies, Inc., Us, [2]Material Research Lab, Pennsylvania State University, Us, [3]Australian Institute of Innovative Materials, University of Wollongong, Au

13:30 – 14:50
Thursday, August 3, 2017
III/V Nitride and Other WBG Semiconductors (3 of 3)

Anasazi Ballroom North

Moderation: Dirk Ehrentraut[1]; Nelson Tansu[2]; [1]SOORA, [2]Lehigh

13:30 - 13:50
PULSED OMVPE GROWTH STUDIES OF INN FOR INTEGRATION IN INGAN ACTIVE REGION
Ioannis Fragkos[1]; Wei Sun[2]; Damir Borovac[1]; Renbo Song[1]; Jonathan Wierer, Jr.[1]; Nelson Tansu[1]; [1]Lehigh University, PA/Us, [2]Lehigh University, Us

13:50 - 14:10
PROPERTIES OF GAN ON HIGH QUALITY ALN SAPPHIRE TEMPLATE BY USING METALORGANIC CHEMICAL VAPOR DEPOSITION
Akira Mishima[1]; Yuji Tomita[1]; Guanxi Piao[1]; Yoshiki Yano[2]; Toshiya Tabuchi[2]; Koh Matsumoto[2]; [1]Taiyo Nippon Sanso corporation., Jp, [2]Taiyo Nippon Sanso, Jp

14:10 - 14:30
DELTA DOPING AND BIASED ENHANCED GROWTH DIAMOND BY HOT FILAMENT CVD TECHNOLOGY
Gary Harris[1]; Aaron Jackson[1]; Amber Wingfield[1]; James Griffin[1]; Crawford Taylor[1]; Marko Loncar[2]; [1]Howard University, DC/Us, [2]Harvard University, MA/Us

14:30 - 14:50
DOPED, HIGH MOBILITY CADMIUM OXIDE FILMS FOR TUNABLE PLASMONICS
Evan Runnerstrom[1]; Jon-Paul Maria[2]; [1]NC State University, Us, [2]North Carolina State University, NC/Us

13:30 - 15:00
Thursday, August 3, 2017
Bulk Growth and Epitaxy for Power Electronics (2 of 3)
Anasazi Ballroom South

Moderation: Michael Dudley; Balaji Raghothamachar; Stony Brook/US

13:30 - 14:00
INFLUENCE OF CARRIER CONCENTRATION ON BULK LIFETIME IN CZ-SI CRYSTAL
Koichi Kakimoto, Research Institute for Applied Mechanics, Kyushu University, Jp

14:00 - 14:30
SIC CRYSTAL GROWTH AND SUBSTRATE TECHNOLOGY FOR DEVICE MANUFACTURING
Robert Leonard; Yuri Khlebnikov; Michael Paisley; Simon Bubel; Jyothi Ambati; Eugene Deyneka; Ian Currier; Valeri Tsvetkov; Jeff Seaman; Adrian Powell; Mike O'Loughlin; Edward Van Brunt; Al Burk; Elif Balkas; Cree, Inc., NC/Us

14:30 - 15:00
OMVPE GROWTH OF AL-RICH ALGAN ALLOYS FOR POWER ELECTRONICS
Andrew Allerman[1]; Mary Crawford[2]; Greg Pickrell[2]; Andrew Armstrong[2]; Robert Kaplar[2]; Jeramy Dickerson[2]; Brianna Klein[2]; Michael King[2]; Michael Van Heukelom[2]; [1]Sandia National Laboratories, Us, [2]Sandia National Laboratories, NM/Us

13:30 - 15:00
Thursday, August 3, 2017
Symposium on Epitaxy of Complex Oxides (8 of 11)
Eldorado Grand Ballroom (A)

Moderation: Ho Nyung Lee[1]; Darrel Schlom[2]; Lane Martin[3]; [1]ONRL/US, [2]Cornell/US, [3]Berkeley/US

13:30 - 14:00
MAESTRO: A SYNCHROTON BEAMLINE FOR ELECTRONIC STRUCTURE DETERMINATION OF IN-SITU GROWN OXIDES AND 2D MATERIALS
Eli Rotenberg, Lawrence Berkeley National Laboratory, CA/Us

14:00 - 14:30
IN SITU X-RAY STUDIES OF EPITAXIAL OXIDE NANOCOMPOSITE FORMATION
Matt Highland[1]; Dillon Fong[2]; Hua Zhou[3]; Carol Thompson[4]; Peter Baldo[5]; Jeffrey Eastman[5]; Paul Fuoss[5]; [1]Argonne National Lab, IL/Us, [2]Argonne National Laboratory, Us, [3]X-ray Science Division, Argonne National Lab, IL/Us, [4]Department Of Physics, Northern Illinois University, Us, [5]Materials Science Division, Argonne National Lab, IL/Us

14:30 - 15:00
ISLAND GROWTH DYNAMICS IN PULSED LASER DEPOSITION OF $SRTIO_3$
Gyula Eres, Oak Ridge National Laboratory, TN/Us

13:30 - 15:00
Thursday, August 3, 2017
Bulk Crystal Growth (4 of 5)
Eldorado Grand Ballroom (B)

Moderation: Robert Feigelson[1]; Aleksandar Ostrogorsky[2]; [1]Stanford/US, [2] IIT/US

13:30 - 14:00
HIGH PRESSURE FLOATING ZONE GROWTH OF CORRELATED ELECTRON TRANSITION METAL OXIDES
John Mitchell; Junjie Zhang; Hong Zheng; Michael Norman; Daniel Phelan; Antia Botana; Argonne National Laboratory, IL/Us

14:00 - 14:15
EFFECT OF MOLTEN-ZONE INSTABILITY ON THE IMPURITY PARTITIONING DURING FZ GROWTH
Satoshi Uda; Yutaroh Takehara; Chihiro Koyama; Tohoku University, Jp

14:15 - 14:30
SEARCHING FOR IDEAL BI-SYSTEM TOPOLOGICAL INSULATOR, PB-SYSTEM TOPOLOGICAL CRYSTALLINE INSULATOR AND THEIR TOPOLOGICAL SUPERCONDUCTOR
Genda Gu, Brookhaven National Laboratory, NY/Us

14:30 - 14:45
GROWTH OF 8-HYDROXYQUINOLINE SINGLE CRYSTAL BY MODIFIED CZOCHRALSKI GROWTH TECHNIQUE AND CHARACTERIZATION
SONU Kumar[1]; Binay Kumar[2]; [1]UNIVERSITY OF DELHI, In, [2]Crystal Lab, Department of Physics & Astrophysics, University of Delhi, Delhi-7, India, In

14:45 - 15:00
GROWTH, INTERNAL STRUCTURE AND MECHANICAL PROPERTIES OF PLATINUM FIBER CRYSTALS BY ALLOY-MICRO-PULLING-DOWN METHOD
Takayuki Nihei[1]; Yuui Yokota[2]; Akihiro Yamaji[1]; Yuji Ohashi[3]; Shunsuke Kurosawa[4]; Kei Kamada[3]; Akira Yoshikawa[1]; [1]Institute for Materials Research, Tohoku University, Jp, [2]Tohoku University, Jp, [3]NICHe, Tohoku University, Jp, [4]Department of Physics, Yamagata University, Jp

15:30 - 17:00
Thursday, August 3, 2017
Industrial Crystal Growth Technologies and Equipment (2 of 2)
Anasazi Ballroom North

Moderation: Matt Whittaker, Gooch & Housego/US

15:30 - 16:00
REFRACTORY METALS - MATERIAL OF CHOICE FOR SINGLE CRYSTAL GROWTH
Heike Larcher, Plansee SE, At

16:00 - 16:15
IMPROVED CARBON AND GRAPHITE MATERIALS FOR CRYSTAL GROWTH
Chong Chen; Helen Mayer; GrafTechAGM, OH/Us

16:15 - 16:30
APPLICATION OF HEATER MAGNET MODULE FOR IMPROVED CRYSTAL GROWTH OF SEMICONDUCTORS
Christiane Frank-Rotsch[1]; Iryna Buchovska[2]; Natasha Dropka[3]; Radoslaw Zwierz[1]; Peter Rudolph[4]; Frank Kießling[2]; [1]Leibniz Institute for Crystal Growth, De, [2]Leibniz Institute for Crystal Growth (IKZ), De, [3]Leibniz Institute for Crystal Growth (IKZ) , De, [4]Crystal Technology Consulting, De

16:30 - 16:45
TEMPERATURE UNIFORMITY OF INDUCTION-HEATED OMVPE SUSCEPTORS AT HIGH TEMPERATURE
Kuang-Hui Li[1]; Hamad Alotaibi[2]; Xiaohang Li[2]; [1]KAUST, Sa, [2]King Abdullah University of Science and Technology (KAUST), Sa

16:45 - 17:00
A SMALL BUSINESS PERSPECTIVE ON INDUSTRIAL CRYSTAL GROWTH
Candace Lynch[1]; Thomas Caughey[2]; Sergey Selin[2]; Tony Inzalaco[2]; [1]Inrad Optics, Inc., Us, [2]Inrad Optics, Inc., NJ/Us

15:30 - 17:20
Thursday, August 3, 2017
Bulk Growth and Epitaxy for Power Electronics (3 of 3)
Anasazi Ballroom South

Moderation: Michael Dudley; Balaji Raghothamachar, Stony Brook/US

15:30 - 16:00
LATEST PROGRESS IN GALLIUM OXIDE EPITAXIAL GROWTH TECHNOLOGIES FOR POWER DEVICES
Masataka Higashiwaki[1]; Yoshiaki Nakata[1]; Man Hoi Wong[1]; Keita Konishi[2]; Takafumi Kamimura[1]; Ken Goto[3]; Kohei Sasaki[3]; Akito Kuramata[3]; Shigenobu Yamakoshi[3]; Hisashi Murakami[2]; Yoshinao Kumagai[2]; [1]National Institute of Information and Communications Technology, Jp, [2]Department of Applied Chemistry, Tokyo University of Agriculture and Technology, Jp, [3]Tamura Corporation, Jp

16:00 - 16:30
FAST CVD CRYSTAL GROWTH OF 4H-SIC FOR POWER DEVICES
Hidekazu Tsuchida[1]; Isaho Kamata[2]; Masahiko Ito[2]; Tetsuya Miyazawa[2]; Norihiro Hoshino[2]; [1]Central Research Institute of Electric Power Industry (CRIEPI), Jp, [2]Central Research Institute of Electric Power Industry (CRIEPI), Jp

16:30 - 17:00
GROWTH AND CHARACTERIZATION OF SIC
Balaji Raghothamachar[1]; Michael Dudley[1]; Yu Yang[2]; Jianqiu Guo[1]; [1]Stony Brook University, NY/Us, [2]Stony Brook University,

17:00 - 17:20

UNDERSTANDING THE MICROSTRUCTURES OF TRIANGULAR DEFECTS IN 4H-SIC HOMOEPITAXIAL LAYERS GROWN BY CVD METHOD
Jianqiu Guo[1]; Yu Yang[1]; Jungyu Kim[2]; Tae Jin Kim[1]; Balaji Raghothamachar[1]; Michael Dudley[1]; [1]Stony Brook University, NY/Us, [2]LG Chem, Kr

15:30 - 17:00
Thursday, August 3, 2017
Modeling of Crystal Growth Processes (1 of 3)
Chapel Room

Moderation: JeffreyJ. Derby, U of Minnesota/Us

15:30 - 16:00
INSIGHTS INTO THE MATERIALS SCIENCE OF COLLOIDAL CRYSTALS FORMED BY DNA-FUNCTIONALIZED PARTICLES
Talid Sinno; Ian Jenkins; Mehdi Zanjani; John Crocker; University of Pennsylvania, Us

16:00 - 16:30
DIRECT CALCULATION OF SOLID-LIQUID INTERFACIAL FREE ENERGIES FROM EQUILIBRIUM MOLECULAR DYNAMICS SIMULATIONS.
Luis Zepeda, Lawrence Livermore National Laboratory, CA/Us

16:30 - 17:00
ANALYSIS OF RE-MELTING PROCESS OF SILICON GROWN BY TRANSVERSE MAGNETIC FIELD APPLIED CZ METHOD
Koichi Kakimoto, Research Institute for Applied Mechanics, Kyushu University, Jp

15:30 - 17:00
Thursday, August 3, 2017
Symposium on Epitaxy of Complex Oxides (9 of 11)
Eldorado Grand Ballroom (A)

Moderation: Ho Nyung Lee[1]; Darrel Schlom[2]; Lane Martin[3]; [1]ONRL/US, [2]Cornell/US, [3]Berkeley/US

15:30 - 16:00
CRYSTALLIZATION BY PARTICLE ATTACHMENT OF METASTABLE
David Geohegan, Oak Ridge National Laboratory, TN/Us

16:00 - 16:30
ENGINEERING DEFECT FORMATION IN FUNCTIONAL OXIDE THIN FILMS AND HETEROSTRUCTURES
Regina Dittmann[1]; Felix Gunkel[2]; Felix Hensling[1]; Chencheng Xu[1]; [1]Forschungszentrum Jülich GmbH, De, [2]Institut f¨ur Werkstoffe der Elektrotechnik II, RWTH Aachen University, De

16:30 - 16:45
TUNING THE SUPERCONDUCTIVITY IN SINGLE-LAYER FESE/OXIDES BY INTERFACE ENGINEERING
Haichao Xu; Rui Peng; Donglai Feng; Fudan University, Cn

16:45 - 17:00
RAPID-ANNEAL SOLID PHASE EPITAXY OF ATOMICALLY FLAT HIGH SURFACE ENERGY RUO_2(001) FILMS
Paul Snijders[1]; Yang Wang[1]; Yang Song[1]; Rui Peng[1]; Andreas Herklotz[1]; Matthew Chisholm[1]; Zili Wu[1]; Thomas Ward[1]; Hanno Weitering[2]; [1]Oak Ridge National Laboratory, Us, [2]University of Tennessee, TN/Us

17:00 - 17:30
Special Q&A session:
What they don't teach you about industrial crystal growth in school
Anasazi Ballroom North

Moderation: Matt Whittaker[1], Candance Lynch[2] , Kevin Zawailski[3], [1] Gooch & Housego/US,
[2]INRAD/US,[3]BAE/US

15:30 - 16:00
Thursday, August 3, 2017
Bulk Crystal Growth (5 of 5)
Eldorado Grand Ballroom (B)

Moderation: Robert Feigelson,Stanford/US

15:30 - 15:45
DETACHED MELT AND VAPOR GROWTH OF INI IN SUBSA FURNACE
Aleksandar Ostrogorsky[1]; Vladimir Riabov[2]; Martin Volz[3]; Lodewijk Van Den Berg[4]; Arne Cröll[5]; [1], , [2]Illinois Institute of Technology, IL/Us, [3]NASA Marshall Space Flight Center, AL/Us, [4]Constellation Technology, FL/Us, [5]NASA MSFC, AL/Us

15:45 - 16:00
EFFECT OF POWER HISTORY ON THE SHAPE AND THE THERMAL STRESS OF LARGE SIZE SAPPHIRE CRYSTAL DURING THE KYROPOULOS PROCESS
Tran Phu Nguyen[1]; Jyh-Chen Chen[2]; Hsiao-Tsun Chuang[2]; Chieh Hu[2]; [1]National Central University, Vn, [2]National Central University, Tw

	Friday 8/4			
Room	Anasazi North	Zia	Eldorado (A)	Eldorado (B)
7:30-8:00	BREAKFAST			
8:00-10:00	MAT'LS FOR PV & ENERGY	NANO 1	Symp Epi Com. Oxide 10	MODELING 2
10:00-10:30	COFFEE BREAK			
10:30-12:00		NANO 2	Symp Epi Com. Oxide 11	MODELING 3

Friday, August 4, 2017

08:00 - 10:00
Friday, August 4, 2017
Materials for Photovoltaics and Energy Technology (1 of 1)
Anasazi Ballroom North

Moderation: JohnF. Geisz, NREL/Us

08:00 - 08:20
LOW COST III-V PHOTOVOLTAICS BY HYDRIDE VAPOR PHASE EPITAXY
Kevin Schulte[1]; John Simon[2]; Nikhil Jain[2]; John Mangum[3]; Corinne Packard[3]; Brian Gorman[3]; Aaron Ptak[2]; [1], , [2]National Renewable Energy Laboratory, CO/Us, [3]Colorado School of Mines Department of Metallurgical and Materials Engineering, CO/Us

08:20 - 08:40
FIRST BIFACIAL GROWTH AND BIFACIAL EPITAXIAL LIFT OFF (B-ELO) OF 3J SOLAR CELLS ON 6 INCH GAAS SUBSTRATES
Kamran Forghani; Andree Wibowo; Chris Stender; Joshua Wood; Noren Pan; MicroLink Devices Inc., IL/Us

08:40 - 09:00
ELECTRON CHANNELING CONTRAST IMAGING OF GAINP/GAAS/SI SOLAR CELLS
Ryan France[1]; Markus Feifel[2]; Jens Ohlmann[2]; David Lackner[2]; Frank Dimroth[2]; [1]National Renewable Energy Laboratory, Us, [2]Fraunhofer Institute for Solar Energy, De

09:00 - 09:20
GROWTH OF GAASPN P-I-N JUNCTIONS ON SI SUBSTRATES WITH LATTICE MATCHING CONDITIONS FOR MONOLITHIC III-V/SI MULTI-JUNCTION SOLAR CELLS
Keisuke Yamane; Kento Sato; Masaya Goto; Kenjiro Takahashi; Hiroto Sekiguchi; Hiroshi Okada; Akihiro Wakahara; Toyohashi University of Technology, Jp

09:20 - 09:40
SELECTIVE AREA GROWTH OF GAAS ON SI FOR PHOTOVOLTAIC APPLICATIONS
Michelle Vaisman[1]; Nikhil Jain[2]; Qiang Li[3]; Kei Lau[3]; Emily Makoutz[4]; William McMahon[4]; Jeramy Zimmerman[5]; Adele Tamboli[4]; Emily Warren[4]; [1]National Renewable Energy Lab, Us, [2]National Renewable Energy Laboratory, CO/Us, [3]Hong Kong University of Science and Technology, Hk, [4]National Renewable Energy Lab, CO/Us, [5]Colorado School of Mines, Us

09:40 - 10:00
SINGLE-CRYSTAL-LIKE THIN FILM III-V MATERIAL DIRECTLY GROWN ON HASTELLOY TAPE FOR FLEXIBLE SOLAR CELLS
Jae-Hyun Ryou[1]; Venkat Selvamanickam[2]; Sara Pouladi[2]; Mojtaba Asadirad[2]; Monika Rathi[2]; Seung Kyu Oh[2]; Devendra Khatiwada[2]; Pavel Dutta[2]; Shahab Shervin[2]; Yao Yao[2]; Yongkuan Li[2]; Jie Chen[2]; [1]University of Houston, TX/Us, [2]University of Houston, Us

08:00 - 10:00
Friday, August 4, 2017
Nanocrystals, Quantum Dots, and Nanowires (1 of 2)
Zia Ballroom

Moderation: Kris Bertness[1]; Daniel Feezell[2]; [1]NIST/US, [2]U of New Mexico/US

08:00 - 08:30
THREE-DIMENSIONAL, HIGH ASPECT RATIO GAN NANOSTRUCTURES BY TOP-DOWN ETCHING

George Wang[1]; Benjamin Leung[2]; Miao-Chan Tsai[2]; Changyi Li[3]; Ganesh Balakrishnan[4]; [1]Sandia National Laboratories, Us, [2]Sandia National Laboratories, NM/Us, [3]The University of New Mexico, NM/Us, [4]University of New Mexico, Us

08:30 - 08:50
EFFECT OF ALGAN UNDERLAYER ON REVERSE-LEAKAGE CURRENT REDUCTION IN GAN/INGAN CORE-SHELL NANOSTRUCTURE LIGHT-EMITTING DIODES
Mohsen Nami[1]; Ashwin Rishinaramangalam[2]; Darryl Shima[1]; Ganesh Balakrishnan[1]; Steve Brueck[2]; Daniel Feezell[2]; [1]University of New Mexico, Us, [2]University of New Mexico, Center for High Technology Materials, Us

08:50 - 09:10
POLARITY INVERSION IN EPITAXIAL ALN: NEW INSIGHTS IN OBTAINING SELECTIVE AREA EPITAXY OF GA-POLAR GAN-ON-SILICON
Kris Bertness[1]; Matt Brubaker[2]; Alexana Roshko[2]; Joel Weber[2]; Todd Harvey[2]; Paul Blanchard[2]; Bryan Spann[2]; Norman Sanford[2]; [1]National Institute of Standards and Technology, CO/Us, [2]NIST, CO/Us

09:10 - 09:30
QUANTUM SIZE CONTROLLED ETCHING OF INGAN QUANTUM DOTS
George Wang[1]; Benjamin Leung[2]; Xiaoyin Xiao[2]; Arthur Fischer[2]; Daniel Koleske[2]; Ping Lu[2]; Miao-Chan Tsai[2]; Michael Coltrin[2]; Jeffrey Tsao[2]; [1]Sandia National Laboratories, Us, [2]Sandia National Laboratories, NM/Us

09:30 - 10:00
SELF-ASSEMBLED GROWTH OF GAN NANOWIRES ON METALLIC SUBSTRATES
Lutz Geelhaar, Paul-Drude-Institut für Festkörperelektronik, De

08:15 - 10:00
Friday, August 4, 2017
Modeling of Crystal Growth Processes (2 of 3)
Eldorado Grand Ballroom (B)

Moderation: Jeffrey Derby, U of Minnesota/US

08:15 - 08:45
PHASE FIELD MODELING OF GRAIN STRUCTURE EVOLUTION DURING DIRECTIONAL SOLIDIFICATION OF MULTI-CRYSTALLINE SILICON SHEET
Chung-Wen Lan; H K Lin; Dept. of Chem. Eng., National Taiwan University, Tw

08:45 - 09:00
OPTIMIZATION OF HEAT TRANSFER DURING THE DIRECTIONAL SOLIDIFICATION PROCESS OF 1600 KG SILICON FEEDSTOCK CAPACITY
Hu Chieh[1]; Jyh-Chen Chen[2]; Thi Hoai Thu Nguyen[1]; Hou Zhi Zhong[1]; Chun Hung Chen[3]; [1]Department of Mechanical Engineering, National Central University, Tw, [2]National Central University, Tw, [3]Research and Development Division, GlobalWafers Co., Ltd., Tw

09:00 - 09:15
CONTROL OF CRUCIBLE MOVEMENT ON MELTING PROCESS AND CARBON CONTAMINATION IN CZOCHRALSKI SILICON CRYSTAL GROWTH
Xin Liu; Xuefeng Han; Satoshi Nakano; Koichi Kakimoto; Research Institute for Applied Mechanics, Kyushu University, Jp

09:15 - 09:30
3D GLOBAL MODELING OF INDUCTION HEATING OF SILICON IN THE FLOATING ZONE PROCESS
Xuefeng Han; Satoshi Nakano; Xin Liu; Koichi Kakimoto; Research Institute for Applied Mechanics, Kyushu University, Jp

09:30 - 10:00
ANALYSIS OF THE V/G CRITERION IN SI SINGLE CRYSTAL GROWTH
Francois Dupret, Université catholique de Louvain, Be

08:30 - 10:00
Friday, August 4, 2017
Eldorado Grand Ballroom (A)
Symposium on Epitaxy of Complex Oxides (10 of 11)

Moderation: Ho Nyung Lee[1]; Darrel Schlom[2]; Lane Martin[3]; [1]ONRL/US, [2]Cornell/US, [3]Berkeley/US

08:30 - 08:45
COMPOSITION CONTROL AND STEP COVERAGE FOR ALD DEPOSITED PBTIO3 AND PZT THIN FILMS
Nick Sbrockey[1]; Gary Tompa[2]; Mark Fanton[3]; Kathleen Trumbull[3]; Robert Lavelle[3]; David Snyder[4]; Ronald Polcawich[5]; Daniel Potrepka[5]; [1]Structured Materials Industries, NJ/Us, [2]Structured Materials Industries, Inc., NJ/Us, [3]Penn State University, Us, [4]Penn State Applied Research Laboratory, PA/Us, [5]U.S. Army Research Laboratory, Us

08:45 - 09:00
EPITAXIAL GROWTH OF CAMN$_7$O$_{12}$ THIN FILMS BY BOTH OZONE-PLD AND OXIDE MBE
Amanda Huon[1]; Ho Nyung Lee[2]; Steven May[1]; [1]Drexel University, PA/Us, [2]Oak Ridge National Laboratory, TN/Us

09:00 - 09:15
SELF-TEMPLATED EPITAXIAL GROWTH OF LOW-SYMMETRY VANADIUM DIOXIDES ON PEROVSKITES
Xiang Gao[1]; Shinbuhm Lee[1]; Matthew Chisholm[2]; Ho Nyung Lee[1]; [1]Oak Ridge National Laboratory, TN/Us, [2]Oak Ridge National Laboratory, Us

09:15 - 09:30
MBE GROWN (LU1-XFEO3)M/(LU1-YMN(1/3)FE(2/3)O3)N SUPERLATTICES
Rachel Steinhardt[1]; Julia Mundy[2]; Megan Holtz[3]; Charles Brooks[1]; Darrell Schlom[3]; [1]Cornell University, NY/Us, [2]berkeley university, NY/Us, [3]Cornell University, Us

09:30 - 10:00
25 YEARS OF PROGRESS IN PEROVSKITE-TYPE SUBSTRATE CRYSTAL GROWTH AT THE LEIBNIZ INSTITUTE FOR CRYSTAL GROWTH
Christo Guguschev[1]; Detlef Klimm[1]; Reinhard Uecker[1]; Mario Brützam[1]; Isabelle Schulze-Jonack[1]; Zbigniew Galazka[2]; Rainer Bertram[1]; Steffen Ganschow[1]; Matthias Bickermann[1]; [1]Leibniz Institute for Crystal Growth, De, [2]Institute for Crystal Growth, De

10:30 - 12:00
Friday, August 4, 2017
Symposium on Epitaxy of Complex Oxides (11 of 11)
Eldorado Grand Ballroom (A)

Moderation: Ho Nyung Lee[1]; Darrel Schlom[2]; Lane Martin[3]; [1]ONRL/US, [2]Cornell/US, [3]Berkeley/US

10:30 - 11:00
CHEMICAL SOLUTION SYNTHESIS OF EPITAXIAL THIN-FILM OXIDES
José Manuel Vila-Fungueiriño[1]; Beatriz Rivas-Murias[2]; Andrés Gómez[3]; Jaume Gazquez[3]; Marti Gich[3]; Adrian Carretero-Genevrier[1]; Francisco Rivadulla[2]; [1]Institut d´Électronique et des Systèmes (IES), Fr, [2]Universidad de Santiago de Compostela, Es, [3]ICMAB, CSIC, Es

11:00 - 11:30

IN SITU OBSERVATION OF LAYER-BY-LAYER MEAN INNER POTENTIAL OSCILLATIONS AND PRECISE GROWTH CONTROL OF OXIDE INTERFACES
Yuefeng Nie, Nanjing University, Cn

11:30 - 12:00
ATOMICALLY ENGINEERED FERROIC LAYERS YIELD A ROOM-TEMPERATURE MAGNETOELECTRIC MULTIFERROIC
Julia Mundy, University of California, Berkeley, CA/Us

10:30 - 11:00
Friday, August 4, 2017
Modeling of Crystal Growth Processes (3 of 3)
Eldorado Grand Ballroom (B)

Moderation: Jeffrey Derby, U of Monnesota/US

10:30 - 10:45
EFFECT OF WETTING ON THE TRANSITION FROM HOMOGENEOUS TO HETEROGENEOUS NUCLEATION OF DEUTERIUM
Luis Zepeda, Lawrence Livermore National Laboratory, CA/Us

10:45 - 11:00
ANALYSIS OF SILICON CARBIDE AND SILICON NITRIDE PARTICLE ENGULFMENT DURING MULTI-CRYSTAL SILICON GROWTH FOR PHOTOVOLTAICS
Yutao Tao[1]; Jeffrey Peterson[1]; Christian Reimann[2]; Jochen Friedrich[2]; Thomas Jauss[3]; Tina Sorgenfrei[3]; Arne Croell[4]; Jeffrey Derby[1]; [1]University of Minnesota, MN/Us, [2]Fraunhofer IISB, De, [3]University of Freiburg, De, [4]University of Alabama in Huntsville, AL/Us

10:30 - 11:30
Friday, August 4, 2017
Nanocrystals, Quantum Dots, and Nanowires (2 of 2)
Zia Ballroom

Moderation: Kris Bertness[1]; Daniel Feezell[2]; [1]NIST/US, [2]U of New Mexico/US

10:30 - 10:50
ELECTRON-BEAM-INDUCED CURRENT IN GAAS/FE CORE-SHELL NANOWIRES
Mingze Yang; Simon Watkins; Karen Kavanagh; Department of Physics, Simon Fraser University, BC/Ca

10:50 - 11:10
MOVPE OF INAS QDS ON INP EMITTING AROUND THE TELECOM C-BAND
Andrey Krysa[1]; Joanna Skiba-Szymanska[2]; Jan Huwer[2]; Tina Müller[2]; M Felle[3]; Brett Harrison[4]; R M Stevenson[2]; Jon Heffernan[4]; Andrew Shields[2]; [1]National Centre for III-V Technologies, University of Sheffield, Gb, [2]Toshiba Research Europe Limited, Gb, [3]Department of Engineering, University of Cambridge, Gb, [4]EPSRC National Centre for III-V Technologies, Dept. of Electronic and Electrical Eng., University of Sheffield, Gb

11:10 - 11:30
LARGE AREA UNIFORM VLSI NANOWIRE GROWTH TOOL
Serdal Okur[1]; Tom Salagaj[2]; Nick Sbrockey[2]; Gary Tompa[3]; Jignesh Vanjaria[4]; Ebraheem Azhar[4]; Hongbin Yu[4]; [1]Structured Materials Industries, Inc., Us, [2]Structured Materials Industries, NJ/Us, [3]Structured Materials Industries, Inc., NJ/Us, [4]Arizona State University, Us

Presentation Abstracts

THERMODYNAMIC CONSIDERATIONS FOR EPITAXIAL GROWTH OF III/V COMPOUNDS

Gerald B. Stringfellow

University of Utah, UT, UNITED STATES OF AMERICA

III/V semiconductor alloys have been extensively studied because of their usefulness for electronic and photonic devices. Nevertheless, the search for new alloys for specific applications continues. Often, thermodynamic factors restrict the compositional range accessible by epitaxial growth processes, particularly when the size difference between atoms mixing on a particular sublattice is large. This causes solid phase immiscibility, leading to important effects on the epitaxial growth, the resultant alloy properties, and, consequently, device performance. Stringent thermodynamic limits exist for a number of alloys being considered for advanced LED, laser, and solar cell applications where the atomic sizes are very dissimilar, such as GaInN, GaAsN and GaAsBi. This paper will review the basic thermodynamics of the epitaxial growth processes and mixing in semiconductor alloys, as well as the causes and consequences of the resultant complex microstructures.

NEW HARD RADIATION DETECTION SEMICONDUCTOR MATERIALS

Mercouri Kanatzidis

Northwestern University, IL, UNITED STATES OF AMERICA

The search for new semiconductors hard radiation detectors for room temperature operation is a challenging endeavor because of the very strict requirements imposed on a candidate material. In addition to requiring suitable energy bandgap and high stopping power, extremely high purity crystals with low carrier trap densities must be grown. We bring to bear a combination of solid state chemistry, crystal growth expertise and materials science approaches to search across the semiconductor phase space and discover or identify new candidate materials which can be developed into high performing g-ray detectors. The search is broad with materials synthesized and evaluated under a host of criteria. Then they are either eliminated from further consideration on selected for further studies aimed at improving the g-ray detection characteristics. This approach has been successful in revealing several entirely new candidates from the class of main-group metal chalcogenides, chalcohalides and halides, which are highly promising in the field of radiation detection. In this talk, I will describe our collaborative efforts and our design and selection strategy, present challenges we have encountered as well as successes achieved in developing promising semiconductor detectors.

TEMPLATED CVD OF LARGE-AREA WS_2 WITH OHMIC GRAPHENE EDGE CONTACTS

Michael S. Fuhrer

Monash Centre for Atomically Thin Materials, Monash University, VIC, AUSTRALIA

Layered transition metal dichalcogenides (LTMDs) are promising new electronic materials, with monolayer $(Mo,W)(S,Se)_2$ showing moderate direct bandgaps and high room-temperature charge carrier mobility. To advance 2D electronics with LTMDs, growth of large-area LTMD layers interfaced with conducting electrodes is desirable. Here, graphene−WS_2 heterojunctions are prepared over large areas on $Al_2O_3(0001)$ substrates using a seedless ambient-pressure chemical vapor deposition technique[1]. As previously shown, the substrate and its hydration condition can be used to control the doping of LTMDs[2]. The heterojunctions are studied as grown on sapphire, as well as transferred to SiO_2 with and without thermal annealing, in order to realise different doping conditions in the WS_2. Kelvin probe force microscopy, photoluminescence spectroscopy, and scanning tunnelling microscopy characterize the doping in graphene−WS_2 heterojunctions. Both *p*−*n* and *n*−*n* junctions are observed, and a flat-band condition (zero Schottky barrier height) is found for lightly *n*-doped WS_2, promising low-resistance Ohmic contacts. This indicates a more favorable band alignment for graphene−WS_2 than has been predicted, likely explaining the low barriers observed in transport experiments on similar heterojunctions. Electrostatic modeling demonstrates that the large depletion width of the graphene−WS_2 junction reflects the unique electrostatics of the one-dimensional junction between two-dimensional materials. 1. C. Zheng et al., *ACS Nano* **11**, 2785 (2017). 2. C. Zheng et al., *Nano Letters* **15**, 3096 (2015).

OPTIMIZING TRANSITION METAL DISULFIDE METALORGANIC CHEMICAL VAPOR DEPOSITION PROCESSES USING NON-DISPERSIVE INFRARED GAS ANALYZERS

James Maslar[1], Berc Kalanyan[1], Brent Sperling[1], William Kimes[1], Ravindra Kanjolia[2]

[1]NIST, UNITED STATES OF AMERICA, [2]EMD Performance Materials, MA, UNITED STATES OF AMERICA

Two dimensional (2D), layered transition-metal dichalcogenides (TMDCs) are of increasing interest for next-generation nanoelectronic and optoelectronic devices. For many applications, high-volume manufacturing of devices based on TMDCs will require techniques that are capable of reproducibly depositing large-area, 2D TMDC films with monolayer control. Metal organic chemical vapor deposition (MOCVD) is a technique that can potentially achieve this goal. However, optimizing MOCVD deposition parameters can be time-consuming. This is particularly problematic when comparing different deposition chemistries, as is the case in this work. To reduce the time involved in optimizing MOCVD deposition recipes, non-dispersive infrared (NDIR) gas analyzers have been developed for use with both transition metal and organo-sulfur precursors. The use of NDIR gas analyzers to optimize our MOCVD processes will be the focus of this presentation. In this work, molybdenum/tungsten sulfide MOCVD processes employing the metal precursors bis(tertbutylimido)bis(dimethylamido) molybdenum and bis(tertbutylimido)bis(dimethylamido) tungsten and the sulfur precursors diethyl disulfide, propanethiol, and dipropyl sulfide are being investigated. These transition metal precursors are low vapor pressure liquids at room temperature. When employing low vapor pressure liquids or solids, it can be difficult to reproducibly deliver a relatively high precursor vapor flux to the deposition surface. Therefore, NDIR gas analyzers were used to characterize the reproducibility of the time-dependent metal precursor flux from the source ampoule, both during a single deposition run and from day-to-day. Furthermore, the correlation between these variabilities and resulting film properties was examined. In contrast, the organo-sulfur compounds exhibit a relatively high vapor pressure and must be delivered in a different manner than the metal precursors, if extreme pressure transients are to be avoided in the process. In order to select an appropriate delivery method, NDIR gas analyzers were used to characterize the time-dependent sulfur precursor flux in different delivery line configurations. In addition, the correlation between the sulfur reactant flux profile and resulting film properties was examined.

OPTIMIZATION OF MOVPE OF 2D MOS_2

M. Heuken, M. Marx, Y.-R. Lin, H. Kalisch, A. Vescan, A. Grundmann

RWTH Aachen University, GERMANY

2D transition metal dichalcogenides (TMDC) offer a wide range of unique electrical and optical properties. Yet, for further systematic scientific studies and implementation in commercial devices, it is necessary to have a reproducible, scalable and homogeneous deposition technique for these materials. For this, chemical vapour deposition based on metal-organic precursors is the premier choice since a metal-organic vapour phase epitaxy process (MOVPE) allows for an optimal control of material flows and gas phase composition during film formation. Additionally, commercial state-of-the-art-tools are available and enable an integration of 2D materials into conventional 3D semiconductors. The direct deposition of MoS_2 via MOVPE is investigated in this work. The experiments are performed in an AIXTRON horizontal hot-wall reactor in 10×2" configuration. Molybdenum hexacarbonyl (MCO) and di-tert-butyl sulphide (DTBS) are used as metal-organic precursors for Mo and S, respectively. Here, we focus on the growth on sapphire (0001) substrates. The deposited layers are characterized via Raman and photoluminescence (PL) spectroscopy, atomic force microscopy (AFM) as well as scanning electron microscopy (SEM). We will show that in order to improve the film quality, a clean surface with a reduced defect and nucleation site density has to be provided for MoS_2 deposition. We address this issue by the choice of the substrate offcut angle and surface pretreatment. The best results are obtained with low offcut angles and a substrate prebake step at 1050°C in a pure H_2 atmosphere. To investigate the 2D growth via MOVPE, a 2-step process is adopted with the intention to initiate MoS_2 nucleation in step 1 and to focus on the growth of existing crystallites during step 2. The influence of various growth parameters such as temperature, pressure and molar flows on the growth in the two steps is discussed. For example, the nucleation site density decreases and the average crystal size increases in step I for higher deposition pressures. However, at the highest pressures (beyond 400 hPa), a less defined crystal morphology and a simultaneous occurrence of triangular and hexagonal crystallites are observed. Further experimental details on the entire growth process will be presented in the paper.

EPITAXIAL GROWTH OF MOLYBDENUM DISULFIDE ON GALLIUM NITRIDE

Robert A. Burke[1], Kehao Zhang[2], Dmitry Ruzmetov[1], Andrew Herzing[3], Glen Birdwell[1], Mahesh Neupane[1], Terrance O'Regan[1], Barbara Nichols[1], Matt Chin[1], Alex Mazzoni[1], Albert Davydov[3], Joshua Robinson[2], Madan Dubey[1], Tony Ivanov[1]

[1]US Army Research Laboratory, MD, UNITED STATES OF AMERICA, [2]The Pennsylvania State University, PA, UNITED STATES OF AMERICA, [3]National Institute of Standards and Technology, MD, UNITED STATES OF AMERICA

To date, transition metal dichalcogenides (TMDs) have been synthesized on a variety of substrates including SiO_2, quartz, sapphire, mica, and gold foils. However, synthesis on these substrates typically leads to polycrystalline films due to the random orientation of the triangular domains. Epitaxial growth has been achieved on annealed sapphire substrates, but sapphire is not a suitable substrate if one wants to explore 2D/3D vertical semiconductor heterostructures. III-nitrides, on the other hand, can be an active component of a 2D/3D vertical heterostructure and also possess a small lattice mismatch with a variety of TMDs. As a result, synthesis of TMDs on III-nitrides can lead to epitaxial growth of aligned triangles on a 3D semiconductor substrate. In this talk, we will discuss the synthesis of molybdenum disulfide (MoS_2) on n-type and p-type GaN via powder vaporization. We will show epitaxial growth of aligned MoS_2 triangles on both n-type and p-type GaN and the importance of sample preparation in achieving the epitaxial growth. We will also present our attempts to control the MoS_2 domain size and coalesce the triangles into continuous films. We will also present our findings from scanning electron microscopy (SEM), atomic force microscopy (AFM), Raman spectroscopy, photoluminescence (PL), conductive atomic force microscopy (CAFM), and transmission electron microscopy (TEM).

ASSEMBLY OF VIRUS NANOREACTORS

Trevor Douglas

Indiana University, UNITED STATES OF AMERICA

The virus like particles (VLP) derived from the bacteriophage P22 provide an opportunity for constructing catalytically functional materials by directed encapsulation of enzymes into the interior volume of the icosahedral capsid. Directed enzyme encapsulation has been genetically programmed allowing biosynthesis and directed self-assembly of desired enzymes within the roughly 60 nm diameter P22 capsid. The self-assembly of these nanoreactors, which encapsulate multiple copies of the cargo enzymes, has a dependent on nature of the cargo. Using these P22 nanoreactors as individual building blocks we can extend the utility of the system towards complex materials fabrication. Through the directed hierarchical assembly of individual P22 particles we can create superlattice materials with long-range order that exhibit complex coupled catalytic behavior through communication between individual P22 nanoreactors.

BIO-INSPIRED CRYSTAL GROWTH OF TRANSITION METAL OXIDES IN CONFINEMENT

Lara A. Estroff

Cornell University, NY, UNITED STATES OF AMERICA

Biomineralization provides examples of strategies for controlling the growth of crystalline materials patterned at the nanoscale. In particular, the concept of crystal growth in confinement has led to many interesting synthetic structures. In this presentation, I will focus on our recent efforts to use confinement within track-etched membranes to force the incorporation of a secondary phase with single crystals and the use of block copolymers to template the surface confined precipitation of crystalline transition metal oxides with periodicities on the order of 50 nm. For both of these strategies, I will present results related to the formation mechanisms, internal structures, and properties of the resulting nanostructured oxides.

NOVEL BIO-INSPIRED SEMICONDUCTOR/AMINO ACID COMPOSITE SINGLE CRYSTALS: FROM CRYSTAL GROWTH TO BAND GAP ENGINEERING

Iryna Polishchuk, Boaz Pokroy

Technion, ISRAEL

Many of the physical properties of biogenic crystals originate from the presence of intracrystalline organic molecules within individual inorganic crystalline hosts. The presence of these molecules has been shown to strongly influence the crystalline host microstructure and structure (anisotropic lattice distortions). Recently, by applying a bio-inspired approach, we have shown that similar microstructures and lattice distortions can be achieved in synthetic calcium carbonate crystals grown in the presence of organic molecules[1]. However, no similar approach has been performed on non-calcium carbonate crystals. In this work, we utilize this bio-inspired approach so as to modify the crystal properties of functional semiconductor material[2,3].

We will show that amino acids can get incorporated into the crystal lattice of semiconductor hosts, similar to the process observed for calcium carbonate. Moreover, not only that such incorporation exists; the resulting lattice distortions are accompanied by a significant band-gap energy shift of the semiconductor host (in some cases up to 17%).

We will discuss possible mechanisms for this phenomenon and show that such bio-inspired organic/inorganic interfaces have much potential for the manipulation of not only structural properties of different crystalline hosts but rather of a variety of functional properties. Moreover, we believe that this research may open a new bio-inspired route for tuning the band-gaps of semiconductors in addition to the ones known and utilized to date.

[1] Borukhin S, Bloch L, Radlauer T, Hill AH, Fitch AN, Pokroy B. Screening the Incorporation of Amino Acids into an Inorganic Crystalline Host: the Case of Calcite. *Advanced Functional Materials* 2012;22:4216.

[2] Brif A, Ankonina G, Drathen C, Pokroy B. Bio-inspired Band Gap Engineering of Zinc Oxide by Intracrystalline Incorporation of Amino Acids. *Advanced Materials* 2014;26: 477.

[3] Brif A, Pokroy B. Bio-inspired Engineering of Zinc Oxide/Amino Acid composite: Synchrotron Microstructure Study. *CrystEngComm* 2014;16: 3268.

DESIGN AND SYNTHESIS OF FUNCTIONALIZED SELF-ASSEMBLED MONOLAYERS (SAMS) AS IN VITRO MODEL OF THE ORGANIC INTERFACES IN THE SITE-SELECTIVE MINERALIZATION PROCESS IN THE CHITON TOOTH.

Linus M. Stegbauer, Derk Joester

Northwestern University, MSE, IL, UNITED STATES OF AMERICA

SAMs allow the precise organization of functionalized molecules on metal surfaces via the formation of thiol-metal bond. In this work a compact Au layer on silicon wafers is utilized as metal surface. SAMs with functionalized tail group allow side- and even face-selective growth of crystal in a bio-inspired setting thereby imitating the protein-crystal interaction.[1] Herein the focus lays on the development of the 'radula teeth' of the chiton, a marine mollusk. Most chitons feed on algae by grazing on and eroding rocks using extremely hard, wear resistant, and self-sharpening 'radula teeth'. The chiton tooth cusp, which is the hardest component of the tooth and one of the hardest biomaterials known, is a sophisticate nanocomposite of magnetite (Fe_3O_4) and fibers of the polysaccharide chitin.[2] The protein-mineral interface is thought to be the key for the specific crystallization of magnetite during the tooth development. Building an in vitro model system to study mechanisms in this biological interface we concentrate on functional groups (FGs) which are known to have beneficial interaction with iron ions in proteins. With the technique of μ-contact printing selective functionalization of the surface with different groups is within reach. Specific parts of the Au surface are functionalized by printing of functionalized SAMs in patterns with the corresponding FG or a mixture of FGs. The residual parts of the Au surface are then passivated non-functionalized alkyl bearing SAMs. Subsequently, the functionalized surface is exposed to an iron-containing aqueous solution enabling the growth of magnetite.[3] The impact of the FGs/ligands on the crystallization to magnetite will be directly studied, together with the final morphology and properties. This will allow not only the identification of the involved FGs but also the direct transfer into application: The assembly of magnetite nanocrystals in a magnetic array in bottom-up fashion. (1) Aizenberg, J.; Black, A. J.; Whitesides, G. M. Oriented Growth of Calcite Controlled by Self-Assembled Monolayers of Functionalized Alkanethiols Supported on Gold and Silver. J. Am. Chem. Soc. 1999, 121 (18), 4500–4509.

(2) Joester, D.; Brooker, L. R. The Chiton Radula. In Iron Oxides: From nature to applications; Faivre, D., Ed.; Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany, 2016; pp 177–206.

(3) Galloway, J. M.; Bramble, J. P.; Rawlings, A. E.; Burnell, G.; Evans, S. D.; Staniland, S. S. Nanomagnetic Arrays Formed with the Biomineralization Protein Mms6. Journal of Nano Research 2012, 17, 127–146.

THE ELIMINATION OF SUZUKI PHASE PRECIPITATES FROM SINGLE CRYSTALS OF DIVALENT-ION-DOPED ALKALI HALIDES: IMPROVED SCINTILLATORS FOR RADIATION DETECTION

Lynn A. Boatner, Eleanor Comer, Gomez W. Wright, Joanne O. Ramey, Richard A. Riedel, Gerald E. Jellison, James A. Kolopus

Oak Ridge National Laboratory, TN, UNITED STATES OF AMERICA

Alkali halide crystals such as LiI, NaI, or CsI that are activated with divalent rare-earth ions such as divalent Eu have not been widely used as scintillators for radiation detection applications due to their incompatibility with the incorporation of divalent activator ions at relatively high levels - nominally between 0.5 and 5.0 %. This is due to the fact that when divalent ions such as Eu(2+) are added during the melt growth of single crystals of monovalent-cation alkali halides at a level of between ~0.5 and 5.0 %, the resulting single crystals are effectively white and opaque due to the formation of so-called Suzuki Phase precipitates. These Suzuki-phase precipitates scatter the scintillator light thereby adversely affecting the light transmission and reducing the overall radiation detection performance (e.g. light yield and energy resolution) of the scintillator crystals – for either gamma-ray detection (or in the case of LiI:Eu(2+) crystals containing preferably isotopically enriched Li(six) as the neutron converter) for thermal neutron detection. Here we describe the crystal growth and post-growth treatment and preparation of heavily Eu-doped alkali halide single crystals where the Suzuki Phase precipitates are eliminated by a two-stage post-growth thermal treatment process that renders the otherwise effectively opaque crystals highly transparent to radiation-induced scintillation light. The application of these methods to the case of divalent europium activated LiI scintillators for neutron detection is presented here as an example of the scintillator performance that can be achieved by eliminating Suzuki Phase precipitate particles. This method of combining high concentration divalent ion doping during crystal growth with the post-growth thermal treatment described here is not limited to divalent europium ions - but is applicable to any divalent rare-earth or iron-group ion, or to any other divalent dopant ion at additive concentrations that result in the formation of Suzuki Phase precipitates in alkali halides - nor is the combined single-crystal growth and post-crystal-growth treatment described here restricted to the formation of scintillator materials for radiation detection applications – but it is potentially applicable to optical materials in general - including lasers, infrared detectors, UV radiation detection, phosphors for solid state lighting or fluorescent lighting applications, optical amplifiers, optical filters, or any other applications requiring optical transparency in heavily divalent-ion-doped alkali halides.

STRUCTURE AND THERMAL EXPANSION OF CSCAI3:EU AND CSSRBR3:EU SCINTILLATORS

Matthew Loyd, Adam Lindsey, Maulik Patel, Charles L. Melcher, Mariya Zhuravleva

University of Tennessee, TN, UNITED STATES OF AMERICA

Using scintillator crystals for national security applications requires growing large size crystals with uniform optical quality. Investigation of crystal structure and thermal expansion behavior of scintillation crystals grown via the vertical Bridgman technique can give insight into residual stress that may have been induced during growth and cooling. $CsCaI_3$:Eu and $CsSrBr_3$:Eu are distorted-perovskite scintillators that both undergo phase transitions that leave them cloudy, but uncracked. Differential scanning calorimetry was utilized to measure the phase transition temperatures. High temperature powder X-ray diffraction was measured on both crystals using a vacuum set up to prevent exposure to the atmosphere. The structure and lattice parameters were determined using sequential refinements in GSAS II. Thermal expansion coefficients for both crystals and each phase were calculated. The information obtained in this work will be used to design a more optimal crystal growth process, including thermal gradients, and cooling and growth rates.

GROWTH AND LUMINESCENCT PROPERTIES OF CS_2HFI_6-BASED SINGLE CRYSTAL SCINTILLATORS

Shohei Kodama[1], Shunsuke Kurosawa[2], Akihiro Yamaji[3], Jan Pejchal[4], Robert Kral[5], Yuji Ohashi[3], Kei Kamada[6], Yuui Yokota[7], Martin Nikl[5], Akira Yoshikawa[3]

[1]Institute for Materials Research, JAPAN, [2]Faculty of Science, Yamagata University, JAPAN, [3]Institute for Materials Research, Tohoku University, JAPAN, [4]Institute of Physics CAS, CZECH REPUBLIC, [5]Institute of Physics, Czech Academy of Sciences, CZECH REPUBLIC, [6]C&A corporation, JAPAN, [7]New Industry Creation Hatchery Center, Tohoku University, JAPAN

Novel halide scintillators have been studied due to their potentially high light output and good energy resolution because of relatively small band-gap energy [1]. However, most of the halide materials have hygroscopic nature. Therefore, degradation due to moisture and resulting demands on crystal growth technique and sealing can limit their application. Recently, Cs_2HfCl_6 has been reported as non-hygroscopic halide scintillator [2]. Cs_2HfCl_6 has a high light output of up to 54,000 photons/MeV, and its energy resolution is estimated to be 3.3% from full width at half maximum (FWHM) at 662 keV gamma-ray. Moreover, Hf^{4+} makes the effective atomic number of Cs_2HfCl_6 as high as 54, and this value is much larger than that for the other conventional halide materials, such as Tl:NaI or Ce:$LaBr_3$. Cs_2HfCl_6 is an attractive heavy scintillation material; however, the density of Cs_2HfCl_6 is generally smaller than that of oxide scintillators. Thus, detection efficiency for gamma-rays is smaller than for some oxide materials. In order to improve the effective atomic number and density, we considered changing the host composition of Cs_2HfCl_6. In this time, we replaced I^- for Cl^- and the effective atomic number of Cs_2HfI_6 is calculated to be 57. We report the scintillation properties for Cs_2HfI_6-based single crystals. Non-doped and Eu-doped Cs_2HfI_6 crystals were grown by vertical Bridgman methodfrom 99.9%-pure (except Zr) HfI_4 and 99.999%-pure CsI as starting materials. The details of the growth are described in [3]. Finally, we succeeded in growing these crystals. Here, the lattice constant was calculated as 11.64±0.01 Å from powder X-ray diffraction (XRD) pattern [4] (in Figure 1), and the crystal system was revealed to be Fm-3m. As shown in Fig. 2, non-doped Cs_2HfI_6 showed broad emission around 650 nm under X-ray excitation. The light output and energy resolution were estimated to be 12,000 photons/MeV and 8.0% at 662 keV (FWHM), respectively. In the case of $Cs_2(Hf_{0.99}Eu_{0.01})I_6$, lattice constant was 11.63±0.01 Å, and it showed the same emission peak as the non-doped Cs_2HfI_6 in X-ray radioluminescence. Its light output and energy resolution were estimated to be 12,000 photons/MeV and 8.1 %, respectively. Thus, we found that the effect of Eu-doping was negligible. [1] P. Dorenbos, *Nucl. Instrum. Methods. Phys. Res. A*, **486** (2002) 208

[2] A. Burger *et. al.*, *Appl. Phys. Lett.*, **107** (2015) 143505 [3] S.Kodama *et al.*, *J. Lumin.*, submitted [4] F. Ackerman, *Mat. Res. Bull.*, **19** (1984) 783-791

CRYSTAL GROWTH OF CESIUM HAFNIUM CHLORIDE SCINTILLATORS

Stephanie Lam[1], Arnold Burger[2], Shariar Motakef[1]

[1]CapeSym Inc., MA, UNITED STATES OF AMERICA, [2]Fisk University, TN, UNITED STATES OF AMERICA

Cesium hafnium chloride (CHC, Cs_2HfCl_6) is a recently-discovered material with superior radiation detection properties relative to the incumbent detectors NaI(Tl) and CsI(Tl). Advantages of CHC include: an excellent energy resolution, no self-absorption, no self-activity, and non-hygroscopicity. Our first-grown crystals were measured to have a light yield of 30,000 ph/MeV and an energy resolution of 3.3%. With a decay time close to 4 μs, CHC is well-suited to most low-count scenarios encountered in homeland security applications. This presentation will address techniques for charge purification and preparation, crystal growth by the Bridgman technique, as well as the challenges associated with handling this line compound. Finally, we will discuss the use of alloying to reduce the decay time to 2 μs. *This work has been supported by the US Department of Energy, under competitively awarded contract DE-SC0015733. This support does not constitute an express or implied endorsement on the part of the government.*

EFFECTS OF CA/SR RATIO CONTROL ON OPTICAL AND SCINTILLATION PROPERTIES OF EU-DOPED LI(CA,SR)ALF$_6$ SINGLE CRYSTALS

Yuui Yokota[1], Chieko Tanaka[2], Shunsuke Kurosawa[3], Akihiro Yamaji[2], Yuji Ohashi[1], Kei Kamada[4], Martin Nikl[5], Akira Yoshikawa[2]

[1]New Industry Creation Hatchery Center, Tohoku University, JAPAN, [2]Institute for Materials Research, Tohoku University, JAPAN, [3]Faculty of Science, Yamagata University, JAPAN, [4]C&A Corporation, JAPAN, [5]Institute of Physics, Czech Academy of Sciences, CZECH REPUBLIC

$LiCaAlF_6$ [LiCAF] and $LiSrAlF_6$ [LiSAF] with the colquiriite-type structure have been investigated as a host material of the neutron scintillator which can be used in the neutron detectors for the applications of the homeland security devices. Especially, the Eu:LiCAF and Eu:LiSAF single crystals demonstrate high light yield under the thermal neutron irradiation. However, there is few reports about the solid solution of the LiCAF and the LiSAF [$Li(Ca,Sr)AlF_6$, LiCSAF] single crystals. In addition, there is no report about the Eu-doped LiCSAF single crystals. Therefore, the purpose of this study is the crystal growth of the Eu:LiCSAF single crystals with various Ca/Sr ratios and investigation of the optical and scintillation properties for the Eu:LiCAF single crystals to reveal the effects of the band-gap modification by the control of Ca/Sr ratio. The Eu:LiCSAF single crystals were grown by the micro-pulling-down [m-PD] method with a vacuum chamber which could grow a fiber fluoride single crystal using a carbon crucible with a hole at the bottom. Starting materials, LiF (^{6}Li 95%, 4N), CaF_2, SrF_2, AlF_3 and EuF_3 (4N purity) powders, were mixed as nominal compositions of $Li(Ca_{0.98-x}Sr_xEu_{0.02})AlF_6$ with x = 0, 0.10, 0.20, 0.25, 0.40, 0.50, 0.75 and 0.98. Crystal growth was performed at 0.1 mm/min growth rate using a platinum wire as a seed. The as-grown Eu:LiCSAF single crystals were cut and polished to prepare specimens for the measurements of their optical and scintillation properties. During the crystal growth, the liquid-solid interface was located just below the bottom of the crucible and the diameter of the grown single crystal was controlled by the hole (outlet). In the result, the as-grown single crystals had approximately f2 mm diameter. There were some cracks around the growth initial parts of the as-grown single crystals and the generation of cracks is due to the use of the platinum wire as the seed. The cracks gradually decreased during the crystal growth and, finally transparent and crack-free parts could be obtained for all Eu:LiCSAF single crystals. All diffraction peaks in the powder X-ray diffraction patterns of the Eu:LiCSAF single crystals could be identified by the colquiriite-type crystal structure and there was no diffraction peak originated from a secondary phase. The lattice parameters were systematically increased with increasing Sr concentration and the result is attributable to the substitution of Ca^{2+} site by the Sr^{2+} ion with larger ionic radius than Ca^{2+} ion. The optical and scintillation properties will be reported.

WHAT DETERMINES A NUCLEATION PATHWAY?

Yuki Kimura

Institute of Low Temperature Science, Hokkaido University., JAPAN

Recent progress in nucleation experiments and theoretical simulations has surprisingly shown an unexpected variety of nucleation pathways to final crystal formation. Even in the vapor phase, the final crystals cannot be directly formed through the classical nucleation mechanism. In the case of homogeneous nucleation from the vapor phase, the size of the critical nuclei can be as small as that of several growth units or even dimer due to extremely high supersaturation (*Science Advances*, 3 (2017) e1601992; *Crystal Growth & Design*, 12 (2012) 3278). Since the size of the critical nuclei can be smaller than the size of a unit cell of the final crystal, the first nucleation stage cannot determine the character of the final crystalline particles. The critical nuclei gradually grow by monomer attachment and cluster adhesion to become a nanoparticle. In many cases, the nuclei grow in the melt, despite the nucleation temperature being lower than that of the corresponding bulk, because the melting point of a nanoparticle decreases depending on its size due to the so-called size effects. The degree of supercooling of the melt is gradually increased by elevating the melting point even at a constant temperature, because the particle grows. Thereafter, the supercooled melt crystallizes through secondary nucleation (*Chemistry of Materials*, 28 (2016) 8732; *The Astrophysical Journal*, 803 (2015) 88). Our systematic nucleation experiments in the vapor phase demonstrate subsequent crystallization in the particle-mediated growth process. The third stage of the crystallization is governed by the singular properties of the nanoparticles and determines the characteristics of the final crystal, whereas secondary nucleation seemed to determine the characteristics of the final particle in many cases. The formation of a crystalline particle from an aqueous solution involves several complex processes because of the hydrated layer surrounding a particle in water. Thus, the dehydration process may pose the greatest hindrance for the crystallization process, and therefore, the growth units nucleate together with the water molecules and form a dense liquid or hydrated amorphous particles (*PNAS*, 114 (2017) 2154). The secondary nucleation accompanied by the dehydration of the non-crystalline particles facilitates the formation of crystalline particles as well as vapor phase nucleation via liquid phase. Further growth by the particle-mediated process including oriented attachments has been reported in many systems. I believe that the diversity of the nucleation process originates from the singularity of the nanoparticles. Based on this concept, I demonstrate the determination of the nucleation pathways.

CLASSICAL OR MULTI-STEP NUCLEATION

Dominique Maes[1], James F. Lutsko[2], Sander Stroobants[1], Mike Sleutel[1], Sudha Chinnu[1], Marco A.c. Potenza[3], Peter G. Vekilov[4]

[1]Vrije Universiteit Brussel, BELGIUM, [2]Universite Libre de Bruxelles, BELGIUM, [3]University of Milano, ITALY, [4]University of Houston, TX, UNITED STATES OF AMERICA

It has become widely accepted that many phase transitions do not follow nucleation pathways as envisaged by the Classical Nucleation Theory. Many substances can traverse intermediate states before arriving at the stable phase. In this talk we will discuss the nucleation of the protein glucose isomerase that follows a classical pathway in two dimensions and has all the characteristic of a two-step mechanism in three dimensions. Molecular resolution atomic force microscopy imaging of the two-dimensional nucleation of glucose isomerase demonstrates that the interior of subcritical clusters is in the same state as the crystalline bulk phase and that glucose isomerase 2D crystals are formed classically. Our observations illustrate the resurfacing importance of the classical nucleation theory by re-validating some of the key assumptions that have been recently questioned. In contrast according to the two-step mechanism of nucleation, protein-rich clusters serve as locations for and precursors to the nucleation of protein crystals. We will report on our characterization of these "mysterious clusters" with Brownian microscopy. Using confocal Depolarized Dynamic Light scattering we were able to follow nuclei at birth. [1] M. Sleutel, J. Lutsko, A.E.S. Van Driessche, M.A. Duran-Olivencia and D. Maes, Nature Communications **5**, 5598 (2014). [2] M.A. Vorontsova, D. Maes and P.G. Vekilov, Faraday Discuss. **179**, 27 (2015). [3] D. Maes, M.A. Vorontsova, M.A.C. Potenza, T. Sanvito, M. Sleutel, M. Giglio and P.G. Vekilov, Acta Cryst. **F71**, 815 (2015).

LA MER BURST NUCLEATION AND GROWTH: ASSUMPTIONS, MODELS, AND DATA

Baron Peters

University of California - Santa Barbara, UNITED STATES OF AMERICA

Recent efforts to synthesize monodispersed nanoparticles have employed in situ reactions to steadily and homogeneously generate a mounting solute supersaturation. As the supersaturation climbs past a critical level in solution, the nucleation rate spikes giving birth to a large population of nuclei over a very short interval of time. Subsequent growth of these nuclei lowers the supersaturation and thereby suppresses further nucleation. The result is a large population of nearly monodisperse particles. Classic experiments by T. Sugimoto and others have been modeled with deterministic models having separate stages of supersaturation build-up, nucleation, growth, and sometimes ripening. We examine assumptions in these models within the context of chalcogenide nanoparticle synthesis (Prof. J. S. Owen) and gold nanoparticle synthesis (Prof. S. L. Scott). We present a fully non-equilibrium stochastic model for LaMer burst nucleation with comparisons to results from simpler models. The results should clarify whether fit parameters from simple models accurately resolve the microscopic nucleation and growth kinetics.

SOME CURRENT DEVELOPMENTS IN HYDROTHERMAL CRYSTAL GROWTH OF BORATES FOR UV NONLINEAR OPTICS

Joseph Kolis, Colin Mcmillen, Rylan Terry, Henry Giesber

Clemson University, SC, UNITED STATES OF AMERICA

The design of nonlinear optical (NLO) crystals with good performance in the UV (355-200) and deep UV (<200nm) of the optical spectrum poses some unique challenges. In particular it is difficult to obtain acentric crystals with sufficiently wide bandgaps (≥6eV), decent NLO coefficients, moderate birefringence for suitable phase matching and good physical properties for processing. Thus far the only class of compounds that can fulfill all of those characteristics are the alkali/alkaline earth borates. The borates have an increased tendency to form acentric crystalline structure types with wide bandgaps and decent NLO coefficients. Currently all commercially available UV NLO crystals are borates, including b-BaB_2O_4 (BBO), LiB3O5 (LBO) and CsLiB6O10 (CLBO). All have their applications but all have significant limitations. Most importantly it is difficult to obtain good performance below 266nm. Several years ago, two new compounds $KBe_2BO_3F_2$ (KBBF) and $Sr_2Be_2B_2O_7$ (SBBO) were reported to have extremely promising UV and deep UV NLO performance. Since that time, considerable effort was spent to develop these materials for commercial application. The original work employed various fluxes to grow the materials, which did lead to single crystals, but the well known tendency of borates to form viscous fluids led to some challenges in the scaled up growth of the crystals. Previous work in our group demonstrated that the hydrothermal method is a suitable pathway for the growth of both KBBF and SBBO single crystals. This originally led to scaleup of KBBF single crystal growth and these efforts will be reviewed. More recently we found that the hydrothermal method leads to growth of a new SBBO phase that eliminates the disorder and ambiguity in the original reports of SBBO. Preliminary work suggests that this leads to significantly improved NLO performance of these new SBBO crystals. Early work on this new phase will be discussed.

SYNTHESIS, GROWTH AND CHARACTERIZATION OF NOVEL NONLINEAR OPTICAL MATERIAL: 4-FLUOROBENZYL TRIPHENYLPHOSPHONIUMCHLORIDE

Arul Haribabu[1], K Sugandhi[1], S Bharathi[2], A Jeya Rajendran[2], K Eswara Moorthi[2], M P Kannan[2]

[1]Department of Science and Humanities, Kumaraguru College of Technology (Autonomous), INDIA, [2]Advanced Materials Research Laboratory, Department of Chemistry, Loyola College, INDIA

Materials with large nonlinear optical susceptibilities are of current interest in the region of second harmonic generation and optical modulation. In recent years, some polar organic crystals form a non-centrosymmetric structure which exhibit second-order nonlinear optical properties; those far surpassed the conventional materials. It leads to the synthesis and evaluation of a wide range of useful single crystals. Materials showing high optical nonlinearity have potential applications in signal transmission, data storage, optical switching, laser printing, displays, photolithography, remote sensing, chemical and biological species detection, high resolution spectroscopy, medical diagnosis and underwater monitoring and communication. Different types of molecular and bulk materials have been examined for nonlinear optical properties. Presently, semi organics are being explored, which can share the properties of both organic and inorganic materials, such as optical transparency, high non-linear susceptibilities, their large birefringence to use as frequency converters and fairly high laser damage thresholds. We synthesized a new promising semiorganic non-linear optical material, 4-fluorobenzyl triphenylphosphoniumchloride and the single crystal was grown by slow evaporation technique at 311 K with dimensions 15 X 14 X 4 mm^3. In the present work, we have reported the material synthesis, crystal growth, structural, thermal, optical, nonlinear optical and dielectric properties for the first time. UV analysis shows that cut-off wavelength of the title compound is 342 nm, which could be an essential requirement of a nonlinear optical material for device fabrication. Thermal stability of the compound was assessed as 210°C using TG-DTA. SHG efficiency shows that 1.3 times than that of standard KDP.

MEASUREMENTS OF D COEFFICIENTS OF SOME CUBIC CRYSTALS AT INFRARED WAVELENGTHS

Joel Murray[1], Jean Wei[1], Shekhar Guha[2]

[1]UES, Inc., OH, UNITED STATES OF AMERICA, [2]Air Force Research Laboratory, OH, UNITED STATES OF AMERICA

With the promise of high power frequency conversion using quasi-phase matched cubic crystals, it has become important to know the values of their d-coefficients at various wavelengths of interest. Since many of these materials are transparent at CO_2 laser wavelengths and are potentially suitable for frequency doubling, tripling or quadrupling processes, a project was undertaken to measure the values of the d-coefficients at the relevant wavelengths. A picosecond duration laser (EKSPLA PL2143 with OPG and DFG units) tunable from 2 to 10 µm was used for the frequency doubling measurements. Single crystal wafers of ZnS, CdS, ZnTe, GaP, CdTe, InP, GaAs and InAs as well as ternary alloys CdZnTe and HgCdTe, each oriented in the 100 or 110 directions, were obtained commercially. The GaAs and GaP wafers were polished to approximately three times the coherence length for maximal second harmonic generation; other samples also generated measurable second harmonic in spite of having various ratios of the measured thicknesses to the coherence length. The samples were mounted on a two axis rotation stage, with the rotation axes being the vertical direction and the wafer normal direction. The wafer normal stayed in the horizontal plane so the wafer surfaces were always in a vertical plane. Using a laser beam (designated the pump) with wavelength 9.334 µm and approximately Gaussian transverse spatial and temporal distribution (149 µm HWe $^{-1}$M spot size and 5.7 ps HWe $^{-1}$M pulse width), second harmonic generation (SHG) was observed in all the samples studied. The SHG energy (E_s) was measured as a function of the irradiance of the pump beam (I_p) incident on the sample and the expected quadratic dependence was observed. From a quadratic fit to the E_s vs I_p plots, the d coefficient can be evaluated if the values of the refractive indices at the pump and the SHG wavelengths are known. From the currently available literature values for the refractive indices of the binary compounds and extrapolated values for the ternary alloys, a set of d coefficients were obtained. From the plot of d coefficient values vs the band gap energies (E_g) of the semiconductors, it was found that d scaled roughly as $E_g^{-2.5}$.

STUDIES OF LOCAL ELECTRONIC PROPERTIES IN GRAPHENE AND 2D MATERIALS

Olga Kazakova

NPL, UNITED KINGDOM

We present a combined study of local and global electronic properties of various types of graphene and graphene-based devices as well as 2D materials and their heterostructures using a combination of Scanning Kelvin Probe Microscopy, electrical and magnetic Scanning Gate Microscopy and transport measurements. We demonstrate that using advanced scanning probe microscopy techniques it is possible to obtain detailed information on the unique sample properties (such as effect of non-uniformity, defective structure, degree of molecular absorption, etc.), which are not available by other more traditional methods. We also consider the effect of environmental doping (soft gating) on the local/global properties of different types of graphene. To demonstrate capabilities of the method, the following cases will be presented: - Effect of environment (humidity and gases); - Carrier type reversal in intercalated graphene; - Effect of graphene bi-layer on electronic and optoelectronic properties. We demonstrate the accuracy of the measurements, which allow us to eliminate the common artefacts, which are not usually taken into account in many other approaches. The present work facilitates development of realistic graphene and 2D materials sensors and their faster and more reliable implementation. 1. V. Panchal, et al., *Scientific Reports* **3**, 2597 (2013) 2. R. K. Rajkumar, et al. *J. of Appl. Phys.* **115**, 172606 (2014) 3. V. Panchal, et al., *Scientific Reports* **4**, 5881 (2014) 4. C. Melios, et al., *Scientific Reports* **5**, 10505 (2015) 5. M. Munz, et al., *ACS Nano* **9**, 8401 (2015) 6. C. E. Giusca, et al. *ACS Nano* **10**, 7840 (2016)

INFLUENCE OF SUBSTRATE ON THE GROWTH AND PROPERTIES OF THIN 3R NBS2 FILMS GROWN BY CHEMICAL VAPOR DEPOSITION.

Azimkhan Kozhakhmetov[1], Tanushree H. Choudhury[2], Zakaria Y. Al Balushi[1], Yixuan Chen[3], Ying Liu[3], Joan M. Redwing[2]

[1]Dept. of Materials Science and Eng., The Pennsylvania State University, PA, UNITED STATES OF AMERICA, [2]2D Crystal Consortium, Materials Research Institute, PA, UNITED STATES OF AMERICA, [3]Department of Physics, The Pennsylvania State University, PA, UNITED STATES OF AMERICA

The different polytypes of layered metallic $NbSe_2$ (2H, 3R and 4H) and NbS_2 (3R and 2H) are well – known for their unique physical properties such as superconductivity and charge density waves. The absence of charge density waves in layered NbS_2 combined with the potential to develop metallic/semiconductor van der Waals heterostructures using NbS_2 provides a compelling motivation to study the synthesis of single crystal NbS_2 thin films with controlled thickness using chemical vapor deposition (CVD) and other vapor transport approaches. Due to the layered crystal structure of van der Waals – bonded transition metal dichalcogenide (TMDC) films, the choice of substrate has a significant impact on the film growth and properties which has not been extensively studied for NbS_2. In this study, the effect of substrate on the texture, morphology, crystallinity and electrical properties of few layer of 3R NbS_2 films was investigated. The NbS_2 films were deposited in a horizontal cold – wall quartz tube reactor at constant 100 Torr reactor pressure using the niobium (v) chloride ($NbCl_5$) and hydrogen disulfide (H_2S) as precursors in a hydrogen carrier gas. Growth temperatures ranging from 400 ºC to 800 ºC and sulfur to niobium ratios (S: Nb) ranging between 640 and 5100 were studied. C – plane sapphire and epitaxial graphene on SiC were used as substrates for the film deposition. Growth on sapphire resulted in small grained polycrystalline NbS_2 films with a rough and irregular surface morphology whereas smooth, planar c – axis oriented triangular domains of NbS_2 were obtained on epitaxial graphene under identical growth conditions. In case of graphene, which was hydrogenated prior to growth to form quasi – free – standing epitaxial graphene, the lack of dangling bonds promote surface diffusion of Nb adatoms and van der Waals epitaxy of few layers of NbS_2 films on the graphene surface. In contrast, Nb appears to interact strongly with the sapphire surface preventing lateral growth of planar domains. Van der Pauw resistivity measurements of 3 – 4 layers of NbS_2 films were carried out at room temperature indicated resistivities in the range 1.9×10^{-3} and 9.0×10^{-4} Ω-cm which are comparable to that reported previously for bulk NbS_2. The growth and properties of NbS_2 on other van der Waals surfaces such as WS_2 and WSe_2 for the fabrication of contact layers and heterostructures will also be discussed.

GROUP IV CHALCOGENIDES: EMERGING 2D AND LAYERED SEMICONDUCTORS

Peter Sutter[1], Yuan Huang[2], Hannu-Pekka Komsa[3], Arkady Krasheninnikov[4], Eli Sutter[1]

[1]University of Nebraska-Lincoln, UNITED STATES OF AMERICA, [2]Brookhaven National Laboratory, UNITED STATES OF AMERICA, [3]Aalto University, FINLAND, [4]Helmholz-Zentrum Dresden-Rossendorf, GERMANY

Metal chalcogenides have received attention as 2D materials beyond graphene. Semiconducting chalcogenides are particularly attractive since they exhibit novel physics such as strongly bound excitons and valley polarization, and promise to enable applications in electronics and energy conversion. While transition metal dichalcogenides (e.g., MoS_2) have been studied extensively as prototype systems, other 2D and layered semiconductors remain much less explored. Here we discuss the fundamental properties and device characteristics of group IV chalcogenides, a family of semiconducting non-transition metal chalcogenides that includes tin sulfides (SnS, SnS_2) and others. We demonstrate the successful isolation of few-layer and single-layer materials by both exfoliation and bottom-up synthesis, and use real-time, *in-situ* low-energy electron microscopy to establish the fundamental processes that govern the growth. Transmission electron microscopy (S/TEM), band structure measurements and STEM cathodoluminescence are used to determine the electronic structure and light-matter interactions of SnS and SnS_2 and their evolution from the bulk to a single layer. Using field-effect transistors, we explore the achievable carrier mobility and light detection and identify the factors that govern performance in (opto-) electronic devices and sensors. Finally, *in-situ* electron microscopy has been combined with *ab-initio* calculations to evaluate defect formation pathways and study possible structural transformations, e.g., from a Sn(IV)-sulfide (SnS_2) to a layered Sn(II)-sulfide (SnS), both across large scales and locally to create heterostructures between different layered semiconductors. This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award # DE-SC0016343.

VAPOR PHASE EPITAXY OF HEXAGONAL BORON NITRIDE ON SAPPHIRE

Anthony Rice[1], Andrew Allerman[1], Mary Crawford[1], Thomas Beechem[1], Taisuke Ohta[1], Douglas Medlin[2], Catalin Spataru[2], Jeffrey Figiel[1], Michael Smith[1]

[1]Sandia National Laboratories, NM, UNITED STATES OF AMERICA, [2]Sandia National Laboratories, CA, UNITED STATES OF AMERICA

Hexagonal Boron Nitride (hBN) is a wide bandgap (~6 eV) semiconductor of interest for use in conventional optoelectronic, quantum optoelectronics, and 2D heterostructures. High quality hBN is currently produced as bulk single crystals or by vapor phase epitaxy (VPE) at ~1000 ˚C on metal catalyst substrates and typically requires exfoliation to integrate with other materials. Consequently, we are investigating the use of VPE at high temperature as a means to produce hBN on non-catalytic oxide or semiconductor substrates to allow for direct growth of heterostructures. In this study, hBN was deposited on c-plane sapphire wafers in a cold-walled, rf-heated reactor using a borazine ($B_6H_{12}N_6$) source with N_2 carrier and diluent at 50 Torr total pressure. Deposition temperatures were varied from 1300 °C to 1600 °C, measured by optical pyrometry of the susceptor, and borazine partial pressures (ρBZ) were varied from 10^{-6} Torr to 10^{-3} Torr. Atomic force microscopy (AFM) characterization of hBN films showed that nuclei density could be controlled by temperature and ρBZ during deposition. For temperatures greater than 1400 °C individual hBN nuclei could be resolved, whereas VPE at 1300 ˚C yielded clusters of ~10 nm diameter grains. Nuclei density decreased with increasing temperature and decreasing ρBZ, as expected from classical nucleation theory, with a minimum nuclei density of ~10^7 cm^{-2}. Nuclei expansion and subsequent film coalescence could also be controlled by temperature and ρBZ. Both isolated nuclei and coalesced hBN films exhibited wrinkles thought to be from thermal expansion mismatch between hBN and sapphire during cooldown. The height of such wrinkles were less than 1 nm for nuclei and films upon coalescence with RMS roughness of ~0.2 nm and ~1 nm for nuclei and films upon coalescence, respectively. Further growth yielded thicker hBN films with larger wrinkles and increasing roughness. Characterization by Raman spectroscopy showed a peak at ~1369 cm^{-1}, consistent with sp^2 BN, with FWHM of ~20 cm^{-1}. For hBN films deposited with temperatures greater than 1500°C room temperature photoluminescence showed spectra with near band edge emission dominated by peaks at 216 nm and 222 nm, thought to be emission of the optical phonon replica of free exciton and defect bound exciton, respectively. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

ANTIMALARIALS INHIBIT HEMATIN CRYSTALLIZATION BY UNIQUE DRUG-SURFACE SITE INTERACTIONS

Peter G. Vekilov

University of Houston, UNITED STATES OF AMERICA

In malaria pathophysiology, divergent hypotheses on the inhibition of hematin crystallization posit that drugs act either by the sequestration of soluble hematin or their interaction with crystal surfaces. We employ physiologically-relevant, time-resolved *in situ* surface observations and show that quinoline antimalarials inhibit hematin crystal surfaces by three distinct modes of action: step pinning, kink blocking, and step bunch induction. Detailed experimental evidence of kink blocking validates classical theory and demonstrates that this mechanism is not the most effective inhibition pathway. Quinolines also form various complexes with soluble hematin, but complexation is insufficient to suppress heme detoxification and is a poor indicator of drug specificity. Collectively, our findings reveal the significance of drug – crystal interactions and open new avenues for rationally designing antimalarial compounds.

THE SECONDARY AND QUATERNARY STRUCTURE OF AMELOGENIN ON HYDROXYAPATITE

Wendy Shaw[1], Rajith Arachchige[1], Sarah Burton[1], Junxia Lu[2], Yimin Xu[1], Jinhui Tao[1], Barbara Tarasevich[1], Garry Buchko[1]

[1]Pacific Northwest National Laboratory, WA, UNITED STATES OF AMERICA, [2]Shanghai Tech, CHINA

Full-length amelogenin is necessary for proper enamel formation, but very little is understood at a mechanistic level about how amelogenin controls crystal growth. Protein structure (secondary, tertiary, and quaternary) is thought to play a key role in the function of amelogenin in enamel formation, and our group has started to provide quantitative insight into the structure of amelogenin in solution and bound to hydroxyapatite (HAP). The wildtype protein has a common lack of structure in solution and in the nanosphere, but becomes structured when bound to HAP along with a reduction in flexibility. The quaternary structure upon binding to HAP is signficantly different than in solution. The goal of these studies is to understand the secondary, tertiary, and quaternary structures of the wildtype protein, to correlate structure and function in enamel development. Using solution and solid state NMR and AFM, the secondary, tertiary, and quaternary structure of two naturally occurring *full-length* amelogenin mutants will be compared in solution, in the nanosphere and bound to HAP, and the intermolecular interaction provides quantitative, atomic level interactions that will help develop a mechanistic understanding of the protein-protein interactions governing biomineral formation. Further, the application of NMR and AFM techniques to allow the investigation of proteins >60 residues represents a major advancement for amelogenin specifically and biomineralization proteins in general.

SPECIFIC AND NON-SPECIFIC INTERACTIONS WITH GROWING CALCITE CRYSTALS - LIVE IMAGING AFM STUDIES

Amir Berman, Bidisha Tah

Ben-Gurion University, ISRAEL

Crystal nucleation and growth is a ubiquitous process with manifestations in biological mineralization as well as in many synthetic and technological aspects. We study calcite crystal growth at near molecular level using in-situ, live imaging AFM. We study crystal growth in the presence of additives and their effects on differential directional step propagation velocities, as well as the integrated volume incremented addition. Phosphoserine (PS) is a documented inhibitor of calcium carbonate crystallization that induce ACC formation and its stabilization. Live imaging AFM depict the details of the crystal inhibition process and the recovery of calcite growth when PS is removed. The mineralization regulatory protein, Pif-80 from the oyster *Pinctada fucata* shell nacreous layer has a DDRK consensus repeat. “DDRK” peptide, derived from Pif-80 was introduced into growing calcite in an AFM live image setup, resulted in unidirectional effect which can be reversed upon peptide removal.

QUANTIFYING CRYSTALLIZATION KINETICS OF AMORPHOUS CALCIUM CARBONATE USING DROPLET MICROFLUIDICS

Jack Cavanaugh, Michael L. Whittaker, Derk Joester

Northwestern University, IL, UNITED STATES OF AMERICA

Many organisms control growth of mineralized tissues through crystallization of a disordered precursor phase. Prominent model systems include the growth of single crystalline calcite via amorphous calcium carbonate (ACC) in larval sea urchin spicules and adult sea urchin spines. It is thought that this transformation may depart considerably from classical models for nucleation and growth of a new phase, and accumulating evidence has supported developing theories of non-classical growth via particle attachment. However, quantitative data to support theories of crystal formation via amorphous precursors remain limited. Characterization of the transformation presents challenges because crystallization proceeds rapidly and heterogeneous nucleation sites remain poorly characterized at relevant time- and length-scales. *In vitro* and *in vivo* studies point to confinement within a small volume of solution as an important biological strategy for prolonging the lifetime of precursor mineral and controlling heterogeneous nucleation sites to direct crystallization. Leveraging the effect of confinement and microfluidics techniques, we built a device to quantify nucleation of crystalline calcium carbonate ($CaCO_3$) in aqueous droplets containing ACC. The device consists of aqueous calcium chloride droplets ~500 picoliters in volume that are “parked” in separate wells along a linear, oil-filled channel. The droplets are exposed to a constant source of carbonate ions delivered via diffusion of carbon dioxide from two adjacent channels. ACC precipitates and grows in all droplets without perceivable delay. However, confinement delays nucleation of crystalline $CaCO_3$ compared to precipitation in bulk and prolongs the lifetime of ACC. This allowed us to extract nucleation rates of crystalline polymorphs of $CaCO_3$ by combination of time-lapse polarized light microscopy and in situ Raman microscopy. We will discuss rate information extracted using our microfluidic device in the context of classical and non-classical nucleation and growth pathways. With facile methods for detecting crystals and identifying polymorphs, the device presented in this study holds promise for quantifying the impact of additives relevant to biomineralization, including proteins and Mg^{2+} ions, on the crystallization of $CaCO_3$ from solution containing ACC.

PHASE EQUILIBRIA AND SEGREGATION IN BRIDGMAN GROWTH OF CS_2LIYCL_6

Frank Ruta[1], **Robert S. Feigelson**[1], Stacy Swider[2], Stephanie Lam[2]

[1]Stanford University, CA, UNITED STATES OF AMERICA, [2]CapeSym Inc., MA, UNITED STATES OF AMERICA

Cs_2LiYCl_6 (CLYC) is a commercial scintillator material having good energy resolution and dual gamma/neutron detection capabilities. CLYC crystals currently used in detectors are grown by the vertical Bridgman method. Boules grown from stoichiometric melts (50% Cs_2YCl_5 + 50% LiCl), however, often contain second phases at the beginning and end of the crystal, suggesting this composition is incongruently melting. Since no phase diagram containing CLYC existed in the literature prior to this study, the Cs_2YCl_5-LiCl phase diagram was explored using differential thermal and x-ray powder diffraction analyses. A CLYC plus liquid two-phase existence region was found to extend from ~50-88% LiCl, below a high-temperature Cs_3YCl_6 plus liquid phase field ending at ~60% LiCl. Based on the derived phase diagram, a melt composition of around 60% LiCl would be optimal for CLYC Bridgman growth at slow growth rates. Several CLYC crystals were then grown from melt compositions of 55%, 60%, 66% and 75% LiCl. As predicted, the boule grown from the 60% melt composition did not contain unwanted secondary phases.

HIGH-THROUGHPUT GROWTH OF SRI_2(EU) AND CLYC SCINTILLATORS BY THE EFG METHOD

Stacy Swider[1], George Calvert[2], Matthew Overholt[1], Frank Ruta[2], Robert Feigelson[2]

[1]CapeSym Inc., MA, UNITED STATES OF AMERICA, [2]Stanford University, MA, UNITED STATES OF AMERICA

SrI_2(Eu) is a promising scintillator having high brightness, 3% energy resolution at 662 keV, and no self-activity. The elpasolite $Cs_2{}^6LiYCl_6$(Ce) (CLYC) has also shown great promise for dual-gamma-neutron detection. While these materials are fairly uncomplicated to grow by the Bridgman technique, is of interest to lower production costs so they may be adopted by mainstream nuclear detection technologies. Features inherent to the Bridgman technique limit the achievement of high throughput. Interactions with the ampoule wall can create defects, and resulting stresses become aggravated by thermal gradients along the boule length. Therefore, growth rates are limited to less than 1 millimeter per hour. With edge-defined film-fed growth (EFG), crystal solidification proceeds from a free surface, which removes the possibility of defect formation at the ampoule wall. The lower density of surface defects in EFG-grown material allows the crystal to tolerate higher stress levels without cracking. SrI_2(Eu) crystals have been grown by EFG at rates 10 times faster than the Bridgman-grown crystals. [1] EFG also allows for near-net shape growth of cuboids, which reduces material loss to machining. We will share our latest results of EFG growth of SrI_2(Eu) and CLYC cylinders and cuboids. We shall discuss considerations for seed orientation, die design, material compatibility, and overall equipment design. In addition, we will complement our discussion with 3D conjugate thermal models of the apparatus. [1] G. Calvert, C. Guguschev, A. Burger, M. Groza, J. J. Derby, R. S. Feigelson, “High speed growth of SrI2 scintillator crystals by the EFG process,” *J. Crys. Growth*, **455**, p 143-151, 2016 This work was supported by US Department of Homeland Security, Domestic Nuclear Detection Office, under the competitively awarded contract HSHQDC-15-C-B0040. This support does not constitute an express or implied endorsement on the part of the Government.

PULSED NEUTRON IMAGING STUDIES OF IN SITU GROWTH OF NEUTRON AND GAMMA DETECTOR MATERIALS

John Z. Larese, Christopher A. Crain, Nicholas Strange

University of Tennessee, TN, UNITED STATES OF AMERICA

We will present the current results of our activities using pulsed neutron, radiographic/resonant-imaging techniques to examine the synthesis of CLYC with a focus on identifying the conditions that favor the production of defect free materials. The studies are aimed at addressing the critical need to develop dependable crystal growth techniques of solid-state materials used as radiation detectors for both national security and medical applications. The goal of these studies is to identify: (1) the thermodynamic and convective conditions that exist at the furnace wall, within the melt and at the crystal-melt interface, (2) the nature and creation of solute segregation, voids, and crystal dislocation networks (3) the variations in crystal stoichiometry and (4) the formation of multi-crystalline domains. Using a pulsed neutron beam and time of flight detection methods we exploit the penetrating power and element/isotope wavelength dependence of neutron absorption and neutron resonances to perform measurements *in-situ* during crystal growth (using a commercial scale, three-zone, Bridgman furnace). Our current efforts concentrate on imaging the evolution of the liquid state and shape of the liquid-solid interface. Modeling studies by Derby and his collaborators indicate that the shape of the solid-melt interface has a dramatic effect on the crystal quality. We note that solid boules can also be examined (*nondestructively and without cutting or segmenting)* either inside the furnace or free standing. The objective of these studies includes: the validation/improvement of the modeling studies of crystal growth behavior, the development of new/improved furnace design, and the identification of optimum growth techniques that enable the production of large boules of defect free, single crystalline materials in a timely and cost effective manner. We will discuss our results to date including: a description of the experimental setup at LANSCE, sample neutron radiographic images (CLYC) and synchrotron based IR images of CZT flat solid plates. Furthermore, we illustrate that the shape of the solid-melt interface has both convex and concave curvature as a function of the thermal status within the furnace. Furthermore, we include MCNP model calculations of optimum incident energy and sample isotopic compositions to guide and enhance the contrast of various elemental components of the materials.

SIMULTANEOUS GROWTH OF 38 MM DIAMETER $KCAI_3$:EU SCINTILLATOR

Matthew Loyd[1], Luis Stand[2], Charles L. Melcher[1], Mariya Zhuravleva[1]

[1]Scintillation Materials Research Center, University of Tennessee, TN, UNITED STATES OF AMERICA, [2]Bredesen Center, University of Tennessee, TN, UNITED STATES OF AMERICA

$KCaI_3$:Eu is a scintillator composition that is promising for national security applications, with a high light yield and good energy resolution (~70,000 ph/MeV and ~3% E.R. at 662 keV, respectively). In addition to its high performance, $KCaI_3$ has been grown at larger sizes (38 mm diameter) without cracking. In this work we utilized a multi ampoule growth station to grow multiple 38 mm diameter crystals simultaneously. Two 26 x 38Ø mm crystals grown together were largely uncracked but showed some inclusions toward the last-to-freeze section. Gamma ray spectroscopy for both yielded energy resolutions < 3.8% at 662 keV. These two crystals were packaged in two different geometries: one in a conventional scintillator package with the crystal closely wrapped in a reflector, and one that utilizes a gap between the crystal and the reflector to maximize light collection and reduce self-absorption. Additionally, we completed growth of four 38 mm diameter crystals of $KCaI_3$:Eu simultaneously.

IMPACT OF ADDITIVES ON THE CRYSTALLIZATION OF PHARMACEUTICAL SUBSTANCES

Lynne S. Taylor

Purdue University, IN, UNITED STATES OF AMERICA

Many new and current drugs are very poorly soluble in water, and therefore to deliver them to the body, solubility enhancing formulations need to be employed. The impact of additives on the crystallization kinetics of drugs from aqueous solutions is important in the context of these solubility enhancing formulations. This is because formulation approaches to enhance delivery of poorly water soluble compounds may result in the generation of supersaturated solutions upon dissolution of the formulation, or supersaturated solutions may evolve during transit along the gastrointestinal tract when pH changes occur. Supersaturated solutions can then undergo crystallization, whereby crystallization kinetics will be dependent on a variety of factors including the composition of the media. Since supersaturated solutions may enhance the absorption of the drug, it is important to consider the impact of additives on the supersaturation duration. Various additives, in particular certain polymers are known to inhibit crystallization, by reducing nucleation and/or crystallization rates. In contrast, other additives may actually enhance crystallization rates. The mechanisms by which additives alter crystallization rates of drug-like moleules are not well understood. In this presentation, we will discuss what is known about drug-additive interactions and how these interactions can alter crystal nucleation and/or crystal growth. Microscopy studies of crystal surfaces grown in the presence of polymers will be used to visually illustrate how polymers can interact with poorly water soluble drugs. Efforts to understand structural features of polymers and other additives that lead to effective crystallization inhibition will also be discussed.

NUCLEATION OF CRYSTALS OF HARD POLYHEDRA

Julia Dshemuchadse, Samanthule Nola, Richmond S. Newman, Sharon C. Glotzer

University of Michigan, MI, UNITED STATES OF AMERICA

Hard particles crystallize into ordered structures solely via entropy. Hard spheres form their well-known cubic close-packing with only isotropic entropic interactions, and a large number of polyhedra assemble the same structure. Polyhedral particles are subject to directional entropic forces that arise from their shape anisotropy. In addition to characterizing free energy barriers and other system parameters, we also quantify these shape-dependent, entropic interactions and therefore the local order around these faceted particles. As a result, we can elucidate the influence of faceting and polyhedral symmetry on the nucleation of entropic crystals.

SMALL-VOLUME NUCLEATION

Stéphane Veesler, N. Candoni, R. Grossier, R. Morin

CINaM-CNRS, FRANCE

The nucleation mechanisms behind crystallized products remain mysterious, mainly due to the fact that experiments on nucleation are generally of a stochastic nature: we do not know where and when an indefinite number of nucleation events will occur. In this presentation, we present experiments performed using small volumes, microdroplets[

ADVANCES IN NONLINEAR OPTICAL CRYSTALS FOR THE MID-INFRARED

Peter Schunemann

BAE Systems, NH, UNITED STATES OF AMERICA

Interest in nonlinear optical (NLO) materials for mid-infrared frequency conversion has exploded in recent years due to the emergence of new laser applications ranging from frequency-comb-based spectroscopy to high harmonic generation. NLO semiconductors such as $ZnGeP_2$ (ZGP) and orientation-patterned GaAs (OP-GaAs) offer transparency deep into the mid-infrared and THz with d-coefficients 5-10 times higher than those of oxides. ZGP and OP-GaAs must be pumped at wavelengths ≥ 1.9 mm, but new analogs for these materials – cadmium silicon phosphide ($CdSiP_2$, or CSP) and orientation-patterned GaP (OP-GaP) – can be pumped with widely-available 1-mm and 1.5-mm lasers. $ZnGeP_2$ remains the NLO material of choice for frequency conversion between 2 and 8 microns. Continued efforts to improve ZGP crystal quality and aperture size for high-energy laser applications are ongoing, enabling record-level peak- and average-output powers in the mid-IR. ZGP, however, still has two main limitations: 1) its transparency and phase-matching range make it incompatible with 1- and 1.5-micron laser pumping; and 2) its usefulness for generating output in the 8-12 micron atmospheric window is limited by severe multi-phonon absorption. $CdSiP_2$ (CSP) is a new bulk birefringent chalcopyrite analog of ZGP grown by horizontal gradient freeze growth in a transparent furnace. Its larger band gap (512 nm) and birefringence (-0.05) allows for 1- and 1.5-mm pumping, and its nonlinear coefficient (d_{14}=85 pm/V) and thermal conductivity (13 W/mK) are dramatically higher than existing materials ($AgGaS_2$, $AgGaSe_2$, and PPLN) that can be pumped at these wavelengths. OP-GaAs and OP-GaP are quasi-phasematched (QPM) NLO semiconductors grown by all-epitaxial processing : first, polar-on-nonpolar MBE produces GaAs (GaP) with an inverted orientation inverted with respect to the substrate which is photo-lithographically patterned, etched with the desired grating structure, and re-grown by hydride vapor phase epitaxy (HVPE) at rates up to 200mm/hr to produce thick (> 1mm), low-loss (< $0.01 cm^{-1}$) QPM layers for in-plane laser pumping. OP-GaAs has the highest gain among all QPM materials (d_{14} = 94 pm/V), and can be pumped at 2-mm to generate 8-12 mm output and beyond, whereas OP-GaP is a low-loss QPM ZGP analog than can be pumped with 1-mm lasers. Numerous OP-GaP device demonstrations have been achieved based on 1-, 1.5- and 2-mm laser pumping, and highly parallel grating propagation during growth promises to extend aperture sizes well beyond 1 mm.

THERMO-OPTIC AND STRESS-OPTIC PROPERTIES OF CADMIUM SILICON PHOSPHIDE

David E. Zelmon[1], William B. Poston[2], John D. Kunkel[2]

[1]Air Force Research Laboratory, UNITED STATES OF AMERICA, [2]US Air Force Research Laboratory, OH, UNITED STATES OF AMERICA

Submitted to public affairs office for approval. Approval will be obtained NLT 30 April

ADVANCES SINGLE CRYSTAL CDSIP$_2$ FOR HIGH ENERGY MID-INFRARED GENERATION

Kevin T. Zawilski[1], Peter Schunemann[1], F. Kenneth Hopkins[2]

[1]BAE Systems, NH, UNITED STATES OF AMERICA, [2]Air Force Research Laboratory, AFRL/RX, OH, UNITED STATES OF AMERICA

CSP is a new non-linear material which is a high temperature analog to ZnGeP$_2$ (ZGP) with a larger bandgap and promising characteristics for IR frequency conversion. CSP has the highest nonlinear coefficent (d36=84.5 pm/V) of any bulk birefringent material for producing mid-infrared pulses from high-energy 1-, 1.5-, or 2-micron laser sources. Crystals are birefringent and are transparent from 0.5 to 9 microns. Its thermal conductivity (13.6 W/mK) is higher than that of YAG, and 10-15 times higher than existing NLO crystals AgGaS2 (1.4 W/mK) and AgGaSe2 (1.0 W/mK) used for shifting 1.06-micron and 1.55-micron lasers into the mid-IR. Laser damage thresholds similar to those for ZGP have been measured. CSP growth presents significant crystal growth challenges compared to ZGP including: a higher melting point and vapor pressure that push the limits of fused silica based growth technology, a higher reactivity with boat materials and fused silica ampoules, an increased incidence of twin formation, and a negative c-axis thermal expansion coefficient making it prone to cracking. Despite these difficulties, recent advances in growth using the horizontal gradient freeze (HGF) technique from stoichiometric melts have resulted in scaling boules to 28mm diameter. In addition, efforts to minimize impurity contamination as well as more precise stoichiometry control continue to reduce extrinsic absorption losses in CSP. Defect studies using electron paramagnetic resonance (EPR) have begun to correlate specific defects to specific types of optical absorption in CSP crystals, and will be useful in further improving crystal quality. Recent laser results will be discussed.

OPTICAL ABSORPTION BANDS IN CDSIP2 CRYSTALS

Elizabeth Scherrer[1], Brant Kananen[1], Nancy Giles[1], Larry Halliburton[2], F. Kenneth Hopkins[3], Peter Schunemann[4], Kevin T. Zawilski[4]

[1]Air Force Institute of Technology, UNITED STATES OF AMERICA, [2]West Virginia University, WV, UNITED STATES OF AMERICA, [3]Air Force Research Laboratory, AFRL/RX, OH, UNITED STATES OF AMERICA, [4]BAE Systems, NH, UNITED STATES OF AMERICA

Single crystals of $CdSiP_2$ are rapidly becoming a useful and versatile nonlinear optical material. When used as an optical parametric oscillator (OPO), $CdSiP_2$ crystals efficiently generate tunable laser output in the mid-infrared. Compared to the widely used $ZnGeP_2$ crystals, $CdSiP_2$ has a higher nonlinear coefficient (d_{36} = 84.5 pm/V), can be pumped at shorter wavelengths (between 1 and 1.5 μm), and can produce non-critically phasematched output near 6.5 μm. The OPO performance of $CdSiP_2$ crystals, however, may be limited by unwanted optical absorption bands that overlap the pump wavelengths. Thus, we have initiated a research program to identify and characterize the primary absorption bands in $CdSiP_2$ that can be photoinduced by changing the charge state of as-grown point defects or that can be formed by irradiation with high-energy particles. The behaviors of these absorption bands at various temperatures (from room temperature to below 77 K) are especially important. A broad defect-related optical absorption band peaking near 800 nm, with a shoulder near 1 μm, can be photoinduced at room temperature in many $CdSiP_2$ crystals. This absorption is produced with 633 nm laser light and decays, at room temperature, with a lifetime of 0.5 s after removal of the excitation light. The 800 nm and 1 μm bands are accompanied by a less intense absorption band peaking near 1.90 μm. Data from eight $CdSiP_2$ crystals grown at different times show that singly ionized silicon vacancies are responsible for the photoinduced absorption. Electron paramagnetic resonance (EPR) is used to directly monitor these silicon vacancies. We also show, in separate experiments, that an irradiation with high-energy neutrons creates a large absorption band in $CdSiP_2$, peaking in the 750-850 nm region with a tail extending to near 1.5 μm. Work is on-going to determine the defects responsible for this neutron-induced absorption.

REMOTE EPITAXY THROUGH GRAPHENE SAVES WAFER COST VIA 2DLT

Jeehwan Kim

MIT, UNITED STATES OF AMERICA

In recent studies, van der Waals epitaxy was investigated on 2D materials grown or transferred on arbitrary substrates with the primary notion that the 2D material is the sole epitaxial seed layer for epitaxy. However, the underlying substrate below 2D materials may still play a role in determining the orientation of the overlayers since the weak van der Waals potential field from 2D materials may barely screen the stronger potential field from the substrates. Here, we reveal that the epitaxial registry of adatoms can be remotely assigned to the underlying substrate even with the gap between the substrate and the epilayer created by 2D material interlayers. Our study shows that epitaxial growth can be performed remotely through the single-atom-thickness gap defined by monolayer graphene at the substrate-epilayer interface. We experimentally demonstrated successful "remote epitaxy" of (100) III-Vs on (100) III-V substrates through monolayer graphene (III-V includes GaAs, InP, and GaP). After growth, the single-crystalline III-V film was released from the van der Waals surface of graphene. Remote epitaxy on graphene suggests that one can copy/paste the crystal structure of any substrate material through the atomically thin gap created by a graphene interlayer and the copied films can be subsequently released and transferred. This offers a universal layer transfer technique, so called 2D material-based layer transfer (2DLT) that can be applied for any material system.

TWO-DIMENSIONAL GALLIUM NITRIDE REALIZED *VIA* GRAPHENE ENCAPSULATION

Zakaria Y. Al Balushi[1], Joshua A. Robinson[2], Joan M. Redwing[2]

[1]Dept. Materials Science and Engineering, The Pennsylvania State University, PA, UNITED STATES OF AMERICA, [2]2D Crystal Consortium, Materials Research Institute, PA, UNITED STATES OF AMERICA

The spectrum of 2D and layered materials “beyond graphene” has been continually expanding. The realization of wide bandgap (E_g) 2D materials “beyond hexagonal boron nitride (hBN)”, however, has been limited. Along similar lines to initial theoretical discovery and subsequent experimental synthesis of “beyond graphene” 2D materials (i.e. silicene and borophene), theoretical studies have suggested that indium nitride (InN), gallium nitride (GaN), and aluminum nitride (AlN) take on a 2D graphitic structure with a thickness tunable E_g (~0.7-7.0 eV) due to quantum confinement. To accomplish this, an alternative growth scheme was developed to realize two-dimensional forms of conventional bulk semiconductors, utilizing the mechanism of adatom intercalation from the vapor phase in an MOCVD growth environment into the interfacial region of graphene formed on SiC. This synthesis process, referred to as “Migration Enhanced Encapsulated Growth” (MEEG)[1], establishes an entirely new platform to realize tunable optoelectronics that may frame next-generation technology. In the case of 2D GaN, a layer of gallium intercalates between the hydrogenated QFEG and the SiC substrate. The intercalated bilayer of gallium is converted to a quintuple monolayer of 2D GaN *via* nitrogen intercalation from decomposed NH_3. Our density functional theory (DFT) calculations suggest that the atomic structure in 2D nitrides considerably impacts the stability and bandstructure. We verify the atomic structure by directly resolving the nitrogen and gallium atomic columns in 2D GaN using aberration corrected scanning TEM (STEM) in annular bright field (ABF) mode with supported ABF-STEM simulations. Our DFT calculations predict an E_g for 2D GaN in the range of 4.79-4.89 eV which correlates well with experimental results from UV-visible reflectance, absorption coefficient and low loss EELS measurements. Vertical transport measurements suggest 2D GaN acts as a Schottky barrier between graphene and SiC. High resolution x-ray photoelectron spectroscopy demonstrates that 2D GaN is stable in air for at least 24 hours after removal of the graphene cap. [1]Z.Y. Al Balushi et al., Nature Materials 15, 1166–1171 (2016).

THE GROWTH AND ELECTRONIC PROPERTIES OF ULTRA-THIN EPITAXIAL TOPOLOGICAL DIRAC SEMIMETAL NA_3BI FILMS

Mark T. Edmonds

Monash University, AUSTRALIA

Topological Dirac semimetals (TDS) are three-dimensional analogues of graphene, with linear electronic dispersions in three dimensions. In this talk I will present our recent efforts to grow thin films of the TDS, Na_3Bi via MBE on both α-$Al_2O_3(0001)$ and Si(111) substrates. Magneto-transport measurements on these films reveal carrier mobilities in excess of 6000 $cm^2V^{-1}s^{-1}$ and carrier densities below 10^{18} cm^{-3} comparable to the best single crystal values. Perfect weak anti-localization behaviour, expected for Dirac fermions in the absence of intervalley scattering, is observed that corresponds to phase coherence lengths in excess of one micron. By utilizing scanning tunnelling microscopy/spectroscopy the potential fluctuations can also be directly measured. We find that the potential fluctuations are significantly smaller than room temperature ($\Delta E_F \approx 5meV=60$ K) and comparable to the highest quality graphene on h-BN; far smaller than graphene on SiO_2, or surface state of a topological insulator. Furthermore, surface Na vacancies show a novel resonance state close to the Dirac point with large spatial extent, offering a means to tune the surface electronic properties of this material.

THE EFFECTS OF COMPOSITION, GROWTH CONDITIONS AND DOPING ON VERTICAL BRIDGMAN GROWTH OF THE TOPOLOGICAL INSULATOR BI2TE2SE

David Snyder[1], Randal Cavalero[1], Robert Lavelle[1], Ron Redwing[2]

[1]Penn State Applied Research Laboratory, PA, UNITED STATES OF AMERICA, [2]Penn State MatSE, UNITED STATES OF AMERICA

In this presentation we describe results of a study the effects of composition and doping from residual impurities on the Vertical Bridgman (VB) growth of the topological insulator Bi2Te2Se. While the binary constituents have been widely studied, there have been few studies of the role of growth process and impurities on the bulk and surface states of the stoichiometric ternary compound, off-stoichiometric grown crystals and Sb and Sn doped crystals. The main interest was to focus on the growth of high resistivity bulk crystals of Bi2Te2Se with low bulk carrier concentrations. We evaluated the effects of compositional variations, growth related impurities and growth conditions on resistivity. Boules of B2Te2S2 of length greater than 100mm were grown using the vertical Bridgman process, sectioned and (001) cleaved crystals were characterized as a function of temperature to determine the effects on resistivity and carrier concentration as a function of boule position. The effects of impurity segregation and compositional variation along the boule length were characterized were characterized using glow discharge mass spectrometry. Ampoule coatings, growth process conditions and doping concentrations were evaluated. Initial results for growth of quaternary compounds containing either Sb or Sn and S will also be presented. Structural, compositional and electrical properties were characterized and the role of residual growth process impurities was correlated relative to compositional and doping levels.

WHAT YOUR MOTHER NEVER TOLD YOU ABOUT APATITE...AND HOW TO EXPLOIT IT

Jill D. Pasteris

Washington University in St. Louis, MO, UNITED STATES OF AMERICA

The calcium phosphate mineral component of bone remains more elusive than one might imagine, given that bone has been studied for centuries. Bone mineral is often referred to simply as hydroxylapatite, $Ca_{10}(PO_4)_6(OH)_2$, which is a designation so oversimplified as to be misleading to medical practitioners, biomaterials developers, and bone(-mineral) modelers. The bioapatite in bone is a hydrated, Ca-deficient, OH-deficient apatite exhibiting several weight% carbonate substitution and whose crystals are of a different shape, size, and solubility than those of hydroxylapatite. The compositional and structural details of bioapatite are important to both those doing biological research on bone (and its pathologies) and those formulating biomaterials to replace or augment bone. Moreover, the connection between the composition and the properties of bioapatite also should be of interest to those involved in the biomimetic development of materials. Among the attributes of bioapatite to be explored in this talk are isomorphous substitution of anions and cations in the apatite structure, the effects of structural incorporation of H_2O in the apatite channels, the controls on and importance of adsorbed species on bone crystallites, and the different steps in and possible different pathways of thermal maturation of bioapatite and its synthetic analogs. As an example of how to make use of one of the often-overlooked "details" of bioapatite, consider the recognized positive correlation between apatite's degree of carbonate substitution and its solubility. As is typical in minerals, composition mediates an important chemical parameter. By imposing a specific concentration of carbonate within synthetic apatite in a biomaterial, one can control the solubility of that apatite in body fluid. Moreover, one could engineer the material to express slow-release capabilities by synthesizing apatite with a specified range of carbonate concentrations, thereby setting up gradients in solubility within the same packet of biomaterial. The possibility of compositional gradients to promote solubility gradients could be tested in natural bone to determine if this mechanism could shed light on the means by which bone acts as a pH buffer for body fluid. Such buffering requires bone apatite, more specifically its carbonate component, to be released into solution during a decrease in pH (as in acidosis). This is just one example of how what otherwise might be perceived as a "bit of trivia" about bioapatite can be explored and exploited for the dual purposes of enhanced biological understanding of bone and creative development of biomimetic materials.

TOOTH ENAMEL FORMATION: THE ESSENTIAL ROLE OF AMELOGENIN PHOSPHORYLATION

Henry C. Margolis[1], Nah-Young Shin[1], Hajime Yamazaki[2], Seth S. Margolis[3], Megan K. Pugach[1], James P. Simmer[4], Elia Beniash[5]

[1]The Forsyth Institute, MA, UNITED STATES OF AMERICA, [2]Harvard School of Dental Medicine, MA, UNITED STATES OF AMERICA, [3]The Johns Hopkins University School of Medicine, MD, UNITED STATES OF AMERICA, [4]University of Michigan School of Dentistry, MI, UNITED STATES OF AMERICA, [5]University of Pittsburgh School of Dental Medicine, PA, UNITED STATES OF AMERICA

Amelogenin, the predominant extracellular enamel matrix protein, has been shown to play an essential role in regulating tooth enamel formation. Tooth enamel is a highly mineralized tissue (>97wt% mineral) comprised of intricate interwoven patterns of individual bundles (prisms) of extremely long and co-aligned crystals of carbonated hydroxyapatite. Prior studies in our laboratory have demonstrated a unique ability of full-length amelogenin to form higher-order assemblies and regulate ordered mineralization *in vitro*, as seen in developing enamel. We have also found that the single-site phosphorylation of serine-16 greatly enhances the capacity of native amelogenins to stabilize nanoparticles of amorphous calcium phosphate (ACP), the first mineral phase in developing enamel, preventing hydroxyapatite (HA) crystal formation. These observations lead us to hypothesize that amelogenin phosphorylation is critical for proper enamel formation. *In vitro* laboratory evidence in support of this hypothesis will be presented, along with our recent results from testing this hypothesis *in vivo.* Working with a commercial laboratory, we generated an amelogenin knock-in (KI) mouse with a targeted serine-16 to alanine point mutation that is phosphorylation-defective. Teeth from KI, heterozygous (Het) and wild-type (WT) littermates were assessed using SEM, TEM, immunohistochemistry (IHC) and µCT. Using this approach, we found that KI, Het and WT littermates were readily generated, although KI mice required a soft diet. Western blot and IHC findings confirmed the absence of amelogenin phosphorylation in KI enamel. In sharp contrast to the WT, KI enamel was brittle and exhibited a marked phenotype in both the initial secretory stage and the maturation stage of enamel development. Mature KI enamel showed a loss of decussating prism patterns found in WT enamel and numerous surface defects (nodules). TEM analyses of secretory and early maturation stages indicate that KI enamel (incisor) is comprised of discontinuous short bundles of aligned HA-like crystals, unlike WT enamel that exhibits extremely long and well-aligned enamel crystals. Het enamel also appeared abnormal, with a variable mosaic appearance with portions of underlying and surface enamel reflecting both WT enamel and KI phenotypes. Based on µCT, KI and Het enamel were significantly under-mineralized, compared to WT enamel. Preliminary evidence suggests that ACP->HA transformation seen in each genotype takes place faster in KI enamel. Based on these findings, we conclude that amelogenin serine-16 phosphorylation is essential for proper enamel formation and, in part, plays a critical role in regulating the appositional growth of forming enamel crystals. Supported by NIDCR grants DE023091 and DE023425.

REGULATION OF COCCOLITH CALCITE FORMATION

Andre Scheffel[1], Sanja Sviben[1], Assaf Gal[1], Damien Faivre[2]

[1]Max-Planck Institute of Molecular Plant Physiology, GERMANY, [2]Max-Planck Institute of Colloids and Interfaces, GERMANY

Coccoliths are complex arrays of calcite crystals that decorate the cell surfaces of unicellular marine algae known as coccolithophores. About 300 distinct coccolith architectures are known to be produced by the extant species. The pathway for intracellular coccolith formation involves a specialized organelle, called coccolith vesicle. Inside the coccolith vesicle calcite crystals nucleate and grow on the rim of an organic scale called base plate. The mature crystals possess convoluted shapes and are only tens of nanometers thick. Many species produce coccoliths containing two differently-shaped crystals, arranged in an alternating order. In these coccoliths, the orientation of the crystallographic *c*-axis of one crystal type is parallel to the coccolith base plate whereas the *c*-axis of the other crystal type is perpendicularly oriented. Coccoliths are a paradigm for the controlled fabrication of complex-structured crystalline materials and identification of the mechanisms underlying their formation may allow for the development of biomimetic approaches for fabricating novel materials. How coccolithophores control the site–specific nucleation of calcite on the base plate, the orientation of the crystals and coccolith architecture remains largely elusive. In this talk I will summarize our recent discoveries regarding the pathway of intracellular coccolith formation and the control of coccolith calcite formation by biomacromolecules.

MITIGATION OF SECOND-PHASE PARTICLES IN SINGLE CRYSTALS VIA POST-GROWTH TREATMENT: TEMPERATURE GRADIENT ZONE MELTING AND ANNEALING

Nathan T. Morgan, Kerry Wang, Jeffrey J. Derby

University of Minnesota, MN, UNITED STATES OF AMERICA

Second-phase particles are often unavoidable during the growth of binary semiconductor crystals from liquids, due to effects arising from non-congruent solidification and thermodynamics of the solid state. This presents a special challenge for the growth of large, high-quality crystals of cadmium telluride (CdTe) and cadmium zinc telluride (CZT) needed for gamma spectrometers, in which tellurium-rich particles are deleterious to the performance of such devices. We first present the most plausible mechanisms by which these second-phase particles arise during the growth of CdTe and CZT from the Bridgman process and the traveling heater method (THM). Since it may not be possible to prevent the formation of these particles during crystal growth, we discuss possible mitigation strategies that involve post-growth processing. Specifically, we analyze and assess post-growth strategies that involve treatment of the crystalline material under controlled temperatures and gas-phase environments over time. We discuss the temperature gradient zone melting (TGZM) technique, whereby particles can be induced to migrate by heating to slightly above the eutectic temperature and applying a temperature gradient across the sample. Under such conditions, the now-liquid particle dissolves on the hot side and re-solidifies on the cool side, with a net effect of the particle migrating toward the hotter region. We next consider how annealing under a cadmium-rich atmosphere can reduce the size of second-phase particles. Finally, we consider the combined strategy of TGZM and cadmium- overpressure annealing. Our assessment relies upon mathematical and computational models for these post-growth treatments. We briefly present the formulation of mathematical models for particle migration via TGZM and particle shrinkage under the effect of solid-state diffusion of an enriched constituent. We provide analytical solutions that give good estimates for the overall outcomes of these strategies. We also describe the implementation of a moving-boundary, finite-element method that solves for particle position and shape, with no simplifying assumptions about mechanistic interactions. This model allows for a computation of the evolution of particle velocity, size, and shape over time and comparison to experimental observations. --------------

This work has been supported in part by U.S. Department of Homeland Security, 2012-DN-077-ARI066-06, and no official endorsement should be inferred.

MODELING AND EXPERIMENTAL ANALYSIS OF ZINC DISTRIBUTION AND DISLOCATION DENSITY EVOLUTION IN CZT BRIDGMAN CRYSTAL GROWTH

Alex Galyukov[1], Vladimir Artemyev[2], Andrey Smirnov[2], Vasif Mamedov[2], Vladimir Kalaev[2], Zhou Changhe[3], Chao Xu[3], Shiwen Sun[3]

[1]STR US, Inc., VA, UNITED STATES OF AMERICA, [2]STR Group, Inc. – Soft-Impact, Ltd., RUSSIAN FEDERATION, [3]Shanghai Institute of Technical Physics, Chinese Academy of Sciences, CHINA

$Cd_{1-x}Zn_xTe$ (CZT) crystals are used for manufacturing of room temperature radiation detectors, IR filters and used as a substrate for epitaxial growth of HgCdTe (MCT). Quality and performance of devices manufactured using CZT crystals and wafers depend on the concentration of crystal defects such as dislocations, inclusions, grain boundaries, and on the homogeneity of Zinc concentration distribution over the crystal volume. The traditional approach for crystal growth technology optimization is experimental. Due to very low growth rate of CZT crystals, such approach is expensive and time-consuming. Accurate and detailed computer models help to significantly reduce the time and cost of process optimization [1]. In the presented work, we demonstrate a detailed computer model of CZT crystal growth. Modeling of the crystal growth is coupled with the computations of the melt flow including the effect of Zn concentration on the melt convection. Results also include distribution of Zn in the grown crystal for the subsequent analysis of the effect of growth conditions on radial and axial uniformity of Zn concentration. Nonuniform temperature distribution in the crystal during growth and cooling stages results in generation of thermal stress and their subsequent release with generation of dislocations. This process is analyzed by computer modeling within modified Alexander-Haasen model [2, 3]. Calculated distributions of dislocation density and zinc concentration in the crystal are compared to experimental data. [1] N. Zhang et al., Journal of Crystal Growth 355 (2012) 113–121 [2] H. Alexander, P. Haasen, Solid State Phys. 22, 27 (1968) [3] O.V. Smirnova et al., Cryst. Growth Des. 2014, 14, 5532−5536

TOWARDS OPTIMIZATION OF ACRT SCHEDULES APPLIED TO THE GRADIENT FREEZE GROWTH OF CADMIUM ZINC TELLURIDE

Mia S. Divecha[1], Jedidiah J. Mccoy[2], Kelvin G. Lynn[2], Jeffrey J. Derby[1]

[1]University of Minnesota, MN, UNITED STATES OF AMERICA, [2]Washington Stat University, WA, UNITED STATES OF AMERICA

Cadmium zinc telluride (CZT) is widely used for advanced gamma ray detectors due to its room temperature operability and high band gap. CZT grown via the gradient freeze method is often plagued by large, tellurium-rich inclusions that are a consequence of a morphologically unstable solid-liquid interface. These inclusions impede detector performance and require lengthy annealing processes to mitigate. Additionally, spontaneous nucleation of new grains can occur at the solidification interface during growth, reducing the yield of single-crystal material. The Accelerated Crucible Rotation Technique (ACRT), which enhances convective mixing in the melt, has been shown to decrease the population of inclusions and improve monocrystallinity. However, no clear guidelines exist on optimal rotation schedules, and, more importantly, there is only limited understanding on what allows ACRT to improve the growth process from a mechanistic and thermodynamic perspective. We aim to address these questions using a comprehensive computational model of the flow, heat, and mass transfer within the VGF-ACRT growth system paired with an experimentally realistic furnace profile. We compute flow patterns, thermal field, composition, and interface shape in order to track thermodynamically undercooled regions of the melt that arise during growth. Using model results, we explain why ACRT is effective at changing the extent of melt undercooling, thus potentially suppressing morphological instabilities of the growth interface. Moreover, we have developed a thermodynamically-consistent metric that allows for the systematic evaluation and optimization of ACRT schedules. Outcomes from growth experiments under different ACRT schedules are presented and compared with model predictions as evidence of improved material quality. -------------- This work is supported by the Department of Energy, National Nuclear Security Administration, under Award DE-NA0002565; no official endorsement should be inferred.

ALTERNATIVE CRYSTAL GROWTH TECHNIQUES FOR THALLIUM BROMIDE SEMICONDUCTOR RADIATION DETECTORS

Amlan Datta, Piotr Becla, Kris Becla, Shariar Motakef

CapeSym, Inc., MA, UNITED STATES OF AMERICA

Thallium Bromide (TlBr) is a wide bandgap, compound semiconductor with high gamma-ray stopping power and promising physical properties. The purification and growth techniques that are being used for this halide compound last for several months, thereby hindering development of a low-cost commercial process. We took the advantage of alternative growth techniques to overcome the different challenges associated with the current known technique. Particularly, we report on the growth of TlBr crystals using physical vapor transport technique for the first time. This process combines purification and growth, and promises to be a faster alternative to current approaches. Using this process, a 1inch x 1inch TlBr single crystal was grown from pre-purified TlBr material in under two weeks. The starting material was purified using low-temperature sublimation. The impurity concentration in the grown crystal is significantly lower than the crystals grown using the existing techniques. The resistivity of the TlBr radiation detector devices fabricated using this crystal is in the order of 10^{11} Ω-cm. The characterization results of these devices will be discussed. This work was supported by the U.S. Department of Homeland Security, Domestic Nuclear Detection office contract SBIR HSHQDN-16-C-00025. This support does not constitute an express or implied endorsement on the part of the Government.

ANISOTROPIC AND TEMPERATURE-DEPENDENT THERMAL CONDUCTIVITY OF LEAD IODIDE

Arne Croell[1], Justus Tonn[1], Ekkehard Post[2], Harald Böttner[3], Andreas Danilewsky[1]

[1]University of Freiburg, GERMANY, [2]Netzsch Gerätebau GmbH, GERMANY, [3]Fraunhofer IPM (retired), GERMANY

Lead iodide (PbI_2) is a promising material for room temperature radiation detectors, with an average Z number of 62.7 and a bandgap of 2.32 eV. The most common growth method is the self-seeding Bridgman-Stockbarger method, although Czochralski growth, zone melting, and vapour growth have also been used. As a layered structure, it exhibits very anisotropic material parameters. Of special importance for crystal growth are thermal parameters such as the thermal expansion and the thermal conductivity. As an example, it has been shown that in Bridgman as well as in vapour growth of PbI_2, the orientation of self-seeded crystals is governed by thermotaxy, i.e. the c-axis of the crystals is oriented perpendicular to the strongest thermal flux. Reliable values of the material parameters are also a necessity for meaningful numerical simulations of the crystal growth process. The anisotropic thermal conductivity is a 2nd rank tensor, but due to symmetry only two independent components exist, $k_{11} = k_{22}$ for the direction perpendicular to the c axis, and k_{33} parallel to the c axis, all other components being 0. Only two values of the thermal conductivity k_{33} at normal conditions can be found in the literature, differing by more than an order of magnitude. No measured values of k_{11} exist for PbI_2 at room temperature or close to melting point temperatures, which is the most important range for crystal growth setups. For these reasons, Laser Flash Analysis (LFA) measurements of both k_{33} and k_{11} have been performed for temperatures between -100°C and +350°C. The temperature-dependent specific heat capacity c_p was determined independently by Differential Scanning Calorimetry (DSC) to calculate the thermal conductivities for PbI_2 from the thermal diffusivity data. At 27°C, the thermal conductivity in the c-axis-direction, k_{33}, is 0.315 $W\ m^{-1}\ K^{-1}$, whereas the component perpendicular to the c-axis, k_{11}, is 0.681 $W\ m^{-1}\ K^{-1}$. The anisotropy ratio k_{33}/k_{11} changes from 1:2 at -100°C to 1:2.4 at +350°C. The temperature dependencies of both k_{33} and k_{11} in this range could be very well fitted with 3rd order polynomials.

CURRENT STATUS & FUTURE CHALLENGES IN CRYSTAL GROWTH PREDICTION

Michael F. Doherty

University of California Santa Barbara, CA, UNITED STATES OF AMERICA

After 70 years of research on the fundamentals of crystal growth at low supersaturation, it is finally becoming a reality to predict accurately the relative growth rates of crystal faces (i.e., crystal shape) for solutes of complex growth units, and absolute growth rates (i.e., crystal size & shape) for simpler systems. We report on recent developments in surface growth physics and solid-state & solution chemistry which make these advances possible. For complex, non-centrosymmetric growth units that generate alternating step-rows with different levels of stability (e.g., [001] step on the (200) face of monoclinic paracetamol), we report on new models for predicting the (relative) step velocity. For simpler systems, the challenge is to bring rare-event molecular simulation and mechanistic growth models together in order to predict absolute crystal growth rates (e.g., in units of nm/s). To accomplish this task, it is necessary to predict the absolute attachment and detachment rates of growth units into kink sites. This can now be done for sodium chloride crystals grown from aqueous solution.

EXPERIMENT AND PREDICTION OF SURFACE TEMPLATED POLYMORPHS AND SOLVATES

Alastair Florence

CMAC, Technology Innovation Centre, University of Strathclyde, UNITED KINGDOM

Control of the solid-state form of active pharmaceutical ingredients (API) during development and manufacture is key to assuring the consistent performance and quality of medicines. With computational approaches for crystal structure prediction developing considerably in recent years, this has created new experimental challenges to explore the crystal energy landscape. The role of crystal surfaces is of particular interest in this context and provides the opportunity to extend traditional solution based screening approaches to more targeted experimental approaches that exploit computationally inspired surface templating. The presentation will highlight two examples where the role of specific crystal forms and crystal surfaces has been investigated. The application of vapour deposition coupled with specific computationally derived template crystals has produced new polymorphic forms of carbamazepine (form V) and cyheptamide (form III) [1]. A robust experimental approach has been developed for the preparation of templated forms by this method and recent investigations into the crystallisation processes at the surface using atomic force microscopy (AFM) and micro-computed tomogaphy will be shown (Figure 1). Secondly, the role of surface templating in the anhydrous-hydrate phase transformation to produced dihydrate form D on the surface of form I olanzapine in aqueous solution is discussed [2]. Olanzapine exhibits rich solid-state diversity with 60 distinct forms identified to date including 3 polymorphic forms (I, II, III), 52 crystalline solvates, 3 polymorphic dihydrates DB, DD, DE, a disordered higher hydrate plus an amorphous form. AFM results of the transformation suggest that the templated formation of olanzapine dehydrate D on the surface of OZPN I may follow a non-classical nucleation mechanism [2].

The structural and energetic aspects of the templating mechanism will also be discussed. (a) (b) (c) Figure. 1: (a) Microscope image of template surface; (b) AFM image of laterally grown CBZ-V crystals on DHC-II surface. (C) Experimental set-up. References: [1] V. K. Srirambhatla, R. Guo, S. L. Price and A. J. Florence , Chem. Commun., 2016, 52, 7384-7386 [2] R. M. Bhardwaj, L. S. Price, S. L. Price, S. M. Reutzel-Edens, G. J. Miller, I. D. H. Oswald, B. F. Johnston, and A. J. Florence, Cryst. Growth Des., 2013, 13(4), pp 1602–1617; M. Warzecha, R. Guo, R. M. Bhardwaj, S. M. Reutzel-Edens, S. L. Price, D. Lamprou and A. J. Florence, In preparation 2017.

UNRAVELING COMPLEXITY IN THE CRYSTALLIZATION OF PHARMACEUTICAL SOLIDS

Susan M. Reutzel-Edens

Eli Lilly and Company, UNITED STATES OF AMERICA

For the vast majority of small-molecule drugs that are delivered to patients in solid oral dosage forms, the identification of a suitable crystalline form of the active ingredient is usually the first step taken to transform a molecule to a medicine. The ability of a drug to crystallize in many different forms (including salts and co-crystals) creates opportunities to design properties into the bulk drug substance, but at the same time introduces challenges in deciding which form to develop, selectively crystallizing the preferred form on a large scale, and establishing control strategies around crystal form in the drug product. Although an ever-expanding range of techniques has been shown capable of producing novel solid forms, practically important ones are not always found in the timescales currently allowed for solid-form screening. Moreover, even relatively small pharmaceuticals by today’s standards continue to amaze us with the complexity of their crystal chemistry. Problems with crystal growth can frustrate attempts to identify new crystal forms generated during ‘polymorph’ screening. Overcoming these challenges reaps dividends, however, in advancing our understanding of how structure and dynamics in ‘real’ molecular crystals underpins the oftentimes bad behaviors that we observe. Here, we present case studies from our laboratory, where detailed experimental investigation and state-of-the-art use of computational chemistry have helped to unravel complexity encountered in crystallizing small-molecule drugs.

GROWTH AND PROCESSING OF ORIENTATION-PATTERNED SEMICONDUCTOR WAVEGUIDES FOR MID-IR FREQUENCY CONVERSION

Peter Schunemann[1], Daniel J. Magarrell[2], Paul R. Moffitt[2], Peter A. Ketteridge[2], Bradley R. Deshano[3], Rita Peterson[4]

[1]BAE Systems, Inc., UNITED STATES OF AMERICA, [2]BAE Systems, Inc., NH, UNITED STATES OF AMERICA, [3]Air Force Research Laboratory (AFRL/RYDH), OH, UNITED STATES OF AMERICA, [4]Air Force Research Laboratory, OH, UNITED STATES OF AMERICA

Orientation-patterned semiconductor waveguides are promising devices for mid-infrared frequency conversion, combining the high nonlinear coefficient of quasi-phase-matched (QPM) materials such as GaAs and GaP with the tight power confinement offered by the waveguide geometry. The ability to maintain high nonlinear gain along the entire optical path in such a waveguide is expected to result in orders of magnitude reduction in pump power requirements for optical parametric oscillation over bulk orientation-patterned gallium arsenide (OPGaAs) and phosphide (OPGaP) devices. A main obstacle to the utilization of efficient OPGaAs and OPGaP waveguide devices has been the relatively high losses of the waveguides produced to date. Here we describe the design, MBE growth, and fabrication of OPGaAs and OPGaP rib waveguide structures based on $Al_xGa_{1-x}As$ and $Al_xGa_{1-x}P$ cladding layers respectively. The best available dispersion data for GaAs, $AlxGa_{1-x}As$, GaP, and $Al_xGa_{1-x}P$ were used to calculate the phase- matching periods for the desired frequency interaction, which were in turn modified by the specifics of the structure, composition, and geometry of the waveguides. QPM OPGaAs and OPGaP template structures were grown by polar-on-nonpolar MBE using established techniques, followed by growth of cladding, core, cladding, and cap layers that were subsequently patterned and etched to produce rib structures. Details of the growth and processing parameters, waveguide structure, and preliminary loss data and frequency conversion results will be presented.

HETEROEPITAXY OF ORIENTATION-PATTERNED NONLINEAR OPTICAL MATERIALS

Vladimir Tassev[1], Shiva Vangala[2], Rita Peterson[1], Michael Snure[1]

[1]Air Force Research Laboratory, OH, UNITED STATES OF AMERICA, [2]Azimuth Corporation, OH, UNITED STATES OF AMERICA

Heteroepitaxy has many contributions to optics and electronics. In this work, heteroepitaxy is used for growth of GaP on GaAs substrates and orientation-patterned (OP) GaAs templates with periods designed for frequency conversion via quasi-phase-matching in the mid- and longwave IR. Due to the lattice mismatch, the layer initially grows homogeneously strained to fit the substrate lattice. After the initial pseudomorphous growth the strain is released via misfit dislocations, whose periodicity depends on the difference in the lattice constants. The sign of the mismatch and the direction of growth have a strong impact as well. Both the thickness of the pseudomorphous growth and periodicity of the misfit dislocations have been studied by SEM, AFM, multi-spot TEM imaging and other techniques as criteria for the applicability of heteroepitaxy in other material systems. Combining two growth techniques, we also grew by HVPE up to 300 µm thick GaP with smooth surface morphology and high crystalline quality on Si using a 250 nm thin MOCVD buffer layer for both electronic and optoelectronic applications. The growths on an OP template resulted in a number of device quality OPGaP grown on OPGaAs with thicknesses in the range of 180 – 300 µm. These are being evaluated in optical parametric oscillator and second harmonic generation devices to confirm the quality of the heteroepitaxially grown material for practical frequency conversion. Using TEM, transmission measurements, and other techniques we also analyzed the growths on OP-templates to verify our hypothesis that polarity alternation may improve material quality. The OP template preparation and the growth process were optimized for HVPE growth on the template directly after patterning, eliminating the customary MBE regrowth layer. The results from heteroepitaxy and homoepitaxy on similarly patterned surfaces are compared and contrasted with regard to material quality and suitability for quasi-phasematching applications.

TUNABLE3-5 AND 7-12 µM PICOSECOND OPTICAL PARAMETRIC AMPLIFIER BASED ON LIINSE2 MID-INFRARED CRYSTAL

Xutang Tao

State Key Laboratory of Crystal Materials, CHINA

Mid-infrared (MIR) nonlinear optical crystal of $LiInSe_2$ (LISe) was grown by modified Bridgman technique on (001) seed. A 7-12 µm widely tunable picosecond (ps) MIR optical parametric amplifier (OPA) based on LiISe2 crystal was demonstrated for the first time. The MIR OPA was pumped by a 30 ps 1064 nm Nd:YAG laser and injected by a b-barium borate (BBO)-based widely tunable near-infrared seed. The idler operating at 7.5 µm with the highest pulse energy of 170 µJ was obtained under a pump energy of 14 mJ. The corresponding energy conversion efficiency is ~1.21% and the photon conversion efficiency is 8.6%. The tunable range of LISe-OPA was from 7 µm to 12 µm for the idler. The output energies were measured to be ~97 µJ at 7 µm and ~21 µJ at 12 µm, corresponding to the peak power of ~3.2 MW and ~0.69 MW, respectively.

GROWTH OF CHROMIUM DOPED FORSTERITE CR:MG$_2$SIO$_4$ LASER CRYSTALS FROM NON-STOICHIOMETRIC MELTS AND THE PROLONGED HIGH-TEMPERATURE OXIDIZING ANNEALING OF THE CRYSTALS AS THE TOOLS FOR CHANGE THE OXIDATION STATES OF CHROMIUM IN THE CRYSTALS

Viktoriia V. Sanina[1], Kirill A. Subbotin[2], Denis A. Lis[1], Evgenii V. Zharikov[1]

[1]A.M.Prokhorov General Physics Institute of Russian Academy of Sciences, RUSSIAN FEDERATION, [2]A.M.Prokhorov General Physics Institute Russian Academy of Sciences, RUSSIAN FEDERATION

Tetravalent chromium doped forsterite Cr^{4+}:Mg_2SiO_4 (Cr-Fo) single crystals are used as the active media of tunable and femtosecond solid-state lasers. Such lasers have great potential of wide application in various fields, including telecommunications, medicine, LIDARs, spectroscopy, photochemistry, etc. Some important drawbacks of Cr-Fo as laser crystal are caused by the presence of chromium in parasitic oxidation states in the crystal, e.g., Cr^{2+}, and Cr^{3+} ions. Our study was aimed to test the possibility to diminish the contents of octahedrally coordinated Cr^{2+}, and Cr^{3+} in the crystals, and to raise the contents of the useful tetrahedrally coordinated Cr^{4+} by usage of non-stoichiometric melts for the crystals growth, and by impact of a prolonged high-temperature oxidizing annealing of the as-grown crystals. We have successfully grown by Czochralski high-quality Cr-Fo single crystals from the melts containing 0.25 – 2 wt. % excess of MgO. Such excess should promote the formation of vacancies in Si^{4+} sub-lattice. This, in turn, should promote Cr^{4+} introduction into the crystal, and inhibit Cr^{2+}, and Cr^{3+} introduction. The prolonged high-temperature oxidizing annealing of Cr^{4+}:Mg_2SiO_4 should lead to the oxidation of Cr^{2+}, and Cr^{3+} ions for Cr^{4+} and, possibly, for more oxidized chromium ions. The dependence of Cr^{4+}, Cr^{2+}, and Cr^{3+} concentrations in the studied crystals on the melt composition is given in the presentation, as well as the evolution dynamics of Cr^{4+}, Cr^{2+}, and Cr^{3+} concentrations in the Cr-Fo crystals, during their prolonged high-temperature oxidizing annealing. The concentrations of each chromium oxidation state were determined from the polarized optical absorption spectra of the crystals.

GROWTH AND MAGNETIC PROPERTIES OF PRCO2 SINGLE CRYSTALS

Yong Liu, Arjun Pathak, Yaroslav Mudryk, Qisheng Lin, Vitalij Pecharsky, Thomas Lograsso

Ames Laboratory, Ames, IA/United States of America

$PrCo_2$ single crystals have been grown from flux starting from $Pr_{0.44}Co_{0.56}$ that was synthesized by arc melting of a stoichiometric mixtures of the elements. The $Pr_{0.44}Co_{0.56}$ ingot was loaded in a Born Nitride (BN) crucible and sealed inside a quartz tube under vacuum. The quartz ampoule was heated up to 1203 K, and then slowly cooled down to 923 K at a rate of 2 K/h. The obtained crystals have octahedral shapes and are of cubic Laves phase with C15 type structure revealed by single crystal diffraction. Magnetic susceptibility data show the Curie temperature T_C= 46.7 K. Following the main ferrimagnetic transition observed at T_C, magnetization measured in magnetic fields below ~0.5 T exhibits additional low-temperature anomalies. Our results suggest that a detailed study of the magnetic structure of $PrCo_2$ should be performed by neutron scattering measurement

GROWTH, MICROSTRUCTURE AND MECHANICAL PROPERTIES OF IRIDIUM FIBER CRYSTAL BY ALLOY-MICRO-PULLING-DOWN METHOD

Yuui Yokota[1], Takayuki Nihei[2], Yuji Ohashi[1], Shunsuke Kurosawa[3], Kei Kamada[4], Akira Yoshikawa[1]

[1]New Industry Creation Hatchery Center, Tohoku University, JAPAN, [2]Institute for Materials Research, Tohoku University, JAPAN, [3]Faculty of Science, Yamagata University, JAPAN, [4]C&A Corporation, JAPAN

Iridium (Ir) and Ir alloys products with various configurations have been used in wide fields due to the high melting point, high chemical stability and high resistance to oxidation. However, the Ir and Ir alloys are difficult workability and the prices of products increases by increasing the cost of forming processes. Therefore, we have developed the growth method of shape-controlled metal and alloy fibers from the melt by the micro-pulling-down (μ-PD) method using a developed ceramics crucible with high durability at the melting points of the Ir (~2447°C). We named it alloy-micro-pulling-down (A-μ-PD) method. In this study, Ir fiber was grown by the A-μ-PD method, and the microstructure and mechanical properties were investigated. Ir pellets were used as a starting material and they were set in a ZrO_2 crucibles. The crucible was placed at the center of the radio-frequency induction coil in a chamber and the crucible was surrounded by the ZrO_2 insulators. A commercial Ir wire of 0.90~0.95 mm in diameter was set below the hole of the crucible as a seed. The pellets were heated directly up to the melting point by the RF induction coil. After the pellets were completely melted, the melt in the crucible was pulled down using the commercial Ir wire through the hole of the crucible. Grown fibers were cooled to room temperature for 2 hours after the growth was finished. The as-grown Ir fiber was cut and polished for the observation of the internal texture and measurements using X-ray. Surfaces of the polished specimens were treated by the Cross section Polisher (CP) with Ar+ ion to observe the internal structures. Local structures on the polished and the CP treated surfaces of the Ir fibers were observed by the scanning electron microscope (SEM). X-ray diffraction (XRD) pattern and Electron Backscatter Diffraction (EBSD) of the fiber was measured on the polished surface perpendicular to the growth direction. We grew the Ir fibers from the melt using the ZrO_2 crucible and their fibers with 1 mm diameter and more than 10 m length could be obtained. The domain structures of the grown fibers were observed by the SEM and the fibers were composed of some domains stretched along to the growth direction. All diffraction peaks in the XRD pattern could be identified by the face-centered cubic structure of the Ir. The mechanical properties of the Ir fiber will be reported.

GROWTH AND INTERNAL STRUCTURE OF CO-CR-MO ALLOY FIBER CRYSTALS BY ALLOY-MICRO-PULLING-DOWN METHOD

Takayuki Nihei[1], Yuui Yokota[2], Akihiro Yamaji[1], Yuji Ohashi[2], Shunsuke Kurosawa[3], Kei Kamada[2], Akira Yoshikawa[2]

[1]Institute for Materials Research, Tohoku University, JAPAN, [2]NICHe, Tohoku University, JAPAN, [3]Department of Physics, Yamagata University, JAPAN

Co-Cr-Mo (CCM) alloys shows high strength, high wear resistance and corrosion resistance, and they have been used as a biomaterial for human body such as spinal-instrumentation surgery rods, artificial hip joint bearings and dental implants. CCM alloys are also expected to apply for the stent and guide wire. However, it is difficult to process them into complicated shapes due to the low ductility of e-hcp phase in the CCM alloys. Therefore, it is necessary that a noble process is used to fabricate the CCM alloys with complicated shapes easily. In our previous studies, the alloy-micro-pulling-down (A-µ-PD) method has been developed to grow alloys with specific shape from the melt directly, and fiber crystals of platinum-group metals could be grown by the A-µ-PD method. In this study, we tried to grow the CCM alloy fibers from the melt by the A-m-PD method and investigated the internal structure. Co, Cr and Mo powders (3N) were mixed as a nominal composition of Co-28Cr-6Mo (mass%) and the mixed powder was melted by the arc melting furnace. The CCM ingot was set in ZrO_2 or Al_2O_3 crucibles with a f1 mm hole at the bottom and it was heated up to the melting point (~1400°C) by high frequency induction heating. After it was completely melted, the melt was pulled down from the hole at 0.5 mm/min pulling rate using an Ir wire as a seed. Crystal growth was performed under Ar + 3%H_2 to prevent from the oxidation of the ingot. At first, we grew the CCM fiber using the ZrO_2 crucible. However, the ZrO_2 crucible was broken just after the ingot was melted. In the result, the melt leaked to the outside of the crucible. The color of the crucible changed to white from light yellow after the growth and it suggests that the ZrO_2 was reduced during the growth and the crucible became fragile. In addition, Cr_2O_3 volatiles were deposited on the side of the crucible due to the oxidization of Cr in the ingot. Therefore, we used the dense Al_2O_3 crucible and carbon insulator to prevent from braking and oxidization. In the result, a CCM alloy fiber crystal could be grown without crucible braking and quantity of the volatiles decreased during crystal growth. We will report details of the crystal growth and the internal structure.

GROWTH AND PIEZOELECTRIC PROPERTIES OF CA3TA(GA1-XSCX)3SI2O14 BULK SINGLE CRYSTALS

Yu Igarashi[1], Yuui Yokota[2], Yuji Ohashi[2], Kenji Inoue[3], Akihiro Yamaji[1], Yasuhiro Shoji[1], Kei Kamada[2], Shunsuke Kurosawa[2], Akira Yoshikawa[1]

[1]Institute for Materials Research, Tohoku University, JAPAN, [2]New Industry Creation Hatchery Center, Tohoku University, JAPAN, [3]Piezo Studio Inc., JAPAN

$Ca_3TaGa_3Si_2O_{14}$ [CTGS] single crystals have been investigated as a piezoelectric material for compact resonator with low power consumption and high stability of temperature coefficient of frequency (TCF) comparable to the conventional quartz. In our previous studies, we have grown Al doped $Ca_3TaGa_3Si_2O_{14}$, $Ca_3Ta(Ga_{1-x}Al_x)_3Si_2O_{14}$ [CTGAS] single crystals, and the e_{11} systematically increased and $|e_{14}|$ decreased with an increase of Al substitution. The results are considered to be attributable to the substitution of Al ion with smaller ionic radius than Ga ion. Therefore, in this study, we grew Sc doped CTGS, $Ca_3Ta(Ga_{1-x}Sc_x)Si_2O_{14}$ [CTGSS] single crystals to expect effects opposite to the Al substitution on the piezoelectric properties by the substitution of Sc ion with larger ionic radius than Ga ion. If the $|e_{14}|$ increases by the Sc substitution, novel piezoelectric devices can be realized using propagation modes and suitable cut angles for the $|e_{14}|$. $CaCO_3$, Ta_2O_5, β-Ga_2O_3, Sc_2O_3, SiO_2 powders (4N) were mixed as nominal compositions of $Ca_3Ta(Ga_{1-x}Sc_x)_3Si_2O_{14}$ [$x = 0$, 0.1, 0.2, 0.3 and 0.4] and mixed powders were sintered at 1200°C in air. CTGSS fiber crystals were grown by the micro-pulling-down [m-PD] method using an Ir crucible and <010> oriented CTGS seed crystal in $Ar+2\%O_2$. In addition, 1 inch CTGSS bulk single crystals with $x = 0.1$ were grown by the Czochralski [Cz] method using a Ir crucible and <010> oriented CTGS seed crystal in N_2 to evaluate the piezoelectric properties precisely. X-ray diffraction patterns of the CTGSS crystals grown by the m-PD method showed that the crystals with $x = 0$ and 0.1 were single phase of langasite-type structure without secondary phase while the crystals with $x = 0.2$, 0.3 and 0.4 included secondary phases in addition to the langasite-type phase. The lattice constants, *a*- and *c*-axes lengths, of langasite-type phase were systematically increased with an increase of x. The increase of the lattice constants is attributable to the Sc ions substitution for the Ga site on the CTGS. The piezoelectric properties of CTGSS crystal grown by the m-PD method were evaluated by the resonance and anti-resonance method, and the CTGSS crystal with $x = 0.1$ showed larger e_{11}^T/e_0, and smaller k_{12} and d_{11} than the CTGS. The effects on the piezoelectric properties by the Sc substitution were opposite to the effects by Al substitution. Details of crystal growth by the Cz method and the piezoelectric properties will be reported.

STUDIES ON GROWTH ASPECTS, PROPERTIES AND EFFECTS OF H^+ ION IMPLANTATION ON ORGANIC SINGLE CRYSTAL: L-HISTIDINIUM SEMISUCCINATE (LHS)

H Arul[1], D Rajan Babu[2], R Ezhil Vizhi[2]

[1]Department of Science and Humanities, Kumaraguru College of Technology (Autonomous),, INDIA, [2]Advanced Materials Research Centre, Department of Physics, School of Advanced Sciences, VIT University, INDIA

Organic crystals have gained a prominent role in the field of nonlinear optics due to their inherent properties, offering an opportunity for theoretical modeling coupled with synthetic flexibility to design and produce novel materials [1]. The low temperature solution growth requires knowledge of essential nucleation parameters to optimize the growth condition and to improve the quality and size of the crystal. An attempt has been made to study the growth kinetics, physiochemical properties and ion implantation effects on organic L-Histidinium semisuccinate single crystal. Growth parameters such as metastable zonewidth and induction period were determined using polythermal and isothermal methods respectively. Single crystal XRD confirmed that the crystal belongs to the orthorhombic system with the non centrosymmetric space group $P2_12_12_1$. Its optical, nonlinear optical, thermal and electrical properties were studied in an extensive manner. Bulk Single crystal of L-Histidinium semisuccinate was synthesized and subsequently grown from solution by slow cooling technique. The Presence of protonated amine group was confirmed by FT-IR spectrum. UV-Vis-NIR spectroscopic study shows that the crystal is possessing transmission in the visible region with the cut-off wavelength of 230 nm. Tauc's plot was used to compute the optical band and it was estimated to be 4.76 eV. Photoluminescence spectrum revealed the material is capable of emitting violet emission at 432 nm. Refractive index was determined as 1.3705 (Fig. 1) using Metricon Prism Coupler. The second harmonic generation efficiency was estimated using Kurtz-Perry test and it was found to be 1.4 times greater than standard KDP. Thermal analysis determined that the material is stable up to 217˚C. Dielectric constant and dielectric loss was calculated and plotted as a function of frequencies for different temperatures. Low energy proton ion implantation was carried out on the grown crystal of LHS and the modifications in absorption edge as well as the refractive indices were discussed. Fig. 1 Refractive index spectrum of LHS crystal [1] P.N. Prasad, D.J. Williams, Introduction to nonlinear optical effects in organic molecules and polymers, Wiley, New York, 1991. **Key Words:** Bulk growth, Refractive index, Ion implantation

SYNTHESIS, GROWTH AND CHARACTERIZATION OF METAL ORGANIC SODIUM HYDROGEN OXALATE MONOHYDRATE SINGLE CRYSTAL

D.S Ajisha[1], R Ezhil Vizhi[1], D Rajan Babu[2], **H Arul**[3]

[1]VIT University, INDIA, [2]Advanced Materials Research Centre, Department of Physics, School of Advanced Sciences, VIT University, INDIA, [3]Department of Science and Humanities, Kumaraguru College of Technology (Autonomous),, INDIA

Nonlinear materials attracted researcher’s interest due to their wide range of potential application in the field of optical and electronic application. Nonlinear materials with large second order non linearity and transparency in the visible and ultraviolet regions are used for optical device applications. Among various nonlinear materials metal organic compounds attracted very much because of their capability of combining the advantages of both organic and inorganic compounds such as high nonlinearity and physical and thermal properties. In the case of metal organic compound, the organic ligand is usually more dominant for NLO effect, since the metal compounds have high transparency in the visible region. Many of the oxalate compounds have good NLO properties. The properties of these compounds can be enhanced by combining these compounds with other metal compounds.A metal organic compound of sodium hydrogen oxalate monohydrate single crystal was grown by slow evaporation method. The grown crystal was characterized by using single and powder X-ray diffraction. The XRD studies show that this crystal belongs to triclinic crystal system. The various functional groups present in the compound were analyzed by using FTIR studies. The optical behavior of the compound has been observed by using UV-Vis absorption spectral analysis which shows that the low cut off wavelength lies at 309.7nm.Thermal stability of the compound was analyzed by TG/DTA analysis. The mechanical strength of the compound was found by using Vickers micro hardness measurement. The second harmonic efficiency of the compound was determined by Kurtz and Perry method.

GROWTH OF DETECTOR GRADE CADMIUM ZINC TELLURIDE VIA IMPLEMENTATION OF CRUCIBLE ROTATION IN MODIFIED VERTICAL BRIDGMAN METHOD

Jedidiah J. Mccoy[1], Saketh Kakkireni[1], Santosh K. Swain[1], Mia S. Divecha[2], Jeffrey J. Derby[2], Kelvin G. Lynn[1]

[1]Washington State University, WA, UNITED STATES OF AMERICA, [2]University of Minnesota, MN, UNITED STATES OF AMERICA

Cadmium Zinc Telluride (CZT) is a promising material for high efficiency, high spatial and temporal resolution gamma ray spectrometers in homeland security application. However, the presence of second phase (SP) defects poses a significant challenge by deteriorating device performance through trapping and scattering of charge carriers. Additionally, Zn segregation and low single crystal yields are inherent to melt based growth of CZT which can further hinder detector yield and performance. To address these issues, a modified growth system has been developed in which the accelerated crucible rotation (ACRT) method is implemented in vertical Bridgman (VB) melt growth. During growth, the crucible is rotated at various speeds to induce fluid flow patterns which homogenize melt composition. For a given rotation scheme (RS), crucible acceleration, deceleration, maximum velocity, and hold times at velocity are distinguishable parameters. Adjustable system variables included RS, growth composition, and growth temperature profile. CZT growth composition was varied between 0.25 and 15 weight percent of excess tellurium. Growth rates were varied between 0.5 and 2.0 mm/hr. A study of nucleation control in seeded vs. self-seeded growth was also conducted. The system was implemented with and without pyrolytic boron nitride (pBN) crucibles. Analysis of SP content within grown ingots revealed ACRT capable of reproducibly minimizing SP defects, shifting both volume and density peaks to smaller diameters. Highly uniform Zn distributions were achieved in asymmetric RS where velocity hold times were zero. Flat to convex solid/liquid interface shapes were achieved within pBN crucibles. Large axial wafers approaching single crystal yields of 100% have been obtained. Fabrication of planar detectors yielded favorable detector properties with some growth composition dependent variation. VB growth of CZT ingots via ACRT under excess Te within pBN crucibles represents a successful technique for large scale production of homogeneous and uniform detector grade CZT single crystals with low SP volumes.

MELT GROWTH OF ZINC ALUMINATE SPINEL SINGLE CRYSTAL BY THE MICRO-PULLING DOWN METHOD UNDER ATMOSPHERIC PRESSURE

Akria Yoshikawa[1], Kei Kamada[2], Yasuhiro Shoji[3], Vladimir V. Kochurikhin[4], Shunsuke Kurosawa[5], Akihiro Yamaji[6], Yuji Ohashi[7], Yuui Yokota[7]

[1]IMR, Tohoku Universiry, JAPAN, [2]C&A corporation, JAPAN, [3]Institute for Materials Research, Tohoku University, JAPAN, [4]General Physics Institute, Russian Academy of Sciences, RUSSIAN FEDERATION, [5]Department of Physics, Yamagata University, JAPAN, [6]Institute for Materials Research, JAPAN, [7]New Industry Creation Hatchery Center, Tohoku University, JAPAN

In recent years, new solid-state laser materials working in the visible region are needed for ultrafast optical devices in science as tunable solid-state lasers, and technology as matrix for fiber-optic temperature sensors or a substrate for microelectronics. The zinc aluminium spinel $ZnAl_2O_4$ is attractive oxide material with a combination of desirable properties of high melting point of around 2000ºC, high strength, high hardness, resistance to corrosion, and low electrical losses.[1] Photoluminescence properties of doped $ZnAl_2O_4$ powders were widely reported such as Cr^{3+} , Mn^{2+} and RE^{3+} luminescence; doping with Eu^{3+}, Er^{3+}/Yb^{3+} . $ZnAl_2O_4$ can be also used as UV-transparent conductor, sensor, and dielectric materials. Bulk single crystal growth of $ZnAl_2O_4$ from the melt is difficult because of high vapour pressure of zinc oxide and lower temperature synthesis such flux, sol-gel method and solid state reaction were reported. Recently Goldstein [2] reported a polycrystalline transparent $ZnAl_2O_4$ ceramics sintered with nano-$ZnAl_2O_4$ powders synthesized by the hydrothermal technique. In this study, melt growth of $ZnAl_2O_4$ under ordinary pressure was performed by the micro-pulling down (m-PD) method. The $ZnAl_2O_4$ spinel single crystal with 4 mm diameter could be successfully grown by the m-PD method by optimization of starting melt composition considering with Zinc oxide evaporation. The 10 minute growth under ordinary pressure permitted the melt growth of $ZnAl_2O_4$ even high vapor pressure of ZnO(1.06 atm at 2248K). The grown crystal showed 234 arcsec of line width of rocking curve. The 1mm thick sample showed the transmittance of 69.5% at 550 nm. These results evidenced potential of the the μ-PD grown $ZnAl_2O_4$ single crystal for application which require oriented bulk crystal.

Figure 1. Photographs of the grown crystals at Molar ratio of ZnO: a-$AlO_{3/2}$ = 2.5:2, and cations distribution along the growth direction measured by the EDX [1]S. Sampath and J. F. Cordaro, J. Am. Ceram. Soc., 81 [3] (1998) 649–54 . [2]A. Goldstein, Y. Yeshurun, M. Vulfson, H. Kravits. J Am Ceram Soc 95 (2012)879–82.

REVISITING CAPILLARITY AND ITS IMPACT ON SHAPE EVOLUTION DURING CZOCHRALSKI CRYSTAL GROWTH

Simon Brandon, Oleg Weinstein

Technion, ISRAEL

Modeling Czochralski (CZ) crystal growth has been discussed in the literature for more than three decades. Although these modeling efforts often (but not always) include capillarity in the analysis, they usually do not provide detailed explanations for the impact of capillarity *combined with heat transfer* on shape evolution. In a recent study [1] of oxide crystal growth via the CZ technique, we observed a particular impact of the growth angle value(a) on crystal shape evolution both in anisotropic and isotropic systems. Specifically, in this system (which is not controlled), the rate of change of crystal diameter was shown to be relatively larger in systems exhibiting relatively smaller growth angle values where in the case of anisotropic materials this was seen to be a local effect. In this contribution we present an analysis of this problem, relying in part on a simplified model of shape evolution which provides partial explanations for the phenomena observed in the full scale model described in [1]. [1] O. Weinstein, W. Miller and S. Brandon, ``Modeling anisotropic shape evolution during Czochralski growth of oxide single crystals'' (to be submitted to the Journal of Crystal Growth). (a) Here the growth angle is the angle between the meniscus (melt/gas interface) and the crystal/gas surface (which is not necessarily vertical) as typically defined in the literature.

CRYSTAL GROWTH AND CHARACTERIZATION OF UNDOPED AND DY-DOPED TLPB2BR5 FOR NUCLEAR DETECTION AND IR LASERS

U. Hommerich[1], Eiei Brown[1], Daniel Hart[1], M. Swain[1], H Chen[2], S B. Trivedi[2]

[1]Hampton University, UNITED STATES OF AMERICA, [2]Brimrose Technology Corporation, MD, UNITED STATES OF AMERICA

We report first results of the crystal growth and characterization of undoped and Dy^{3+} doped thallium lead bromide ($TlPb_2Br_5$) for applications in nuclear radiation detection and IR solid-state lasers. The development of room temperature operated nuclear detection devices continues to be of great current interest for applications in homeland security, nuclear medicine imaging, and scientific research. Compared to scintillation based detector materials, semiconductors can directly convert high energy radiation into electron-hole pairs and provide advantages in energy resolution, sensitivity, and compactness. TlBr has received significant attention in recent years for high-energy radiation detection, but it is soft, moisture sensitive, and suffers from polarization effects which degrade detector performance over a long time period. In this work, we investigated the ternary lead halide crystal $TlPb_2Br_5$ (TPB) as a potential room temperature nuclear detection material with increased mechanical stability, no moisture sensitivity, and high energy resolution. The undoped TPB crystal was grown using purified starting materials of TlBr and $PbBr_2$. Following multiple re-crystallization steps, TPB was grown using a two-zone vertical Bridgman station. Furthermore, a Dy^{3+} doped TPB sample was prepared by adding 1-2% of $DyBr_3$ during synthesis. Initial gamma ray detection experiment using undoped TPB revealed energy resolutions of ~1% for Cs-137 and ~2% for Am-241 under non-optimized conditions. The Dy: TPB samples was evaluated for possible mid-IR laser applications and exhibited efficient emission in the 3-5 µm region using a 1.3 µm diode laser as pump source. This work was supported by the National Science Foundation under grants 1649150 and 1137747.

ZONE-REFINEMENT PURIFICATION, FILTERING METHOD AND GROWTH DIFFICULTIES OF EUROPIUM DOPED STRONTIUM IODIDE (SRI_2:EU^{2+}) SCINTILLATOR SINGLE CRYSTAL FOR RADIATION DETECTION APPLICATIONS

A. Raja[1], D. Joseph Daniel[2], P. Ramasamy[1], S. G. Singh[3], S. Sen[3], S. C. Gadkari[3]

[1]SSN College of Engineering, INDIA, [2]Kyungpook National University, KOREA, REPUBLIC OF, [3]Bhabha Atomic Research Centre, INDIA

The parent compound of Strontium Iodide (SrI_2) and Europium Iodide (EuI_2) was purified by homemade Zone-refinement experimental set-up [1]. Insoluble impurities were filtered by specially designed dual chamber quartz ampoule with frit filter method. Europium doped strontium iodide (SrI_2:Eu^{2+}) single crystal was grown by Modified vertical Bridgman – Stockbarger technique [2]. Thermal properties of the SrI_2:Eu^{2+} crystal were investigated by thermogravimetry / differential thermal analysis (TG/DTA). Photoluminescence (PL) excitation and emission (PLE) was measured for Eu^{2+} doped SrI_2 crystal. The sharp emission was recorded at 432 nm. X-ray excited radioluminescence was recorded and the emission was at 435 nm. Scintillation properties of the SrI_2:Eu^{2+} crystal were checked by the gamma ray spectrometer inbuilt ^{137}Cs gamma source. the energy resolution of the grown crystal was 5.1% at 662 KeV. Scintillation decay profile was also analyzed. The scintillation decay time of Eu^{2+} ion was calculated to be 1.09 μs for SrI_2:Eu^{2+} single crystal.

PALLADIUM OXIDE THIN FILMS FOR OXIDIZING GASES DETECTION

Alexander M. Samoylov[1], Valentin M. Ievlev[2], Stanislav V. Ryabtsev[1], Alexey V. Shaposhnik[3], Alexey A. Sinelnikov[1]

[1]Voronezh State University, RUSSIAN FEDERATION, [2]Moscow State University, RUSSIAN FEDERATION, [3]Voronezh State Agricultural University, RUSSIAN FEDERATION

Because of health problems and noxious effects on vegetation caused by atmospheric pollution in industrialized countries, air quality control is becoming of great interest. Three out of six common air pollutants (also called as “criteria pollutants”) are oxidizing gases: nitrogen oxides, low level ozone (or tropospheric ozone), and sulfur dioxide [1]. The monitoring of ozone and nitrogen dioxide concentration in the atmosphere is a critical task for human health protection. For this reason recently various types of binary, ternary and quaternary metal-oxide semiconductors have widely been used for oxidizing gases detection [2]. Palladium oxide thin films have been presented as perspective materials for detection of oxidizing gases. PdO films were prepared by thermal oxidation of previously formed Pd layers on different substrates: SiO_2/Si (100), Si (100), optical quality quartz, and KCl (100) with buffer layer of amorphous carbon. By X-ray analysis, reflection high-energy electron diffraction, and high resolution transmission electron microscopy investigations it has been established that homogenous polycrystalline PdO films (thickness was about 5 – 40 nm) were formed by oxidation at dry oxygen at temperatures T = 770 - 870 K (Fig. 1). The experimental results of X-ray analysis and transmission electron microscopy have shown that the increase in oxidation temperature led to uniformity and enlargement of crystalline grains in homogeneous PdO films. The results of Seebeck coefficient and Hall effect measurements have shown that homogeneous PdO films prepared by oxidation at T = 870 - 1017 K had p-type conductivity. It has been established that the energy band gap values increased monotonically from ΔE_g = 2.15 eV to 2.3 eV for PdO films with *p*-type conductivity oxidized at T_{an} = 670 K and 1070 K, respectively. At ozone detection PdO films fabricated on polished poly-Al_2O_3 have shown high values of sensitivity, signal stability, and reproducibility of sensor response (Fig. 2). For fabrication of gas sensors PdO thin films have some advantages in comparison with other materials because PdO films have shown good values of sensor functional parameters, and their synthesis procedure is rather simple and is compatible with planar processes of the microelectronic industry also. References [1] Estimating Mortality Risk Reduction and Economic Benefits from Controlling Ozone Air Pollution. Report of the US National Academies of Sciences. The National Academies Press, Washington, 2008. [2] A.V. Marikutsa, M.N. Rumyantseva, A.M. Gaskov, A.M. Samoylov, Inorganic Materials, 51 (2015) 1329–1347.

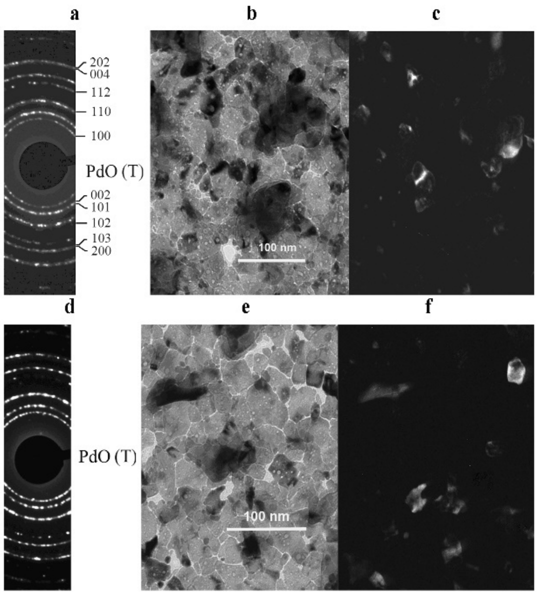


Fig. 1. TEM micro diffraction (*a*, *d*), bright-field image (*b*, *e*), and dark-field image (*c*, *f*) of PdO film (thickness ~ 25 nm) prepared by oxidation at dry oxygen: *a*, *b*, *c* – T_{an} = 770 K (500 °C); *d*, *e*, *f* – T_{an} = 870 K (600 °C).

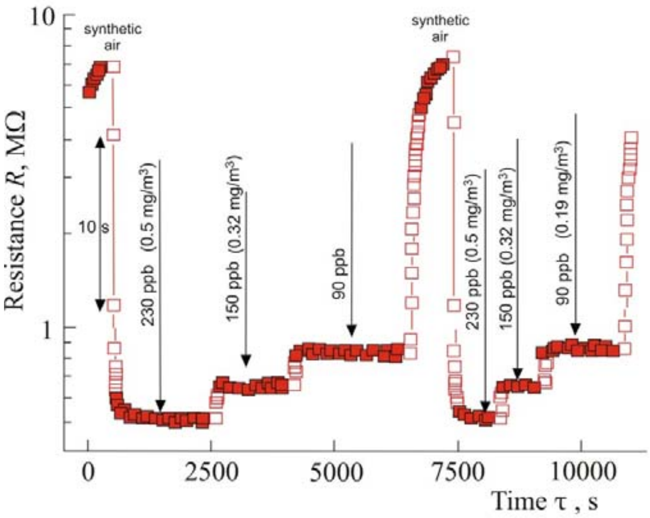


Fig. 2. Time dependence of PdO film (thickness ~ 30 nm) sensor resistance at different ozone concentrations (operating temperature T_d = 490 K.

BORON CODOPING OF CZOCHRALSKI GROWN LUTETIUM ALUMINUM GARNET AND THE EFFECT ON SCINTILLATION PROPERTIES

Camera Foster[1], Merry Koschan[2], Chuck Melcher[1], Yuntao Wu[1]

[1]University of Tennessee, UNITED STATES OF AMERICA, [2]Scintillation Materials Research Center, TN, UNITED STATES OF AMERICA

Lutetium aluminum garnet (LuAG), $Lu_3Al_5O_{12}$, is a commercially available scintillator for use in high energy gamma and x-ray detection because of its high density and effective atomic number. Because LuAG is not an efficient intrinsic scintillator, dopants such as cerium or praseodymium are utilized to enhance scintillation. Cerium doping provides bright, fast scintillation attributed to the characteristic 4f-5d transition of the cerium activation center. Along with doping with activators such as cerium, codoping can be utilized to modify not only the scintillation properties of the crystal but also its mechanical properties and behavior during the growth process, such as growth stability and surface tension of the melt. In particular, boron has been shown to improve the light yield and energy resolution of other garnet scintillators, like GGAG and YAG, when incorporated into the lattice via codoping. In this study, single crystals of LuAG: 0.2 at% Ce codoped with varying concentrations of boron were grown via the Czochralski method at a rate of 1.2 mm/h. Results will show the effect boron codoping has on the scintillation properties of LuAG:Ce, including light yield, energy resolution, and decay time as well as the effect boron codoping has on the CZ growth process.

CRYSTAL GROWTH OF KCAI3:EU AND KSR2I5:EU SCINTILLATORS USING THE MICRO-PULLING-DOWN METHOD

Mariya Zhuravleva[1], Robert Kral[2], Matthew Loyd[1], Chuck Melcher[3], Shunsuke Kurosawa[4], Akira Yoshikawa[5]

[1]Department of Materials Science and Engineering, University of Tennessee, TN, UNITED STATES OF AMERICA, [2]Institute of Physics of the Czech Academy of Sciences, CZECH REPUBLIC, [3]Scintillation Materials Research Center, University of Tennessee, TN, UNITED STATES OF AMERICA, [4]Faculty of Science, Yamagata University, JAPAN, [5]Institute for Materials Research, Tohoku University, JAPAN

Our group at the University of Tennessee has recently developed new ternary halide scintillators $KCaI_3$:Eu and KSr_2I_5:Eu that are very competitive with SrI_2:Eu and $CeBr_3$ for gamma-ray spectroscopy applications. Single crystals up to 2” in diameter produced via the vertical Bridgman method have high scintillation light output of ~90,000 ph/MeV and energy resolution of <4% at 662 keV. Compositional non-uniformity of the crystals caused by axial segregation of the Eu dopant (in case of $KCaI_3$) and by incomplete mixing of the binary starting materials in the melt can be responsible for poor scintillation non-proportionality, which is a critical characteristic that affects energy resolution. The micro-pulling-down (m-PD) method developed at Tohoku University allows the growth of high quality crystals of hygroscopic scintillators with excellent compositional homogeneity. Due to the unique geometry of the solid-liquid interface and the fast pulling rates commonly employed by the m-PD method, Eu dopant segregation is expected to be insignificant as opposed to conventional directional solidification such as the Bridgman method. The objective of this collaborative work is to demonstrate crystal growth of the ternary halide scintillators using the m-PD method and to improve compositional uniformity by exploring faster growth rates. Using radiofrequency heating, carbon crucibles and Pt wire as a seed, we grew 2 mm dia and ~15 mm long cylindrical crystals of $KCaI_3$:Eu and KSr_2I_5:Eu at pulling rates up to 0.09 mm/min, which is ~3-5 times faster than the typical growth rates used for such materials in the Bridgman method. Polycrystalline ingots with compositions of $KCa_{0.97}Eu_{0.03}I_3$ and $KSr_{1.92}Eu_{0.08}I_5$:Eu were pre-synthesized form stoichiometric mixtures of the binary iodides and used as starting materials for growth experiments. The grown crystals had good optical transparency. Scintillation light output, decay time, and non-proportionality were measured and the results were compared to the crystals of the same compositions grown via the Bridgman method.

SPATIAL DISTRIBUTION OF EU IN BABRCL:EU SINGLE CRYSTAL ASSESSED BY LASER INDUCTED BREAKDOWN SPECTROSCOPY (LIBS)

Tetiana Shalapska, Didier Perrodin, Jhanis Gonzalez, Dayana Oropeza, Xianglei Mao, Vassilia Zobra, Gregory A. Bizarri, Edith Bourret-Courchesne

Lawrence Berkeley National Laboratory, UNITED STATES OF AMERICA

Barium-based mixed halides activated with Eu, $BaX_{1-x}Y_x$ (X and Y = Cl, Br or I) is class of scintillator materials that are of interest to the scintillator community due to their excellent performance. For homogeneous scintillation performance, uniformity of Eu in the host crystal is critical, affecting both the light output and the energy resolution. We report on the use of LIBS (Laser Induced Breakdown Spectroscopy) to acquire quantitative data on the spatial distribution of Eu at the microscopic scale in a crystal of BaBrCl:Eu (5%Eu). The crystal was grown via vertical Bridgman–Stockbarger technique in a glassy carbon crucible sealed in an

evacuated quartz tube to prevent oxidation and hydration [1]. Figure 1. LIBS 2D and 3D maps for BaBrCl:Eu (2x5mm) LIBS for chemical analysis requires minimal sample preparation, provides high spatial resolution (single digit micrometers to tens of nanometers, for lateral and depth respectively), single digit ppm limit of detection for most elements, and delivers fast measuring time (few seconds per location) compared to other elemental analysis techniques [2]. 2D chemical maps of the elements of interest were acquired over a 2x5 mm area (10x25 locations) with a lateral resolution of 100 µm. Depth-resolved elemental mapping with and axial resolution of 600 nm was enabled by using multiple laser pulses for every lateral sampling location. The impact of Eu spatial distribution will be discussed. [1] E. D. Bourret-Courchesne G.A. Bizarri, R. Borade, G. Gaudian E. Samulon, S. DerenzoJ. of Crystal Growth 352 (2012) 78-83. [2] V. Zorba, J. J. Gonzalez, G. C. Y. Chan, X. Mao and R. E. Russo, in Encyclopedia of Spectroscopy and Spectrometry, Elsevier, 2017, pp. 571–578.

CZOCHRALSKI GROWTH AND SCINTILLATION PROPERTIES OF CE DOPED GADOLINIUM SCANDIUM ALUMINIUM GARNET SINGLE CRYSTALS

Kei Kamada[1], Vladimir V. Kochurikhin[2], Shunsuke Kurosawa[3], Yuji Ohashi[4], Yuui Yokota[5], Akira Yoshikawa[6]

[1]C&A corporation, JAPAN, [2]General Physics Institute, Russian Academy of Sciences, RUSSIAN FEDERATION, [3]Faculty of Science, Yamagata University, JAPAN, [4]NICHe, Tohoku University, JAPAN, [5]New Industry Creation Hatchery Center, Tohoku University, JAPAN, [6]Institute for Materials Research, Tohoku University, JAPAN

Oxide materials based on garnet structure single crystals are promising candidates for scintillator applications because of well mastered technology developed for laser hosts and other applications, optical transparency and easy doping by rare-earth elements. After a decade of R&D of the gadolinium gallium garnet based single crystal scintillators, new material concept was defined, based on multicomponent $(Gd,RE)_3(Ga,Al)_5O_{12}$ host, Re= Lu, Y. Doped by Ce^{3+}, the Gd- and Ga rich host compositions showed amazingly high light yield up to almost 50,000 phot/MeV[1]. On the contrast to the gadolinium gallium garnet based scintillator, scandium substituted garnet ceramics such $Ce:Gd_3Sc_2Al_3O_{12}$ (GSAG) were reported and GSAG showed interesting scintillation properties such light yield of 7,500 phot./MeV and density of 5.77g/cm^3 [2]. However, details about scintillation properties using the bulk single crystal were not reported. In this study we grew $Ce:Gd_3(Sc, Al)_5O_{12}$ (GSAG) single crystals by Czochralski (Cz) method with different Sc concentration. $Ce1\%:Gd_3Sc_x,Al_{5-x}O_{12}$ (x= 1.5, 2, 2.5) crystals were grown by the Czochralski (Cz) method (Fig.1). Powder XRD measurement and chemical composition analysis were performed in order to investigate Sc substitution effect on garnet structure. The x= 2 sample showed single garnet phase and the x= 1.5 and 2.5 sample showed perovskite phase as a secondary phase. The excitation and emission spectra of the sample set are presented in figure 4. The 4f-5d$_{1,2}$ excitation bands of Ce^{3+} center at 440 and 330 nm was observed at 530nm excitation. The light yields of x= 1.5 and 2 samples were around 6,400 and 7,600 photon/MeV, respectively. The scintillation decay times of the x=2 was 212 ns (47%) 1023 ns (53%), respectively. [1] K. Kamada, et al,. Crystal Growth & Design, vol. 11, pp. 4484-4490, 2011. [2] N. J. Cherepy, et al. IEEE Trans. Nucl. Sci., vol. 56, pp. 873-880, 2009.

BULK GROWTH OF THE CSPBBR$_3$ PEROVSKITE, STRUCTURE AND OPTICAL PROPERTIES

Didier Perrodin, Roberto Reis, Tetiana Shalapska, Stephen Derenzo, Edith D. Bourret, Gregory A. Bizarri

Lawrence Berkeley National Laboratory, CA, UNITED STATES OF AMERICA

Due to its direct bandgap value of 2.25eV, $CsPbBr_3$ is being investigated for solar energy harvesting because of its excellent optoelectronic properties [1]. We demonstrate that this material can also be used as a semiconductor scintillator. Semiconductor scintillators exemplify the highest luminosities and shortest decay times of all known scintillators [2]. For that application, bulk crystals have been grown (Fig 1) and the purification and growth processes will be presented. The structure of the crystals was analyzed by TEM (Fig 2) and found to be I4/mcm tetragonal. Luminescence maps were used to identify parasitic phases and allowed us to improve the crystal synthesis. The temperature dependence of the X-ray luminescence shows an emission peak centered at 543nm and gives access to the IR emission trend. For semiconductor scintillator application, single crystals with low defect

concentration are needed, which we evaluate using thermo luminescence. [1] M. Grätzel, Nature Materials **13**, 838 (2014). [2] S. Derenzo et al., “Bright and ultra-fast scintillation from a semiconductor?” Nuclear Instruments and Methods in Physics Research A 805 (2016) 36–40. This work was supported by the US Department of Homeland Security/DNDO and carried out at Lawrence Berkeley National Laboratory under Contract no. DE-AC02-05CH11231. This work does not constitute an express or implied endorsement on the part of the government.

LI+, NA+ AND K+ CO-DOPING EFFECTS ON SCINTILLATION PROPERTIES OF CE:GD3GA3AL2O12 SINGLE CRYSTALS

Masao Yoshino[1], Kei Kamada[2], Vladimir V. Kochurikhin[3], Mikhail Ivanov[4], Martin Nikl[5], Satoshi Okumura[6], Seiichi Yamamoto[6], Jung Yeol Yeom[7], Yasuhiro Shoji[8], Shunsuke Kurosawa[9], Yuui Yokota[10], Yuji Ohashi[8], Akira Yoshikawa[8]

[1]IMR, Tohoku University, JAPAN, [2]NICHe, Tohoku University, JAPAN, [3]C&A corporation, JAPAN, [4]General Physics Institute, Russian Academy of Sciences, RUSSIAN FEDERATION, [5]Institute of Physics, Czech Academy of Sciences, CZECH REPUBLIC, [6]Graduate School of Medicine Department of Radiological and Medical Laboratory Sciences, Nagoya University, JAPAN, [7]Korea University, KOREA, REPUBLIC OF, [8]Institute for Materials Research, Tohoku University, JAPAN, [9]Department of Physics, Yamagata University, JAPAN, [10]New Industry Creation Hatchery Center, Tohoku University, JAPAN

Scintillator materials used to detect high energy photons. In the last two decades, great R&D effort brought several new material systems, namely the Ce-doped orthosilicates as Gd_2SiO_5 (GSO), $(Lu_{1-x}Y_x)_2SiO_5$ (LYSO), pyrosilicates based on $RE_2Si_2O_7$ (RE=Lu, Y,Gd). Oxide materials based on garnet structure single crystals are promising candidates for scintillator applications due to well-mastered technology developed for laser hosts and other applications, optical transparency and easy doping by rare-earth elements. At the $(Gd,RE)_3(Ga,Al)_5O_{12}$ garnet, Re= Lu, Y. Doped by Ce^{3+}, the Gd- and Ga-rich host compositions showed amazingly high light yield up to almost 50,000 ph/MeV which is the value exceeding by 30-40% the best Ce:LYSO materials ever seen. Recently, our group reported about the Czochralski (Cz) growth of 2inch size $Ce:Gd_3Al_2Ga_3O_{12}$ (GAGG) single crystal and scintillation response of about ~90 ns at emission around 520 nm, an excellent light yield of about 56000 photon/MeV, and density of 6.7 g/cm^3. In the silicate, perovskite and garnet scintillators the slow tunneling-driven radiative recombination between Ce emission centers and nearby lying electron traps can deteriorate scintillation performance. Improvement of scintillation performance by co-doping with divalent alkali earth (AE) ions in Ce-activated scintillators such as LSO:Ce,Ca, LYSO:Ce,Ca , and LuAG:Ce,Mg . Very recently, such an approach has been used in Mg or Ca co-doped Ce:GAGG single crystals. The scintillation decay time of which was accelerated and the presence of Ce^{4+} was clearly identified by its characteristic charge transfer (CT) absorption in the near ultraviolet (UV) range below 350 nm. It was reported that charge compensation by divalent alkali earth metal ions co-doping generated emission process though Ce^{4+} state. Acceding to this mechanism, there is a possibility that monovalent ions also effective to improve scintillation properties of Ce-doped garnet materials. In this study, Li^+, Na^+ and K^+ co-doped Ce:GAGG crystals were grown by the micro-pulling down (μ-PD) method in order to investigate the monovalent alkali metal ions co-doping effects on scintillation properties of Ce:GAGG. Furthermore, Li+ co-doped Ce:GAGG single crystal was grown by the Cz method. As the result, Li^+, Na^+ and K^+ 500 at.ppm co-doped Ce0.5%: Ce:Gd3Ga3Al2O12(GAGG) single crystals were grown by means of the micro-pulling down method. The smooth Ce^{4+} charge transfer absorption below 350nm was observed and decay time acceleration was observed in Li co-doped sample. Furthermore, Li^+ 500 at.ppm co-doped Ce0.5%:GAGG single crystals were grown by the Czochralski method. Scintillation properties and timing resoution properties were evaluated to investigate univalent alkali metal ions co-doping on Ce:GAGG scintillator.

Fig.1 Photographs of the Li, Na and K co-doped Ce:GAGG single crystals grown by the m-PD method.

Fig.2 Absorption spectra of the Li, Na and K co-doped Ce:GAGG single crystals grown by the m-PD method.

BRIDGEMAN GROWTH AND CHARACTERIZATION OF PYN-PMN-PT FERROELECTRIC SINGLE CRYSTALS

Samuel Taylor[1], Jun Luo[1], Wes Hackenberger[1], Shujun Zhang[2], Thomas Shrout[3], Fei Li[3]

[1]TRS Technologies Inc., PA, UNITED STATES OF AMERICA, [2]University of Wollongong, AUSTRALIA, [3]Pennsylvania State University, PA, UNITED STATES OF AMERICA

Relaxor-based ferroelectric single crystals have become the next generation of piezoelectric materials for transducer and actuator devices. Binary $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) and ternary $Pb(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$ -$PbTiO_3$ (PIN-PMN-PT) single crystals as large as 100mm in diameter have been produced by TRS Technologies, Inc. Although PIN-PMN-PT crystals have improved stability under high temperature and electric field over PMN-PT crystals, its cost is also much higher than that of PMN-PT, owing to the expensive In2O3 in the raw material. TRS is currently exploring new crystal compositions to expand the operational domains of relaxor-PT single crystals.. High temperature binary $Pb(Yb_{1/2}Nb_{1/2})O_3$- $PbTiO_3$ (PYN-PT) single crystals cannot be grown by the Bridgman process. Adding $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN) into the PYN-PT system stabilizes the perovskite phase, allowing for bulk PMN-PYN-PT crystals to be grown from the melt by the Bridgman process. 10-15mm diameter PYN-PMN-PT crystals with PYN and PT concentrations ranging 2-26mol% and 31-33mol% respectively, have been grown successfully by a self-seeded Bridgman process. To facilitate composition selection process, multiple single crystal boules were produced in each of the run. All of these crystals have a lighter color than a typical PMN-PT crystal. Some PYN-PMN-PT crystals showed promising coercive field values, as high as 3-4kV/cm for the 6-7mol% crystals. Other electrical properties, including the phase transition temperatures, were similar to normal PMN-PT single crystals; even though it was expected that the phase transition temperatures may be elevated by increasing PYN content in the system. Simply increasing the PYN content, but keeping the PT content constant, drives the system towards tetragonal phase and makes a single crystal more difficult to grow.

SURFACE FREE ENERGY AND THE MORPHOLOGY OF FLUORITE CRYSTALS

Takaomi Suzuki, Ayano Tsukagoshi

Faculty of Engineering, Shinshu University, JAPAN

Specific surface free energy (SSFE) is significant value to explain the morphology of crystals. The relationship between SSFE and growth length of crystal face is considered to be proportional, which is known as Wulff's relationship, and well accepted for thermodynamic interpretation of crystal growth theoretically. Though Wulff's relationship is well accepted for theoretical analysis, experimental measurement of SSFE for crystal face is very few. According to Young's equation, SSFE of solid face can be introduced from contact angle of liquid on the solid face, and we observed SSFE of some crystals, for example, apatite[1], ruby[2], and quartz[3]. However, the SSFEs of crystal face have wide distribution even for a flat face of the crystal. Such wide distribution of observed SSFE was considered to result from steps on the crystal face. In this work, we observed SSFEs of apatite and fluorite crystals in order to demonstrate the effect of steps on the SSFE. Contact angle of water and formamide droplet on crystal face was observed using digital camera. SSFE was calculated using Fowkes approximation and Wu's harmonic mean equations. Though the crystals we experimentally obtained were growth form, the relationship between SSFE and the growth rate was almost proportional, which looks to satisfy Wulff's relationship qualitatively. Natural fluorite crystal was cut and polished for (100), (110), and (111) faces. SSFE can be separated to dispersion component which results from van der Waals force and polar components which results from interaction between permanent dipole moments. The polar component of SSFEs on (100) and (111) faces were smaller then have large rate of dispersion component of than that on (110) face, because (100) and (111) faces are polarized face. Although the SSFE of real crystal is calculated from macroscopic value such as contact angles of liquid droplets, the SSFE reflects microscopic surface structure such as steps and the ionic morphology of the crystal face. [1] T. Suzuki, et. al., J. Crystallization Process and Technology, 3 (2013) 119-122. [2] T. Suzuki and M. Oda, J. Cryst. Growth, 318 (2011) 76-78. [3] T. Suzuki, et. al., J. Crystallization Process and Technology, 4 (2014) 177-184.

APPLICATION OF ULTRASOUND FOR CONTROL OF THE SUGAR CRYSTALLIZATION PROCESS

Zdenek Bubnik, Vladimir Pour, Andrea Hinkova, Svatopluk Henke, Evzen Sarka

University of Chemistry and Technology, Prague, CZECH REPUBLIC

The paper deals with the study and development of methods that use ultrasound to control the process of crystallization of sugar. This research is a continuation of previous work of the authors and its main objective is to expand and improve ultrasonic management procedures. Applications of the ultrasonic technique for concentration measurement are described for many saccharides; mono- and disaccharides (fructose, glucose, xylose, galactose, mannose, sucrose, etc.), alcohol solutions and solutions containing alcohol and sugar (e.g. fermentation media). Main part of the paper deals with an application of the Low Intensity Ultrasonic Technique for metastable zone width measurement during the cooling sugar crystallisation and for dry solid determination. The metastable zone width was measured for pure sucrose solutions and for concentrated raw juice. The accuracy of this method is sufficient for a control of an industrial process. The ultrasonic device was also successfully used for the crystallization control of pure and technical sugar solutions.

GROWTH AND SCINTILLATION PROPERTIES OF CE:LACL$_3$/AECL$_2$ (AE=MG, CA, SR, BA) EUTECTICS FOR X-RAY IMAGING APPLICATIONS

Akria Yoshikawa[1], Kei Kamada[2], Yuki Furuya[3], Shunsuke Kurosawa[4], Akihiro Yamaji[5], Yasuhiro Shoji[5], Yuji Ohashi[6], Yuui Yokota[6]

[1]IMR, Tohoku Universiry, JAPAN, [2]C&A corporation, JAPAN, [3]Institute for Materials Research (IMR), JAPAN, [4]Department of Physics, Yamagata University, JAPAN, [5]Institute for Materials Research, Tohoku University, JAPAN, [6]New Industry Creation Hatchery Center, Tohoku University, JAPAN

In the X-ray imaging applications, radiation imaging sensors were composed of photodetector arrays and indirect flat panel detector (FPD) coupled with a scintillator plate such as Tl:CsI or Gd2O2S:Tb (GOS). Improvement in the spatial resolution is required in this application. However, CsI:Tl columnar grown Tl:CsI reduce the spatial resolution, because light scattering in the micro-meter size Tl:CsI fiber crystals. Light diffusion through scintillatior materials on photodetector degrade resolution of radiation imaging sensors and limit the sensitivity. Recently, pixilated photodetector arrays has been improved to achieve a micrometer scale special resolution. However, pixel size of scintillator arrays and the light diffusion limit the spatial resolution. Currently, submicron-diameter phase-separated scintillator fibers (PSSFs) were reported and they have both characteristics of optical fiber and a radiation-to-light conversion. The PSSFs were realized by a directionally solidified eutectic (DSE) growth in previous research [4-8]. In PSSFs, the emitted scintillation is confined and transported along the eutectic structure by a total reflection mode, so that light diffusion can be reduced and high-resolution imaging can be achieved. Up to now, research on PSSFs such GAP/α-Al2O3[1], SrHfO3/Al2O3[2] and LiF/ CaF2/LiBaF3 [3] have been already reported by our group. Here, Ce:LaCl3 scintillator has attracted attention due to its high light yield of 50,000 photons/MeV and fast decay time of 25 ns even it is hygroscopic[4]. In this research, exploration of PSSFs by directional crystal growth method for Ce doped LaCl3/AECl2 (AE=Mg, Ca, Sr, Ba) was reported. Example photograph of the eutectic was shown in Fig.1. The sample showed optical transparency like bundle optical fibers and the background line is visible on the surface through the transparent rods grown in the material. The grown eutectic structure showed mixture of rods and plates shape of LaCl3 phase surrounded by CaCl2 matrix. This mixed structure of LaCl3 was aligned with length of around 300 μm. The expected 350 nm emission of Ce3+ 4f5d transition was observed in the all samples. Investigations of their crystal structure and eutectic phase were performed. Luminescence and scintillation properties were also evaluated. [1]Y.Ohashi et al., App. Phy. Lett. 102, (2013) 05197. [2]K. Kamada, et al., J. of Phys. Conference Series, 619 (2015) 012036 [3]K. Kamada, et al., Opt. Mater.41 (2015) 41-45 [4]K. Hishinuma et al., Jpn. J. Appl. Phys. 54 (2015) 04DH04 [5]J. T. M. d. Haas et al., IEEE Trans Nucl Sci, 55 (2008)1086-1092

HIGH-QUALITY N-TYPE GAN GROWN BY HVPE: SI VS O DOPING AND THERMAL CONDUCTIVITY

Tania Paskova[1], Plamen Paskov[1], Michael Slomski[1], Jacob Leach[2], John Muth[1]

[1]North Carolina State University, UNITED STATES OF AMERICA, [2]Kyma Technology, UNITED STATES OF AMERICA

Native GaN substrates are the ideal foundation for III-nitride electronic and optoelectronic devices. Many devices benefit from their low-dislocation density and high thermal conductivity, as well as the close match of the lattice and thermal expansion coefficient between the epitaxial layers and the GaN substrates. Although several techniques are currently under intensive development, native GaN substrate product is still very limited and is dominated by substrates produced using hydride vapor phase epitaxy (HVPE). Recent advances in the HVPE growth of bulk GaN substrates resulted in significantly reduced defect density, including both the dislocation density (down to mid 10^5 cm^{-2}) and point defect densities (down to 10^{15} cm^{-3}). Another strong advantage of the HVPE GaN is the ability of the method to produce material with controllable doping and to achieve electrical conductivity variation in wide range. Conductive n-type substrates are required for light-emitting diodes and laser diodes, which also necessitate high thermal conductivity. The incorporation of dopants into the GaN lattice impacts the thermal conductivity, however, it likely proceeds via a complex and not well-understood interplay of the scattering mechanisms acting simultaneously – namely phonon-phonon, phonon-impurity, phonon-electron, phonon-dislocation scattering. In this work we report on two doping alternatives for producing high-quality HVPE-GaN substrates and their effect on the thermal conductivity. Two dopants, silicon and oxygen, have been used to achieve n-type substrates with free-electron density varied from $1x10^{16}$ cm^{-3} to $8x10^{18}$ cm^{-3}. The structural and optical properties were only moderately affected and the high crystalline quality of the material was maintained within the doping levels used. The thermal conductivity was measured by using 3-omega technique at room temperature, as well as at elevated temperatures which are particularly relevant for devices operating at high power regimes. Our results indicate that: (i) the thermal conductivity decreases with increasing the doping concentration and with increasing the temperature; (ii) the thermal conductivity is more significantly influenced by Si doping, as compared to the O doping; (iii) the temperature decreasing slope of the thermal conductivity decreases in samples with higher doping. In order to explain the experimental observations and to speculate on the weight of different scattering mechanisms on thermal conductivity of GaN samples with different doping, we compared our experimental results with theoretical calculations based on a modified Callaway-Holland model. The importance of the results will be discussed in terms of their practical implications for better thermal management and device performance.

SCALING AND SCINTILLATION PERFORMANCE OF TL2LIYCL6:CE

Ivan Khodyuk, Stacy Swider, Shariar Motakef

CapeSym, UNITED STATES OF AMERICA

Crystalline scintillators with high Z numbers, good energy resolution, and the ability to detect neutrons are highly attractive for threat discrimination and special nuclear materials identification. Traditional scintillators NaI and CsI have effective Z numbers of 50 and 54. However, they do not offer neutron detection. CLYC (Cs_2LiYCl_6:Ce) scintillator [1] offers gamma energy resolution near 4%, thermal neutron detection when enriched with ^{6}Li [2], and fast neutron detection when enriched with ^{7}Li [3]. Being a cubic system, it is also relatively easy to grow, therefore its production has scaled rapidly over the last three years, both in terms of size and availability. But at Z=45, and relatively low density of 3.3 g/cc, more material is needed to absorb gamma radiation, as compared to NaI or CsI. In this paper, we will discuss scaled growth and scintillation performance - of a relatively new scintillator, TLYC (Tl_2LiYCl_6:Ce), first presented by Kim *et. al* at SCINT 2015 [4] and later discussed by Hawrami *et. al* [5]. With cesium replaced by thallium, the material becomes 33% more dense (4.58 g/cc) and the Z number increases from 45 to 69. With higher density and effective Z, less TLYC is required to achieve the equivalent stopping power compare to CLYC. Our preliminary results with a small 10 mm in diameter and 20 mm long crystal show 4.1% energy resolution, a brightness of 22,500 ph/MeV at 662 keV, and FOM of 1.87 for thermal neutron detection. In the paper, we will present results of TLYC enriched with ^{6}Li or ^{7}Li to provide dual or tri-mode (γ/n) detection through the well-known pulse shape discrimination technique [6]. References: 1. C.M. Combes, P. Dorenbos, C.W.E. van Eijk, K.W. Krämer, H.U. Güdel, J. of Lum. 82 (1999) 299. 2. C.W.E. van Eijk, A. Bessiere, P. Dorenbos, Nuclear Instruments and Methods in Physics Research Section A 529 (2004) 260. 3. N. D'Olympia, P. Chowdhury, C.J. Lister, J. Glodo, R. Hawrami, K. Shah, U. Shirwadkar, Nuclear Instruments and Methods in Physics Research Section A 714 (2013) 121. 4. H. Kim1, G. Rooh, S. Kim, H. Park, SCINT 2015, Berkeley CA, USA. 5. R. Hawrami, E. Ariesanti, L. Soundara-Pandian, J. Glodo, and K. S. Shah, IEEE Transactions on Nuclear Science 63-6 (2016) 2838. 6. Carel W. E. van Eijk, IEEE Transactions on Nuclear Science 59-5 (2012) 2242.

EFFECT OF (Incomplete Title)

Farit K. Urakaev

Sobolev Institute of Geology and Mineralogy of the Siberian Branch of the Russian Academy of Sciences, RUSSIAN FEDERATION

A comparative study is made regarding the effect of “pollution-free” mechanical activation (**MA**) of $BaCO_3$-HBO_2/H_3BO_3 and $BaCO_3$-Na_2CO_3-NaF-(HBO_2/H_3BO_3) systems on the synthesis of β−BaB_2O_4 and $Ba_2Na_3[B_3O_6]_2F$. MA was used to prepare $YSc(BO_3)_2$ and $Y_3Sc(BO_3)_4$ borates from the Y_2O_3-Sc_2O_3-HBO_2 system. The existence of two series of solid solutions of yttrium-scandium borates based on the YBO_3 or $ScBO_3$ structure is established. It is shown that a morphotropic transition occurs in the range of Y/Sc = 1.5÷1. $ScBaNa(BO_3)_2$ and $YBaNa(BO_3)_2$ were prepared by two-step synthesis and by annealing after MA. Crystal growth was performed from solutions of (Sc/Y)BO_3-BaO-B_2O_3−Na_2O systems. A study also was performed on the influence of MA in Na_2CO_3-$(Bi/In)_2O_3$-WO_3 systems on synthesis and the properties of the charge for growing of bulk crystals. By machining Na_2CO_3-In_2O_3-WO_3 system revealed the formation of $NaIn(WO_4)_2$ nanocrystals at 425°C. Finally, we studied the influence of anomalous anisotropy in the elastic constants of paratellurite (α−TeO_2) on the rate of the following mechanochemical reactions: $Bi_2O_3 + SeO_2 = Bi_2SeO_5$; $SeO_2 + TeO_2 = TeSeO_4$; $Bi_2O_3 + TeO_2 = Bi_2TeO_5$. The formation of the next noncentrosymmetrical compounds was registered by means of X-ray analysis and thermal annealing: Bi_6SeO_{11}, $TeSeO_4$, and Bi_2TeO_5.

INVESTIGATION OF ACTIVATORS FOR SCINTILLATION IN LANTHANUM IODIDE

Mariya Zhuravleva[1], Robyn Collette[1], Daniel Rutstrom[1], Matthew Loyd[1], Luis Stand[2], Chuck Melcher[1]

[1]Department of Materials Science and Engineering University of Tennessee Knoxville, TN, UNITED STATES OF AMERICA, [2]Bredesen Center, University of Tennessee, TN, UNITED STATES OF AMERICA

LaI_3 has the potential to be a promising scintillator, having a high theoretical light yield of 174,000 photons/MeV, but is unused due to lack of a suitable activator. Density Functional Theory DFT calculations showed that Bi^{3+} and Sb^{3+} may be suitable activators due to their ground state and excited state positions within the band gap of LaI_3 [1]. DFT calculations also show that a mixed compound, $LaBr_xI_{3-x,}$ may be a promising scintillator when activated with Eu^{2+} [1]. In this work, we investigated Bi^{3+} and Sb^{3+} as an activator in LaI_3 and Eu^{2+} as an activator in $LaBr_xI_{3-x}$. Bi^{3+} and Sb^{3+} proved to be difficult to incorporate into the LaI_3 matrix due to their boiling points, 542°C and 401°C, being much lower than the melting point of LaI_3, 778°C. The ratio between bromine and iodine in $LaBr_xI_{3-x}$ was varied between x=0 and x=3 to determine an optimal ratio for scintillation performance when doped with Eu^{2+}. Hygroscopicity measurements revealed that LaI_3 was very hygroscopic when compared to a NaI standard and therefore needed to be handled very carefully. Crystals with a diameter of 7 mm were grown by vertical Bridgman technique at a rate of 0.5 mm/hr and cooled over several days. All crystals luminesced under 254 nm ultraviolet light. LaI_3: 0.5% Bi crystals exhibited radioluminescence spectra peaks at 465, 542, 597, and 672 nm. $LaBr_xI_{3-x}$:0.1% Eu crystals exhibited a single radioluminescence spectra peak around 355 nm. [1] Wu, Dangxin, et al. "First-principles search for efficient activators for LaI3." *Journal of Luminescence* (2016): 227-234. Web.

EFFECT OF MASK ORIENTATION AND GROWTH PARAMETERS ON THE EPITAXIAL LATERAL OVERGROWTH OF GAN ON FREE-STANDING NONPOLAR SUBSTRATES

Saadat M. Mishkat-Ul-Masabih, Andrew Aragon, Morteza Monavarian, Daniel Feezell

University of New Mexico, Center for High Technology Materials, UNITED STATES OF AMERICA

One of the main challenges faced by GaN-based vertical-cavity surface-emitting lasers (VCSELs) is the incorporation of the bottom cavity feedback, provided by a distributed Bragg reflector (DBR). Few groups have demonstrated epitaxial DBRs using III-nitride alloys of aluminum with GaN. However, the refractive index difference between these layers is not large, thus requiring more than 30 pairs to reach high-reflectivity. In addition, the number of layers that can be grown is further limited by lattice mismatch between the layers. Alternatively, dielectric DBRs can be used and exhibit a high refractive index difference and a wide stop-band. However, the use of dielectric DBRs necessitates complex processing techniques to allow access to the bottom side of the VCSEL cavity. Often flip-chip and substrate removal is required to deposit the DBR, which itself can pose a significant fabrication challenge. Epitaxial lateral overgrowth (ELO) enables the accommodation of dielectric DBRs in VCSEL structures without the need for difficult fabrication processes. A dielectric DBR may be deposited on the substrate and then n-GaN may be laterally overgrown on top of the DBR, followed by the active region and p-side of the device. This provides a buried dielectric DBR and also significantly lowers the extended defect density of the overlying material. The ELO growth of *c*-oriented GaN has been thoroughly investigated and the growth mechanisms are well-understood to obtain the highest lateral to vertical growth rate ratio. The use of nonpolar *m*-plane freestanding substrates is of interest due to the higher gain and the elimination of polarization-induced quantum confined Stark effect. However, the shape and morphology of the grains resulting from ELO conditions are different and not very well-studied compared to those for *c*-plane. In this work, the crystal morphology of ELO growth on a SiN_x patterned *m*-plane GaN template is studied to optimize the lateral-vertical growth rate ratio (L/V). The SiN_x mask design (i.e. stripe window width and separation) was demonstrated to significantly affect the overall growth rate, as well as L/V. We observe that by reducing the window size from 8 to 2 μm and increasing the separation between stripes from 20 to 50 μm, the L/V was increased by a factor of 6 while maintaining the same overall growth rate for a certain stripe orientation. The effect of SiN_x mask orientation is also considered along with other growth parameters such as temperature, pressure, V/III ratio, and continuous/pulsed growth mode.

GAN EPITAXY ON GLASS USING A (111) SILICON SEED LAYER FORMED BY ALUMINUM-INDUCED CRYSTALLIZATION

Mel F. Hainey Jr.[1], Zakaria Y. Al Balushi[1], Ke Wang[2], Nathan Martin[1], Anushka Bansal[1], Joan M. Redwing[1]

[1]Dept. of Materials Science and Eng., The Pennsylvania State University, PA, UNITED STATES OF AMERICA, [2]Penn State University, Materials Characterization Laboratory, UNITED STATES OF AMERICA

The integration of group III-nitride epilayers on glass is highly desirable for LED applications, as it is a low-cost and transparent substrate, however, direct growth of c-axis oriented GaN on glass is difficult due to the amorphous nature of the glass surface. In this report, we demonstrate a novel approach to this problem using a highly oriented polycrystalline silicon seed layer fabricated directly on glass using a process called aluminum-induced crystallization (AIC). In AIC, an aluminum film is first deposited on glass, followed by a brief air exposure. Amorphous silicon is then deposited over the oxide, and the stack is annealed in nitrogen. For thin (<50 nm) aluminum and silicon films, silicon diffuses through the aluminum and crystallizes at the glass/Al interface, producing a polycrystalline silicon thin film with a uniform Si(111) surface orientation. After removing the aluminum from the silicon film, GaN growth is performed using metalorganic chemical vapor deposition (MOCVD). An aluminum nitride (AlN) buffer layer was grown initially at low temperatures (550°C), followed by high temperature recrystallization and further growth at 1100°C. A 2μm thick GaN layer was grown over the AlN using a two-step process to form a GaN thin film. The GaN films grown on the AIC (111)Si templates are textured with coalesced regions greater than 1mm^2 in size that consist of large GaN grains (40-50 μm) with a uniform (0001) surface orientation and random in-plane orientation. Cross-section transmission electron microscopy confirms the GaN grains contain mostly mixed a+c type dislocations with a few a- and c-type dislocations as well. The silicon seed layer, while defective, has most of its defects in-plane, limiting propagation into the AlN and GaN layers and blocking out-of-plane defects from reaching the Si/AlN interface. Critically, AlN grown directly on the silicon seed layer is observed to overgrow gaps in the silicon, allowing for continuous GaN growth even from non-continuous silicon seed layers. Room temperature photoluminescence confirms strong near-band edge emission using a 266nm UV source, and low emission at longer wavelengths corresponding to deep-levels. These results demonstrate that GaN growth on Si seed layers can produce large grained c-axis textured GaN films on glass substrates. While these initial results are demonstrated on glass, AIC can be used to prepare Si seed layers on a variety of other substrates including oxidized Si(001), potentially allowing for integration with standard electronics and providing a generalizable approach to integrate GaN on unconventional substrates.

STRESS ENGINEERED ALGAN/GAN POWER ELECTRONIC DEVICE STRUCTURES

Isra Mahaboob[1], Kasey Hogan[2], Emma Rocco[1], **Fatemeh Shahedipour-Sandvik**[2]

[1]Colleges of Nanoscale Science and Engineering, NY, UNITED STATES OF AMERICA,
[2]Colleges of Nanoscale Science and Engineering, UNITED STATES OF AMERICA

AlGaN/GaN based power-electronic devices have emerged as the next generation technology platform and are believed to have a similar significance as MOSFETs did by replacing BJTs in 1970s. The interest in this technology has increased tremendously due to several key performance advantages such as high-power density, low on-resistance, high-mobility, large breakdown-voltage and low-thermal resistance. GaN-on-Si technology has a rising demand as it enables low-cost/large-scale manufacturing. However, obtaining good quality GaN-on-Si wafers is challenging due to lattice and thermal-mismatch between III-Nitrides and Si. In our work, we employ MOCVD technique to grow stress-engineered/high-quality HEMT-on-Si devices. Here we describe two methodologies to obtain thick buffer layers with reduced stress levels which are desirable to obtain high breakdown voltage structures. To engineer the stress in layers, K-Space *in-situ* stress-monitoring system is used during the growth to monitor stress evolution in the films and to optimize the stress level. Conventional-planar-HEMTs are grown with stress-engineered AlGaN-interlayers. AlGaN-interlayers mitigate the challenges caused by thermal induced cracking and dislocation density due to lattice-mismatch. The addition of AlGaN layers is also beneficial in improving the vertical breakdown-voltage. With *in-situ* stress monitoring system, we have been successful in incorporating sufficient compressive stress in the AlGaN buffer layers to counter the thermal tensile stress that occurs upon cooldown. HEMTs fabricated from these structures show a maximum power-density of 3W/mm and an off-state breakdown voltage > 400V. The second methodology used here to achieve thick buffer/template layer is growth of HEMT device structure by selective area epitaxy technique. PECVD deposited SiO_2/SiN mask on GaN template is used to enable selective growth. The opening in mask areas followed specific active device geometric designs. In SAG structures the effects of stress due to lattice-mismatch and wafer-bowing are mitigated which enables growth of thicker buffer layers with reduced stress. Selectively grown HEMT structures showed 25X increase in GaN growth-rate enabling thick, crack-free buffer/template layers with high quality surfaces ideal for high-breakdown operation.

INFLUENCE OF THE SUBSTRATE ORIENTATION ON STRUCTURAL AND ELECTRICAL PROPERTIES OF HOMOEPITAXIAL β-GA_2O_3 THIN FILMS GROWN BY MOVPE

Guenter Wagner, Martin Albrecht, Michele Baldini, Andreas Fiedler, Zbigniew Galazka, Klaus Irmscher, Robert Schewski

Institute for Crystal Growth, GERMANY

Gallium oxide is one of the most emerging compound among transparent semiconducting oxides, thanks to its distinctive physical properties. The most stable monoclinic β-phase is characterized by a large bandgap (E_g = 4.8 eV), an extremely high breakdown field (8 MV/cm) and a widely tunable *n*-type conductivity (10^{16}–10^{19} cm^{-3}). The most promising application fields of ß-Ga_2O_3 are high power devices and solar blind UV photodetectors. In this contribution, we report on the growth of high quality n-type ß-Ga_2O_3 layers on ß-Ga_2O_3 substrates with different orientations by using Metal Organic Vapor Phase Epitaxy (MOVPE). Bulk, 2 inch diameter ß-Ga_2O_3 single crystals for the substrates were grown in our institute by the Czochralski method. The MOVPE growth was carried out in a vertical reactor using triethylgallium (TEGa) and tetraethylorthosilicate (TEOS) as organometallic sources for Ga and Si and pure oxygen as oxidant. We present how the MOVPE growth of β-Ga_2O_3 layers leads to dramatically different results depending on the orientation of the substrates. We investigated the growth of ß-Ga_2O_3 layers on misoriented (100) on (010) and (001)-oriented ß-Ga_2O_3 substrates in order to decrease the defect density. The layers were studied by different characterization methods (AFM, Hall- measurements, HRTEM, SEM, SIMS). With increasing miscut angles of the (100) substrates the step-flow growth mechanism is triggered, hindering the formation of planar defects (Fig. 1). At the maximum misorientation of 6° towards the [001] direction the structural and electrical properties of the layers are comparable to those of the bulk material. Another successful approach to decrease the defect density of the layers is the growth on (010)-oriented substrates, since double positioning does not occur on the (010) surface of the substrates. Layers grown in this way show a very high crystalline perfection that leads to a wide doping range of $1x10^{17}$- $8x10^{19}$ cm^{-3} and electron mobilities up to 130 cm^2/Vs (Fig. 2). However, the use of (010)-oriented substrates is not ideal since the wafering is hampered by the easy cleavage of ß-Ga_2O_3 crystals parallel to (100) and (001) planes. The growth of ß-Ga_2O_3 layers on (001)-oriented substrates has only recently been investigated (Fig. 3). The preliminary results are very promising, indicating the absence of double positioning also on this substrate orientation. Nevertheless, other types of defects are visible in the layers. The nature of these defects and their influence on the electrical layer properties are currently under investigation. .

GROWTH OF GAN ON 2D BN BY MOCVD FOR FLEXIBLE ELECTRONICS

Michael Snure, Nicholas R. Glavin, Kelson D. Chabak, Qing Paduano

Air Force Reseach Laboratory, OH, UNITED STATES OF AMERICA

Two dimensional (2D) surfaces such as graphene and BN are attractive for growth of GaN films and device structures. The weak inter-planar van der Waals (vdW) bonding between 2D layers allows for easy mechanical separation of GaN films from the growth substrate for transfer to a flexible one. This approach offers a viable way to producing produce flexible RF electronics suitable for wireless and radar applications. In this paper, we describe the growth of high quality GaN and AlGaN/GaN high electron mobility (HEMT) structures on few layer BN on sapphire substrates. The effects of nucleation and BN template morphology are discussed demonstrating how AlGaN/GaN heterostructures with threading dislocation densities < 3 x10^8 cm^2 and 2DEG mobility > 2,000 cm^2/Vs (at room temperature) can be grown on a 2D BN surface. We will then describe fabrication of AlGaN/GaN-HEMTs, designed for RF application at frequencies > 10 GHz, and their transfer to flexible substrates. Taking advantage of the weak vdW interactions we transfer T-gated RF devices using a simple PDMS stamp mechanical process from our ridged growth substrate to a flexible 3M tape. These devices demonstrate exceptional RF performance with f_T and f_{max} greater than 34 GHz and 75 GHz, respectively. Lastly we will describe the effects of uniaxial strain up 0.9% on the 2DEG transports properties and HEMT device performance.

GAN P-I-P-I-N SEPARATE ABSORPTION AND MULTIPLICATION ULTRAVIOLET AVALANCHE PHOTODIODES BY METALORGANIC CHEMICAL VAPOR DEPOSITION

Mi-Hee Ji[1], Jeomoh Kim[2], Theeradetch Detchprohm[1], Shyh-Chiang Shen[1], **Russell Dupuis**[1]

[1]Georgia Institute of Technology, GA, UNITED STATES OF AMERICA, [2]LG Electronics, KOREA, REPUBLIC OF

Ultraviolet avalanche photodiodes (UV-APDs) based on III-nitride materials are of great interest for many applications in military systems, medical systems, environmental monitoring, and space research because of their promising advantages of low dark current, high detection sensitivity, and high optical gain. In recent years, separate absorption and multiplication (SAM) APDs employing impact-ionization engineering have been extensively studied to achieve low multiplication noise and high maximum gain. However, the development of high-performance GaN-based UV-APDs has been hampered by the lack of lattice matched substrates. The high threading dislocation densities are resulting from heteroepitaxial growth on lattice-mismatched foreign substrates, which may cause device failure by premature microplasma breakdown. In this study, the epitaxial structure of GaN *p-i-p-i-n* UV-APDs with separate absorption and multiplication (SAM) regions were grown by metalorganic chemical vapor deposition (MOCVD) on a *c*-axis *n*-type bulk and free-standing GaN substrates with dislocation densities $< 5\times10^4$ cm^{-2}, which is beneficial in reducing defect densities of the UV-APDs. For a front-illuminated UV-APD structure, a *p*-$Al_{0.05}Ga_{0.95}N$:Mg window layer was introduced instead of a *p*-GaN:Mg layer in order to obtain high-responsivity in the UV spectral region. The epitaxial layer structure consisted of a 1-μm thick *n*-GaN:Si layer (n~5.0×10^{18} cm^{-3}), a 0.21-μm thick *i*-GaN:ud layer as multiplication layer (n~1.3×10^{16} cm^{-3}), a 90-nm thick *p*-GaN:Mg with grading [Mg] up to ~5.0×10^{18} cm^{-3}, 0.24-μm thick *i*-GaN as absorption layer ([Mg]~1.0×10^{17} cm^{-3}), a 30-nm thick *p*-$Al_{0.05}Ga_{0.95}N$:Mg window layer ([Mg]~1.0×10^{19} cm^{-3}) and a 20-nm thick heavily doped *p*-$Al_{0.05}Ga_{0.95}N$:Mg metal contact layer ([Mg]~1.0×10^{20} cm^{-3}). The optimized growth and doping conditions for each epitaxial layer were carefully modified. The GaN *p-i-p-i-n* SAM UV-APDs were fabricated into circular and square mesas with various device areas using standard photolithography and inductively coupled plasma (ICP) etching with a Cl_2/He carrier gas mixture, followed by deposition of a SiO_2 passivation layer using plasma-enhanced chemical vapor deposition. Ti/Al/Ti/Au and Ni/Ag/Ni/Au metal stacks were evaporated and annealed on the *n*-type and *p*-type contact layers, respectively. Under illumination at λ~340 nm, the measured UV-APDs with mesa size of 30-μm-diametaer exhibited a maximum avalanche gain of 7.4×10^6 at the reverse bias of 72.5 V. Also, no microplasmas were visually observed after multiple reverse-bias *I-V* scans. The detailed growth, fabrication, and device characterization of the GaN *p-i-p-i-n* UV-APDs will be further discussed in the conference.

UV AIR-GAP/AL$_X$GA$_{1-X}$N DISTRIBUTED BRAGG REFLECTORS FABRICATED USING CONDUCTIVITY-SELECTIVE ELECTROCHEMICAL ETCHING

Youngjae Park[1], Theeradetch Detchprohm[1], Oliver Moreno[1], Karan Mehta[1], Yuh-Shiuan Liu[1], Shuo Wang[2], Shyh-Chiang Shen[1], P. Douglas Yoder[1], Fernando Ponce[2], **Russell D. Dupuis**[1]

[1]Georgia Institute of Technology, GA, UNITED STATES OF AMERICA, [2]Arizona State University, AZ, UNITED STATES OF AMERICA

Vertical-cavity surface-emitting lasers (VCSELs) have been widely used in optical fiber data transmission, high density optical data storage, solid-state lighting and chip-scale atomic clocks. One of the main challenges for III-nitride VCSELs is to realize the high-reflectivity semiconductor mirrors. Some groups have used dielectric distributed Bragg reflectors (DBRs) on both sides, which requires complex fabrication processes. The epitaxial growth of high-reflectivity DBRs in III-nitride based VCSEL has been also demonstrated using AlN/GaN and AlInN/GaN. However, the former DBR's layers have a large lattice mismatch, which degrades material quality and leads to the formation of cracks. The latter DBR uses AlInN which is challenging to grow due to the greatly different optimum growth condition for AlN and InN. For the chip-scale atomic clock application, 369.5nm VCSEL is required in the cooling process and any semiconductor DBR containing GaN or lower bandgap material cannot be employed due to high optical absorption loss. In this study, we report on the fabrication of a five period AlGaN based air-gap DBR for use in UV VCSELs using a conductivity-selective electrochemical (EC) etching process. The epitaxial growth was performed using an AIXTRON 3x2" close-coupled showerhead metalorganic chemical vapor deposition (MOCVD). The DBR structure consisted of a five periods of 277 nm n+$Al_{0.05}Ga_{0.95}N$ (n = 2E+19 cm^{-3}, sacrificial layer)/ 103.6 nm $Al_{0.05}Ga_{0.95}N$ (unintentionally doped) grown on a 3 µm GaN template. The thickness of each layer ($d_{1,2}$) was estimated by the center wavelength of the DBR as $d_{1,2}=3\lambda_0/4n_{1,2}$ where $n_{1,2}$ is refractive index of each layer. The DBR can theoretically achieve a peak reflectivity exceeding 99% due to the high refractive index contrast between air and the $Al_{0.05}Ga_{0.95}N$. Subsequently, an $Al_xGa_{1-x}N$ spacer layer, five periods $In_yGa_{1-y}N/Al_zGa_{1-z}N$ MQWs designed for an emission wavelength of 369.5 nm and a thin $Al_xGa_{1-x}N$ cap layer were grown on the DBR template. The air-gap layers were obtained by laterally etching the n+$Al_{0.05}Ga_{0.95}N$ layers using a conductivity-selective electrochemical etching process. Photolithography followed by dry etching was performed to expose the sidewall of the sacrificial layers that allowed the EC etching to begin. The air-gap layers around the via holes that were formed by eliminating the n+$Al_{0.05}Ga_{0.95}N$ layers were spread outwards with increasing etching duration. We will deposit a dielectric DBR comprising of ten pairs of HfO_2/SiO_2 on this structure as a top mirror to test an optically pumped VCSEL. More details about the growth process, DBR design and optical characterization will be presented.

NUCLEATION AND GROWTH OF WSE_2: ENABLING LARGE GRAIN TRANSITION METAL DICHALCOGENIDES

Christopher Hinkle

University of Texas at Dallas, TX, UNITED STATES OF AMERICA

In this work, we demonstrate the high-quality MBE heterostructure growth of various layered 2D materials by van der Waals epitaxy (VDWE). The coupling of different types of van der Waals materials including transition metal dichalcogenide thin films (e.g., WSe_2, WTe_2, $HfSe_2$) and topological insulators (e.g., Bi_2Se_3) allows for the fabrication of novel electronic devices that take advantage of unique quantum confinement and spin-based characteristics. We demonstrate how the van der Waals interactions allow for heteroepitaxy of significantly lattice-mismatched materials without strain or misfit dislocations. Yet, at the same time, the VDW interactions are strong enough to cause rotational alignment between the epi-layer and the substrate, which plays a key role in the formation of grain boundaries. Small TMD grain sizes have been the limiting factor in the investigation of their intrinsic properties and high-performance nanoelectronic, optoelectronic, and photovoltaic device applications. To enable larger grains, limit grain boundary formation, and investigate the kinetic issues related to TMD growth, we combined a detailed and systematic experimental design with first-principles kinetic Monte Carlo modeling for the WSe_2 system. These complementary techniques indicate that, in contrast to TMD growth attempts reported in the literature, drastically lowering the metal flux in conjunction with an elevated substrate temperature in a very Se-rich environment reduces nucleation density and promotes 2D growth. We describe how the application of conventional materials growth modes, such as Volmer-Weber, are not applicable to 2D material systems such as TMDs and TIs. We will present a detailed discussion of the growth mechanism, quantitative kinetics data, and strategy for large-area growth of TMDs and other 2D materials by MBE and CVD providing a path to getting scalable 2D materials for important device applications.

NUCLEATION AND GROWTH KINETICS OF MONOLAYER TUNGSTEN DISELENIDE (WSE_2) FILMS ON SAPPHIRE

Xiaotian Zhang[1], Tanushree H. Choudhury[2], Bhakti Jariwala[1], Fu Zhang[1], Nasim Alem[1], Joshua A. Robinson[2], Joan M. Redwing[2]

[1]The Pennsylvania State University, PA, UNITED STATES OF AMERICA, [2]2D Crystal Consortium, Materials Research Institute, PA, UNITED STATES OF AMERICA

Monolayer two-dimensional (2D) materials, particularly the family of transition metal dichalcogenides (TMDCs) have been a focus of intense interest since the discovery of graphene. Monolayer semiconducting TMDCs such as MoS_2 and WSe_2 exhibit good carrier mobility as well as mechanical flexibility, which would greatly benefit flexible electronics technology. Prior studies demonstrated that chemical vapor deposition (CVD) and metalorganic CVD (MOCVD) are promising approaches to provide large-scale TMDCs films, but control of the film growth rate at the monolayer and few-layer level remains a challenge. In this work, we investigate the nucleation and growth kinetics of single crystal WSe_2 films deposited on sapphire by MOCVD using tungsten hexacarbonyl ($W(CO)_6$) and hydrogen selenide (H_2Se) in a cold wall vertical reactor at 700 Torr. A three-step process was developed to control nucleation density and size and the lateral growth rate of domains. Initially $W(CO)_6$ is introduced into the reactor at a higher flow rate (~1.2×10^{-3} sccm) for various time periods at 800^{o}C to drive nucleation followed by an annealing period in H_2Se to enable W adatom diffusion and ripening to form oriented WSe_2 islands with uniform size. The $W(CO)_6$ flow rate is then reduced (~4.2×10^{-4} sccm) to limit further nucleation and promote lateral growth and coalescence of domains to form a continuous monolayer film while minimizing secondary layer nucleation. The results demonstrate that the density of WSe_2 nuclei on sapphire increases in proportion to the duration of the nucleation step where the density of nuclei increases from ~5/μm^2 to 100/μm^2 as the nucleation time is increased from 30s to 5min. Annealing the WSe_2 nuclei at 800^{o}C in H_2Se for periods ranging from 5 to 50 minutes results in an initial increase in the average domain size due to ripening followed by small decrease in size likely due to W desorption from the surface. After annealing, film growth occurs laterally from the domain edges at a rate of ~0.01-0.03 monolayer/min at 800^{o}C resulting in coalesced monolayer films with a low density of bilayer coverage after ~45 minutes. High resolution transmission electron microscopy and selected area diffraction analysis of monolayer WSe_2 removed from the sapphire indicate that the films are predominately single crystal, due to preferential orientation of the domains on sapphire, with some low angle grain boundaries. This work shows the potential to obtain high quality monolayer TMDC films over large substrate areas via controlled nucleation and lateral growth in the MOCVD process.

ATOMIC LAYER AND METALORGANIC CHEMICAL VAPOR DEPOSITION OF MOS_2 AND WS_2 FROM BIS(TERT-BUTYLIMIDO)-BIS(DIALKYLAMIDO) COMPOUNDS

Berc Kalanyan[1], James Maslar[1], William A. Kimes[1], Brent A. Sperling[1], Ravindra Kanjolia[2]

[1]National Institute of Standards and Technology, MD, UNITED STATES OF AMERICA, [2]EMD Performance Materials, UNITED STATES OF AMERICA

Layered 2D transition-metal dichalcogenides (TMDs) are finding use in nanoelectronic and optoelectronic applications due to their thickness dependent optical and electrical properties. Scalable fabrication of TMD-based devices requires vapor-phase deposition routes that can produce continuous and uniform films with sub-nanometer thickness control. Atomic layer deposition (ALD) is a desirable route for the synthesis of 2D TMDs and heterostructures due to digital thickness control achieved by sequential self-limiting surface chemistry. However, since ALD conditions are only met at relatively low deposition temperatures, most ALD films are amorphous. Some will consider this a useful feature of ALD, since the growth rate and the structural development of the films can be decoupled by separating the deposition and crystallization steps. In contrast, metalorganic chemical deposition (MOCVD) enables direct growth of crystalline films, but requires careful process control and precursor selection to achieve the required level of thickness control. The tradeoffs between direct CVD growth and post-sufurization and annealing of amorphous/metallic films is the focus of this work. In this paper, we present a comparison of process characteristics and film properties, including growth rate, film thickness, morphology, composition, and crystallinity, as a function of two potential deposition routes: ALD and MOCVD. We deposited thin films using $(N^tBu)_2(NMe_2)_2M$ and 1-propanethiol, where M={Mo,W}, at wafer temperatures of 200°C to 400°C for ALD and 400°C to 900°C for pulsed MOCVD on SiO_2/Si substrates. Precursor saturation conditions were evaluated using non-dispersive infrared optical flow measurements and *ex situ* X-ray photoelectron spectroscopy. As-deposited and sulfur annealed films were further evaluated using X-ray diffraction, Raman spectroscopy, photoluminescence, and atomic force microscopy. As-grown ALD films were amorphous and included a mixture of a sulfide and a conductive phase, likely a nitride. Below 300°C, deposition was limited to a thin surface oxide. Higher temperatures resulted in an increase in growth rate, which also introduced a weak CVD component to the growth. Deposition rates were <0.5 Å/cycle at 350°C. As-deposited films were successfully annealed to 2H-MoS_2 under a sulfur atmosphere, which also removed residual ligands, including nitrogen-containing groups. As-grown MOCVD films were polycrystalline 2H-MoS_2 at 600°C. Pulsed injections of precursor enabled approximately Å-level control over aggregate film thickness. For both ALD and MOCVD, wafer-scale growth and uniformity in a perpendicular flow reactor were demonstrated on 50 mm substrates. In this paper, we will also present similar results and process characteristics for the WS_2 route and discuss initial results from MoS_2/WS_2 nanolaminates.

EFFECT OF SAPPHIRE SUBSTRATE ORIENTATION ON NUCLEATION AND GROWTH OF TRANSITION METAL DICHALCOGENIDES

Tanushree H. Choudhury, Xiaotian Zhang, Joan M. Redwing

The Pennsylvania State University, PA, UNITED STATES OF AMERICA

The role of the substrate in controlling the orientation of films deposited by chemical vapor deposition is well established. The weak out-of-plane bonding in two-dimensional layered chalcogenides allows the growth of these materials on a variety of substrates in spite of large lattice mismatch. It has, however, been demonstrated that the substrate is able to influence the orientation of 2D domains. For instance, for growth on C-plane sapphire, the domain orientations satisfy the weak van der Waals interaction, which locks the orientation at 0° and 60°.[1] In addition, annealing of C-plane sapphire causes step bunching which, in some cases, is shown to aid the growth of oriented domains. It has been observed that nucleation begins at the step edge and growth occurs in one direction.[2] Given the evidence, we investigate the effect of different orientations of sapphire, A-, R- and M-plane in addition to C-plane, on the growth of these materials. The difference in lattice spacing, crystal symmetry and surface energy of these planes could have considerable impact on nucleation and growth. We investigate the growth of WSe_2 and WS_2 on C-, A-, R- and M-planes of sapphire with and without pre-growth annealing. The growth temperature investigated is 600-900°C in the pressure regime of 100-700 Torr. $W(CO)_6$ has been used as the metal precursor while H_2Se and H_2S serve as the chalcogen precursor. The $W(CO)_6$ concentration was maintained at 1.6´10^{-4} sccm to maintain a low nucleation rate, which is crucial in determining the impact on nucleation. The H_2Se and H_2S flow was varied from 4-20 sccm to confirm the effect of chalcogen to metal ratio. Preliminary results show that the nucleation on R-plane sapphire is very dense and mostly localized along the substrate steps, but the TMD grows on both sides of the step. This is unlike C-plane sapphire, where the nucleation is sparse. Additional details will be provided on the effects of substrate orientation and growth conditions on the nucleation density, orientation and growth of the films. Reference: 1. D. Dumcenco et al, *ACS Nano*, 9(4), **2015**, 4611–4620. 2. L. Chen et al, *ACS Nano***,** *9* (8),**2015**, 8368–8375.

EPIGROWTH CHALLENGES FOR HIGH-VOLTAGE SIC POWER DEVICES

James A. Cooper

Sonrisa Research, Inc., UNITED STATES OF AMERICA

Silicon carbide (SiC) power devices entered commercial production in 2001, and are increasingly displacing silicon parts in medium-voltage (900 - 1700 V) power systems. However the full advantage of SiC is most apparent at higher voltages, in the range 3.3 - 25 kV. The most promising voltage-controlled devices in this regime are insulated-gate bipolar transistors (IGBTs) and superjunction (SJ) MOSFETs. Both have long been available in silicon, but both present unique challenges for epigrowth in SiC. SiC superjunction devices can be formed either by repeated epigrowth and implant steps, or by filling deep trenches with epigrown material. In either case, precise and repeatable control of epilayer doping is critical. IGBTs require layer-by-layer control of both doping and ambipolar lifetime, with desired lifetimes ranging from ~100 ns in the non-punchthrough buffer layer to 2 - 5 μs in the overlying drift layer. Recent developments in Japan have resulted in a viable method for lifetime control, making high-voltage SiC IGBTs a practical option. In this talk I will summarize the present state-of-the-art in SiC power switching devices and discuss the epigrowth needs from a device designer's perspective. The SiC power device field is just transitioning from infancy into adolescence, and we have many years of discovery and innovation ahead of us.

IMPACT OF TRANSITION METAL IMPURITIES ON NITRIDE DEVICES

Darshana Wickramaratne

Materials Department, UC Santa Barbara, UNITED STATES OF AMERICA

The application space for power electronics continues to grow and III-nitride based high-electron mobility transistors (HEMTs) are playing an increasingly important role. To achieve the applications envisioned for III-nitride power electronic devices, degradation mechanisms such as current collapse due to carrier trapping should be mitigated. Degradation in the performance of nitride HEMTs has been closely associated with the concentration of iron [1]. Despite the widespread use of iron in nitride HEMTs to achieve semi-insulating substrates, the microscopic understanding of the properties of Fe in the III-nitrides and carrier trapping processes involving Fe remains incomplete. This talk will explore the structural and electronic properties and nonradiative recombination dynamics due to Fe in the III-nitrides using sophisticated first-principles calculations based on density functional theory with a hybrid functional. I will present calculations of the thermodynamic transition levels, optical transition levels and the stability of substitutional and interstitial Fe and its complexes with oxygen and hydrogen in the III-nitrides. For the case of substitutional iron in GaN I will report on a novel mechanism that leads to rapid nonradiative carrier trapping processes [2]. In traditional semiconductors such as silicon, transition metal impurities are known to act as efficient nonradiative carrier recombination centers by introducing midgap defect levels. Iron impurities in GaN do not follow this pattern: their defect level is close to the conduction band. Since nonradiative carrier trapping rates decrease exponentially with the energy of the transition, iron would not be expected to act as a strong nonradiative recombination center. We demonstrate that the high efficiency of iron as a nonradiative center is due to a recombination cycle involving excited states. Our calculations provide insight into the properties of iron in the III-nitrides and the mechanisms of nonradiative carrier trapping processes due to Fe in GaN, which is essential for engineering improved materials to be adopted in efficient devices. This work was supported by the Department of Energy (DOE) and was performed in collaboration with J.-X. Shen, C. E. Dreyer, G. Kresse, S. Marcinkevicius, A. Alkauskas, and C. G. Van de Walle. [1] S. Mukherjee *et al.*, IEEE Trans. Electron Devices, vol. **63**, no. 4 (2016)

[2] D. Wickramaratne *et al.*, Appl. Phys. Lett. **109**, 162107 (2016).

GROWTH OF GA_2O_3 FOR DEVICE PRODUCTION

Serdal Okur[1], Nick Sbrockey[1], Tom Salagaj[1], Gary Tompa[1], Yao Yao[2], Robert Davis[2], Lisa Porter[2], Luke Lyle[2]

[1]Structured Materials Industries, Inc., UNITED STATES OF AMERICA, [2]Carnegie Mellon University, UNITED STATES OF AMERICA

Having one of the widest energy bandgaps (~4.9 eV) – larger than SiC (3.3 eV) or GaN (3.4 eV) – Ga_2O_3 has many attractive properties not only for power devices but also for gas sensors, TCOs, and solar- or visible-blind UV sensors, among others. The growth of thick, low-doped Ga_2O_3 drift regions in is still a challenge. The present primary growth rate limiting factor is the growth chemistry; however, as processes are explored, many process parameters remain to be optimized; such as temperature, pressure, precursors, and chemical ratios. We have introduced Hydride Organometallic Vapor Phase Epitaxy (HOVPE) and Hydride Vapor Phase Epitaxy (HVPE) techniques to our core Metalorganic Chemical Vapor Deposition (MOCVD) Ga_2O_3 process technology to extend operations to address low (MOCVD), medium (HOVPE), and high (HVPE) growth rates in a single rotating disc reactor (RDR), wherein a chlorine source can be introduced with metalorganics to achieve an accelerated growth rate in our in-house RDR using a 13" platter. The growth rate of Ga_2O_3 films was investigated for different growth modes using HCl flow rates varied between 0 and 60 sccm with triethyl gallium (TEGa) and Ga on sapphire substrates. O_2 is used as the oxygen source. The growths include (i) TEGa+O_2+HCl (0 – 60 sccm) at 650 °C and (ii) Ga+O_2+HCl at 650-800 °C. XRD analysis showed that different growth modes and parameters provided α-, β- and ε-phases. TEGa+O_2 provided β-phase togher with some mixed phases, whereas Ga+O_2 provided predominantly α- and ε-phases. The possible explanation for the difference of the α- and ε-phases in HVPE runs might be due to one order of magnitude difference of oxygen used; 80 vs 800 sccm, respectively. The growth rate showed an exponential increase when HCl flow increased from 5 sccm to 30 sccm (up to 0.8 μm/h) followed by a sharp decrease with additional HCl. HVPE mode produced growth rates up to 3.2 μm/hour at same substrate temperature (650 °C). 800 °C provided lower growth rate than 650 °C reaching up to 2 μm/hr. Additionally, SIMS analysis provided that the chlorine concentration in 650 °C sample varied between $\sim 2\times10^{17}$ and $1\times10^{18}/cm^3$, while it was hovered around $1\text{-}2 \times 10^{16}/cm^3$ in 800 °C sample, both of which produced ε-phase. Both ε-phase samples contained higher Cl concentrations than the α-phase sample grown at 650 °C. All experiments show that the growth of Ga_2O_3 films is very sensitive to growth mode and parameters.

CONTROLLING SCINTILLATOR PROPERTIES VIA CODOPING: AN OVERVIEW

Chuck Melcher, Merry Koschan, Mariya Zhuravleva, Adam Lindsey, Yuntao Wu, Harold Rothfuss, Fang Meng, Sam Donnald, Kan Yang, Jason Hayward, Lars Eriksson

Scintillation Materials Research Center, TN, UNITED STATES OF AMERICA

Scintillation materials that lack intrinsic luminescence centers must be doped with optically active ions in order to provide luminescent centers that radiatively de-excite as the final step of the scintillation process. Codoping, on the other hand, can be defined as the incorporation of additional specific impurity species usually for the purpose of modifying the scintillation properties, mechanical properties, or the crystal growth behavior. In recent years codoping has become an increasingly popular approach for engineering scintillators with optimal performance for targeted applications. This report reviews several successful examples together with their underlying physical mechanisms. Codoping has been used successfully to improve the proportionality of the scintillation light yield with respect to absorbed gamma-ray energy and thus improve energy resolution that is needed for reliable spectroscopic identification of radioisotopes. Codoping has been used to control the trapping of free electrons, thus affecting the kinetics of energy transfer through the crystal lattice to luminescence centers. Both the rise time and the decay time of the scintillation time profile may be modified in this way. Codoping can have a profound effect on the scintillation mechanism itself by changing the valence of the luminescence centers. Optically active codopants can be used to shift the emission wavelength of the scintillation light. The sensitivity to radiation damage of certain scintillators has been dramatically reduced by codoping, and codoping has also been used to improve the mechanical properties of some scintillators. Crystal growth stability can be improved in some cases by controlling heat transport via codopants that absorb in the infrared and by codopants that increase surface tension in Czochralski growth.

INFLUENCE OF CODOPING, NON-STOICHIOMETRY AND GA ADMIXTURE ON LUAG:CE SCINTILLATION PROPERTIES

Jan Pejchal[1], Vladimir Babin[1], Alena Beitlerova[1], Romana Kucerkova[1], Petr Prusa[1], Dalibor Panek[2], Tomas Parkman[2], Kei Kamada[3], Akira Yoshikawa[4]

[1]Institute of Physics CAS, CZECH REPUBLIC, [2]Faculty of Biomedical Engineering, Czech Technical University, CZECH REPUBLIC, [3]NICHe, Tohoku University, JAPAN, [4]Institute for Materials Research, Tohoku University, JAPAN

We focused on study of the influence of Mg codoping, non-stoichiometry and Ga-admixture on the scintillation and luminescence characteristics of Ce-doped lutetium-aluminum garnet crystals (LuAG), the stability of the Ce valence and role of defects. The LuAG single crystals were grown by micro-pulling-down method with radiofrequency inductive heating using an iridium crucible with a die of 3 mm in diameter. The growth was performed from slightly overheated melt to decrease the melt viscosity and increase wettability allowing the melt to spread over the whole diameter of the die. The hot-zone and afterheater were modified to keep a very steep vertical temperature gradient and mild radial gradient to improve the crystal quality. The Ce-doped LuAG crystal rods with a diameter of 3 mm and 35 to 45 mm in length were successfully prepared. The Mg codopant concentration ranged from 0 to 3000 ppm. Two Ce, Mg-codoped samples grown from Al-rich melt (1at% and 3at% excess) were prepared to study the influence of non-stoichiometry. Ga admixed LuGAG crystals with the same Ce and Mg concentrations were grown as well together with the Al-rich analogs. Regarding the Ce-doped LuAG samples, codoping of Mg at a concentration around 300 ppm led to improvement of overall scintillation efficiency, which is in accordance with previous studies and can be attributed to an alternative scintillation mechanism involving Ce^{4+} stabilized by Mg^{2+}. Higher Mg concentrations around 3000 ppm did not bring any further improvement. When the non-stoichiometry of the LuAG matrix for the Ce0.2% Mg 300 ppm sample was 1at%, practically no influence was observed yet, while very significant improvement of the overall scintillation efficiency (almost a factor of 2) when compared to the stoichiometric sample was observed for the Ce0.2% Mg 300 ppm sample with 3at% nonstoichiometry. Light yield increase was observed as well. The highest Mg concentration brings additional slow components to the scintillation decay. Very similar trends were observed for the Ga-admixed LuGAG, but the luminescence related to the exciton trapped at the anti-site defect was strongly suppressed. Suppression of this competitive luminescence channel led to further improvement of the overall scintillation efficiency. The steady-state and time-resolved photoluminescence and scintillation measurements on the above samples will be presented in the relation with composition and crystal growth condition and the scintillation mechanism will be discussed.

CRYSTAL GROWTH AND TEMPERATURE DEPENDENCE OF LIGHT OUTPUT OF CE-DOPED (GD, LA, Y)$_2$SI$_2$O$_7$ SINGLE CRYSTALS

Takahiko Horiai[1], Shunsuke Kurosawa[2], Rikito Murakami[3], Yasuhiro Shoji[1], Jan Pejchal[4], Akihiro Yamaji[1], Yuji Ohashi[5], Kei Kamada[5], Yuui Yokota[5], Tomohiro Ishizu[6], Yasuo Ohishi[6], Taisuke Nakaya[6], Akira Yoshikawa[5]

[1]IMR, Tohoku University, JAPAN, [2]Faculty of Science, Yamagata University, JAPAN, [3]C&A Corporation, JAPAN, [4]Institute of Physics CAS, CZECH REPUBLIC, [5]NICHe, Tohoku University, JAPAN, [6]Hamamatsu Photonics K. K., JAPAN

Scintillation crystals are used in several fields, and one of the application fields is oil well logging operating at high temperatures over 150°C. Thus, the scintillation crystals are required high light outputs even at high temperature. To satisfy this requirement, Ce-doped (Gd,La)$_2$Si$_2$O$_7$ (Ce:La-GPS) has been investigated. Ce:La-GPS has a light output at room temperature of ~42,000 photons/MeV and fast decay time of ~63 ns, and the light output remained even at 150°C [1-3]. Here, in previous study, the thermal quenching of Y admixed Ce-doped Lu$_2$SiO$_5$ was suppressed compared to before Y^{3+} substitution [4,5]. Thus, in this study, we focused on Y admixed Ce:La-GPS to improve temperature dependence. First of all, (Ce$_{0.01}$ Gd$_{0.59\text{-}x}$ La$_{0.4}$ Y$_x$)$_2$Si$_2$O$_7$ (x=0.00, 0.05, 0.10, and 0.15) single crystals were grown by the micro-pulling-down (μ-PD) method. After growth, we evaluated single phases by the powder X-ray diffraction analysis for these samples. In addition, we measured optical and scintillation properties. Finally, we estimated the temperature dependence of light outputs within 25-175°C using a ^{137}Cs gamma-ray source. Thereafter, we grew a 1-inch crystal using the Czochralski (Cz) technique to obtain better quality of a crystal than crystals grown by the μ-PD method. The light output values of Y 0%, Y 5%, Y 10%, and Y 15% admixed Ce:La-GPS grown by the μ-PD method were determined to be ~42,000, ~43,000, ~36,000, and ~33,000 photons/MeV, respectively. Moreover, the light outputs of Y 0%, Y 5%, Y 10%, and Y 15% admixed Ce:La-GPS at 175ºC were 80%, 93%, 94%, and 73% of that at 25ºC, respectively. From these results, we considered (Ce$_{0.01}$ Gd$_{0.54}$ La$_{0.4}$ Y$_{0.05}$)$_2$Si$_2$O$_7$ (Ce:LaY-GPS) was the most suitable for the use of oil well logging. Therefore, we grew a 1-inch crystal about Ce:LaY-GPS. Here, Fig. 1 shows the photograph of a Ce:LaY-GPS single crystal grown by the Cz technique, and we succeeded in growing a transparent sample. In this work, we report the crystal growth and discuss the optical and scintillation properties

[1] A. Suzuki, A. Yoshikawa, et al., Appl. Phys. Express **5** (2012) 102601. [2] S. Kurosawa, A. Yoshikawa, et al., Nucl. Instrum. Methods Phys. Res. A **772** (2015) 72. [3] T. Horiai, A. Yoshikawa, et al., Opt. Mat. **65** (2017) 56. [4] H. Suzuki, et al., IEEE Trans. Nucl. Sci. **40** (1993) 380. [5] L. Pidol, et al., IEEE Trans. Nucl. Sci. **51** (2004) 1084.

GROWTH AND SCINTILLATION PROPERTIES OF DIRECTIONALLY SOLIDIFIED CE:LABR3/AEBR2 (AE=MG, CA, SR, BA) EUTECTIC SYSTEM

Akria Yoshikawa[1], Yuki Furuya[2], Kei Kamada[3], Hiroyuki Chiba[2], Shunsuke Kurosawa[4], Akihiro Yamaji[5], Yasuhiro Shoji[5], Yuji Ohashi[5], Yuui Yokota[6]

[1]C&A Corporation, JAPAN, [2]Institute for Materials Research (IMR), JAPAN, [3]C&A corporation, JAPAN, [4]Department of Physics, Yamagata University, JAPAN, [5]Institute for Materials Research, Tohoku University, JAPAN, [6]New Industry Creation Hatchery Center, Tohoku University, JAPAN

In the X-ray imaging applications, radiation imaging sensors were composed of photodetector arrays and indirect flat panel detector (FPD) coupled with a scintillator plate such as Tl:CsI or Gd2O2S:Tb (GOS). Improvement in the spatial resolution is required in this application. Recently, pixilated photodetector arrays has been improved to achieve a micrometer scale special resolution. However, pixel size of scintillator arrays and the light diffusion limit the spatial resolution.

So far, submicron-diameter phase-separated scintillator fibers (PSSFs) were reported [1]. They have both characteristics of optical fiber and a radiation-to-light conversion. In PSSFs, the emitted scintillation is confined and transported along the eutectic structure by a total reflection mode, so that light diffusion can be reduced and high-resolution imaging can be achieved. The PSSFs were realized by a directionally solidified eutectic (DSE) growth in previous research [2].

In order to find good combination of eutectic structure with PSSFs, choice of scintillator materials is important. In this research, Ce doped LaBr3/AEBr2 (AE = Mg, Ca, Sr, Ba) eutectics were explored. Ce:LaBr3 is a promising scintillator which has high light yield of over 74,000 photons/MeV and fast decay time of around 20 ns with enough density of 5.1 g/cm3 for low energy X-ray detection even it is hygroscopic [3]. We designed matrix AEBr2 phase and scintillation LaBr3 fibers at the eutectic point of LaBr3/AEBr2. Crystal growth was performed by Bridgman–Stockbarger (BS) method in a quartz ampoule with 4mm inner diameter. The eutectic showed optical transparency like bundle optical fibers (Fig. 1). Investigations of their crystal structure and eutectic phase were performed by XRD. Luminescence and scintillation properties were also evaluated. Grown Ce doped LaBr3/CaBr2 eutectic shows 355 nm emission ascribed to Ce3+ 4f-5d transition under X-ray excitation. The light yield of Ce: LaBr3/CaBr2 was around 1/2 of Ce:Lu2SiO4 (LYSO) standard and 13,500 photon/MeV. Scintillation decay time under 662keV gamma-ray was 22.4 ns (60%) 185 ns (40 %). Growths and characterizations of other material LaBr3/AEBr2 (AE = Mg, Sr, Ba) will be discussed in the presentation.

Fig. 1. BEI of the polished LaBr3/CaBr2 eutectic crystal, a) transverse cross-section and b) vertical cross-section along growth direction. Reference

[1] Ohashi, Yoshikawa et al., Applied Physics Letters, 102 (5) 051907
[2]J. Llorca and V. Orera, Prog. Mater Sci. 51 (2006) 711

[3] E. V. D. van Loef, P. Dorenbos, et al., Transactions on Nuclear Science, Nucl. Inst. Method A486 (2002) 254-258

CRYSTAL GROWTH AND SCINTILLATION PROPERTIES OF ND-DOPED (GD, LA)$_2$SI$_2$O$_7$ CRYSTAL AS INFRA-RED SCINTILLATOR

Shunsuke Kurosawa[1], Toetsu Shishido[2], Takahiko Horiai[2], Shohei Kodama[3], Takamasa Sugawara[3], Kunio Yubuta[2], Akihiro Yamaji[3], Yuji Ohashi[3], Yuui Yokota[4], Kei Kamada[5], Akira Yoshikawa[3]

[1]Faculty of Science, Yamagata University, JAPAN, [2]Institute for Materials Research,Tohoku University, JAPAN, [3]Institute for Materials Research, Tohoku University, JAPAN, [4]New Industry Creation Hatchery Center, Tohoku University, JAPAN, [5]C&A corporation, JAPAN

Scintillators are applied to several fields such as medical imaging and high-energy physics as radiation detectors. Radiation therapy has been widely used to treat the tumor. However, it is said that some medical accidents occur due to over dose [1]. Thus, real-time dose-monitoring system is expected to save the accident. Here, human body has an optical transparent area around near infra-red region (650 to 1200 nm), and using this “window”, a novel real-time dosimeter system can be developed with infra-red emission scintillators; When X rays or other radiation particles for medical use generate the scintillation light in the infra-red scintillator, the luminosity or count rate of infra-red scintillation light can be read out of the patient. Since the dose is related to the luminosity or count rate, we can measure the dose with a real time Recently, novel scintillator, $(Ce_{0.01},Gd_{0.90},La_{0.09})_2Si_2O_7$ (Ce:La-GPS: Cerium-doped lanthanum-gadolinium pyrosilicate) was found to have a high light output of roughly 35,000 – 42,000 photons/MeV and energy resolution (FWHM) of ~5% at 662 keV [1,2]. Here, typical emission wavelength of Nd-doped scintillators or phosphors are located at around 850 – 1100 nm. Thus, Nd-doped samples are the candidate for the above application (real time monitor). In this paper, we show the crystal and scintillation properties of $(Nd_{0.01}\quad Gd_{0.90}\quad La_{0.09})_2Si_2O_7$ grown by floating zone (FZ) method. The crystal was grown by the FZ method under argon atmosphere, with a pulling down rate of 1 ~ 5 mm/hour and rotation rate of 20 rpm. As-grown crystals were cut into a 1-mm thickness and then polished to a mirror gloss. We confirmed the sample has a single phase and monoclinic crystal system by X-ray diffraction pattern. Photo-luminescence and radio-luminescence emission spectra were measured. Infra-red emissions originated from Nd^{3+} 4f-4f (e.g. $^4F_{3/2}$à $^4I_{11/2}$ and $^4I_{9/2}$) transitions were observed around 900 and 1050 nm when the sample was excited by X rays. Thus, this material was fond to be one of the candidate for the real time monitor in medical use. In this paper, we show the above results and temperature dependence of the light output, and discuss several optical properties such as the energy transfer Gd^{3+}-to-N^{d3+}. [1] A. Suzuki, *et al.*, APEX, 5, p. 102601 (2012). [2] S. Kurosawa, *et al.*, NIMA, 744, 30–34 (2014)

IN-SITU ATOMIC FORCE MICROSCOPY STUDIES OF POLYMER MICELLE-CALCITE INTERACTIONS

Lara A. Estroff, Coit Hendley

Cornell University, NY, UNITED STATES OF AMERICA

Incorporating guest materials into single crystals is of significant interest because of the potential for synthesizing composites with emergent properties. Calcite serves as an ideal model system for studying additive-crystal interactions because it is cheap, abundant, and relatively easily incorporates a range of additives. Previous work has used in situ AFM to study the modification of calcite growth by atomic substitutions, small molecules, and peptides. More recently, ex situ growth of calcite with polymeric micellar particles >10 nm in diameter has demonstrated that incorporation amounts depend strongly on the surface chemistry of the particles. I will present our recent *in situ* AFM studies of the population dynamics of polymer micelles with varying surface chemistries as they interact with growing calcite hillocks. We have identified three possible behaviors of the micelles at the crystal surface: attaching and detaching, becoming incorporated into the crystal, or “hovering” on the surface. We show that the micelle charge corona plays the most important role in determining which type of interaction dominates for a given particle chemistry. For micelles with polyelectrolyte stabilizer chains, we propose a two-state binding model in which the micelle-crystal interactions are governed by a transition from an extended state to a collapsed state of the polyelectrolyte chains. This work explores the role of the coronal charge, solution ionic strength, and supersaturation in determining the interaction between individual micelles and calcite growth hillocks. These results have the potential to lead to design criteria for polymer-reinforced crystalline materials with unique structure-property relationships.

NUCLEATION AND GROWTH OF CRYSTALLINE CARBONATES FROM AMORPHOUS PRECURSORS

Derk Joester

Northwestern University, IL, UNITED STATES OF AMERICA

Energy-efficient synthesis of materials locked in compositional and structural states far from equilibrium remains a challenging goal. Biomineralizing organisms routinely assemble such materials with sophisticated design and advanced functional properties, often using amorphous precursors. Organic macromolecules and inorganic additives such as magnesium ion are thought to play an important role in controlling phase transformations in these systems. However, it has proven extremely challenging to accurately describe pathways and determine mechanisms, even for extensively studied system such as amorphous calcium carbonate (ACC). I will discuss recent work in my laboratory in which we use liposomes and microfluidic droplets as nano-to-microscale reactors to study the impact of confinement, biomolecules, and inorganic additives on the kinetics of crystallization of ACC and its barium-substituted derivative (ACBC). In the course of this work, we discovered bulk syntheses leading to two other metastable, yet crystalline carbonates that we call balcite and gortotowskite. Balcite is isostructural with a high temperature modification of calcite and has exceptional hardness; its kinetics of formation hint on a complex, possibly non-classical mechanism. Gortotowskite on the other hand is a barium carbonate monohydrate that crystallizes in quasi-two-dimensional habit. These findings demonstrate that microfluidic devices are a powerful tool in the study of phase transformations of the rich chemistry of metastable carbonates.

GUINIER-PRESTON ZONES WITHIN A BIOGENIC SINGLE CRYSTAL: A BIOLOGICAL PRESTRESSING STRATEGY

Boaz Pokroy

Technion Israel Institute of Technology, ISRAEL

Crystals produced by organisms, in contrast to a large portion of synthetic crystals, are formed in ambient conditions and with a limited selection of elements. Nevertheless, living organisms reveal elegant strategies for achieving specific functions, ranging from skeletal support to mastication, from sensors and defensive tools to optical function. In this talk will show that utilizing state-of-the-art characterization techniques, we observed a remarkable biostrategy, hitherto unidentified, for strengthening and toughening the otherwise brittle calcite optical lenses found in the brittlestar *Ophiocoma wendtii*. This intriguing process employs coherent nanoprecipitates to induce compressive stresses on the host crystal matrix, functionally resembling the Guinier–Preston zones known in classical metallurgy. We believe that these calcitic nanoparticles, being rich in magnesium, segregate during or just after transformation from amorphous to crystalline phase, similarly to segregation behavior from a supersaturated quenched alloy.

ENGINEERING CORRELATED DIRAC ELECTRONS IN SRIRO$_3$/SRTIO$_3$ SUPERLATTICE

Hidenori Takagi[1], Daigorou Hirai[1], Naoka Hiraoka[1], Jobu Matsuno[2]

[1]Department of Physics, University of Tokyo, JAPAN, [2]RIKEN, JAPAN

In 5d Iridium oxides, a large spin-orbit coupling of l_{so}~0.7 eV, inherent to heavy 5d elements, is not small as compared with other relevant electronic parameters, including Coulomb U, transfer t and crystal field splitting D, which gives rise to a variety of exotic electronic states. In the layered perovskite Sr_2IrO_4, a spin-orbital Mott state with $J_{eff}=1/2$ is realized due to the interplay of lso and U [1,2]. The three-dimensional analog of Sr_2IrO_4, $SrIrO_3$, distorted perovskite, is a correlated semimetal with Dirac nodes protected by crystalline symmetry [3]. Using $(SrIrO_3)_m/SrTiO_3$ (m: number of $SrIrO_3$ layers) super-lattice structure on $SrTiO_3$ (001) substrate, we could have controlled successfully the dimensionality and hence increasing effective Coulomb U [4]. With decreasing the number of $SrIrO_3$ layers, we observe a Dirac semimetal to insulator transition at m=3, accompanied with the onset of canted antiferromagnetism. This can be understood as a gapping of the Dirac nodes by breaking time reversal symmetry with magnetic moments. At m=1, the single layer, the transport remains insulating even above the magnetic ordering temperature, indicative of the increased spin-orbital Mott character as in Sr_2IrO_4. Electron doping for m=1 was attempted by doping La for Sr, which made system almost metallic. No trace of superconductivity was observed. (111) superlattice $(Sr_{0.5}Ca_{0.5}IrO_3)_m/(SrTiO_3)_2$ was also successfully fabricated [5]. We observed analogous behavior as observed for (001) superlattice. Dirac semimetal-magnetic insulator transition was observed at m=6 with decreasing m. The bilayer m=2 film, pointed out theoretically to have a possible topological state [6], was insulating all the way up to room temperature. 1) B. J. Kim *et al.*, *Phys. Rev. Lett.* **101**, 076402 (2008). 2) B. J. Kim *et al.*, *Science* **323**, 1329 (2009). 3) Chen, Y. et al. ,Nat. Commun. 6:6593 doi: 10.1038/ncomms7593 (2015). 4) J. Matsuno *et al.*, *Phys. Rev. Lett.* **114** 240749 (2015). 5) D. Hirai *et al*, APL mat **3**, 041508 (2015).2015) 6) D.Xiao *et al.,* Nature Communications 2:596 (2011).

EPITAXIAL GROWTH OF LOW VALENCE TRANSITION-METAL OXIDES EXHIBITING NOVEL ELECTRONIC STATES

Akira Ohtomo

Tokyo Institute of Technologuy, JAPAN

The early transition-metals (such as Ti, V, and W) form oxides with a variety of crystal structures as well as oxidation states. The connectivity of the oxygen octahedra network and *d*-band filling are known to play an important role in the electronic phase stability. In this context, there has been continued focus on, for example, controlling competition between Mott/Pierels insulators and correlated metals, because novel phenomena such as superconductivity and a metal-insulator transition often emerge at the phase boundaries. On the other hand, conventional approaches for growing low valence (and often lower symmetry) materials suffer from very high oxygen affinity of those metals. Here we present our recent study on epitaxial growth of low valence transition-metal oxides exhibiting novel electronic states. Starting preparation of reduced source materials, pulsed-laser deposition are conducted on selected substrates under Ar atmospheres. We also implement a Li-ion battery structure for intercalation of the Li ions (*i.e.*, post-growth doping). Our findings upon non-equilibrium thin-film synthesis are summarized as follows. (1) Superconductivity in Ti_4O_7 and gamma-phase Ti_3O_5 with the transition temperatures of 3.0 K and 7.1 K, respectively, both of which have insulating ground states in bulks. (2) Strain induced metal-insulator transition in a perovskite titanate, which has metallic ground states in a free-standing bulk. Similar strain induced effects are seen for perovskite vanadates. (3) Complete and reversible superconductor-insulator transitions in $LiTi_2O_4$ films induced by Li-ion electrochemical reaction. Our approach is a suitable way to demonstrate the unpreceded phenomena in early transition-metal oxides. This work was supported by MEXT Elements Strategy Initiative to Form Core Research Center.

WHAT TO DO WHEN YOUR IDEAL SINGLE CRYSTAL SUBSTRATE IS NOT AVAILABLE: HOW COMBINATORIAL SUBSTRATE EPITAXY OPENS NEW DOORS TO EPITAXIAL SYNTHESIS.

Paul A. Salvador[1], Gregory S. Rohrer[1], John R. Kitchin[1], Wilfrid Prellier[2]

[1]Carnegie Mellon University, UNITED STATES OF AMERICA, [2]Laboratoire CRISMAT, CNRS UMR 6508, ENSICAEN, Universite de Basse-Normandie, FRANCE

Over the past few decades, advancement in epitaxial growth of complex oxides has been remarkable. Surprisingly, most of these advances have been made using a surprisingly small number of commercially available single crystal substrates. Only a few compositions of single crystals are available in very common oxide structures (perovskite, fluorite, corundum, rock salt, etc.); for less common structures there are often none available. If appropriate substrates were available across all interesting structural families, we would vastly expand our abilities to fine tune the design and synthesis of metastable and artificial crystals with structures and properties not found in nature. We have been developing a new approach to epitaxial stabilization for the synthesis of novel materials (metastable polymorphs) that cannot be and/or have not been fabricated through other synthesis techniques. We call this approach Combinatorial Substrate Epitaxy (CSE). In CSE we use epi-polished polycrystalline ceramics as substrates and automated electron backscatter diffraction as a non-destructive local structural characterization method. We map the orientation of hundreds of substrate grains prior to growth, then map film orientations on those same grains after deposition, and use in-house programs to determine the epitaxial orientation relationships (ORs) across all of orientation space (in a single experiment). I will review the primary observations we have made using CSE, both benchmarking it against standard epitaxial growth on single crystals and highlighting novel materials generated owing to the expansion of substrate families. In general, each grain in a polycrystal behaves as an individual single crystal substrate, usually exhibiting grain-over-grain epitaxial growth. A bit surprisingly, there are only a small number (one or two) of epitaxial ORs observed across orientation space, which are largely independent of the surface orientation. On substrates where competitive polymorph nucleation occurs, the winner of the competition can be rationalized using observed ORs and planar matching on low-index orientations. Because of this, we have been able to develop a computational method that guides epitaxial synthesis. Density functional theory computations are combined with continuum models of nucleation to guide the selection of thermodynamically accessible materials and polymorph directing substrates. I will use a variety of film / substrate structural pairs to make these points, including BO_2, B_2O_3, ABO_3, A_2BO_4, and $A_2B_2O_7$. I will describe how CSE opens the door for the predictive design of materials with new properties and the synthesis pathways to make them, as well as validation methods needed to measure both structures and properties.

GROWTH-MICROSTRUCTURE-(ELECTRONIC)PROPERTY CORRELATIONS IN 2D MATERIALS.

Srinivasan Raghavan

Indian Institute of Science, INDIA

In the emerging field of 2-D materials, controlled number of monolayers are required over large areas for device applications. These monolayers are polycrystalline and are formed by nucleation and coalescence of islands. Controlling nucleation density and edge growth rates during deposition help to tailor the grain boundary density length per unit area. While sensor applications prefer more grain boundary length and hence larger nucleation density, transistors demand the exact opposite. In addition, to grain boundary length, the structure of the grain boundary itself significantly modifies transport properties and is affected by growth conditions. In graphene, for instance, monolayers that do not show any dissimilarities when characterized by Raman or scanning electron microscopy, show a 40 fold reversible change in mobility depending on growth conditions. The talk will discuss the correlations between growth parameters, graphene structural changes, methods of characterizing them in large area graphene and these mobility changes that can only be detected by electrical probing. In multi-element systems such as MoS_2, the preferred semiconductor of the 2D world, in addition to grain boundaries, stoichiometry plays a significant role. the growth space and chemistry are also more complicated. Following the discussion on graphene, the conductor of the 2-d world, the abilty to control island sizes form values as low as 30 nm to as large as 100 microns by controlling kinetics in thermodynamically predicted windows will be demonstrated. In the thermodynamic windowns the effect of supersaturations established in the vapor phase, the resultant steady state potentials on the growth surface and their effect on the structure, stoichiometry and device characteristics of MoS_2 will be used to compare and contrast the challenges in growing these two important materials.

GROWTH OF LARGE-AREA, SINGLE-CRYSTAL GRAPHENE AND GRAPHENE BILAYERS FOR ELECTRONIC DEVICES

Yufeng Hao

Nanjing University, CHINA

As first truly and the most important two-dimensional material, graphene keeps standing at the frontier

of two-dimensional materials research field. Therefore, growth of high-quality and layer number controlled graphene films is of great value for scientific research and various applications. In this presentation, I will focus on the recent progress in the identification of new growth mechanisms towards large-area single-layer graphene single crystals and millimeter-size bilayer graphene domains (grains) on Copper: Multiple control experiments and first-principles calculations are used to support the proposed mechanisms. We emphasize that trace amount of oxygen impurities on Cu surface are critical to initiate graphene growth and affect the growth kinetics. Furthermore, contrary to the traditional viewpoint that graphene growth is always surface-limited process, our new observations strongly suggest that metal bulk plays a role to feed carbon species for the growth of additional graphene layers. State-of-the-art structural characterizations and electrical transport measurements of the CVD graphene layers will be presented as well. Ref 1. Y. F. Hao et al., Oxygen-Activated Growth and Bandgap Tunability of Large Single-Crystal Bilayer Graphene,

Nature Nanotechnology 2016,11,426-431.(Cover Story)

Ref 2. Y. F. Hao et al., The Role of Surface Oxygen in the Growth of Large Single-Crystal Graphene on Copper,

Science 2013, 342, 720-723.(Cover Story)

SYNTHESIS AND CHARACTERIZATION OF GRAPHENE BASED THERMOACOUSTIC DEVICES

Nick Sbrockey[1], Tom Salagaj[1], Thottam Kalkur[2], Gary Tompa[1]

[1]Structured Materials Industries, NJ, UNITED STATES OF AMERICA, [2]University of Colorado at Colorado Springs, UNITED STATES OF AMERICA

Thermoacoustic devices create sound waves by thermal heating of the surrounding medium. This differs from conventional acoustic transducers, which use mechanical displacement to create sound waves. Building a thermoacoustic device requires a material with a very low heat capacity, so that it can thermally cycle at audible frequency. The material must also have a low (but finite resistance), so that it can be Joule heated. The material must also be strong and resistant to degradation at moderate temperatures in the acoustic medium. Graphene is a nearly ideal thermoacoustic material. Graphene films of a few atomic layer thickness have low resistivity and very small heat capacity. Graphene is also strong and resistant to oxidation in air at temperatures up to about 300 C. Graphene based thermoacoustic devices have several potential advantages over traditional loud speakers and acoustic transducers; including light weight, flexibility, high efficiency, large surface area and installation over complex geometries. Graphene based thermoacoustic devices could provide significant advantages for applications in entertainment, audio, public address, noise cancellation and sonar systems. This presentation describes fabrication and characterization of thermoacoustic devices based on few layer graphene films. The graphene films were grown by chemical vapor deposition on nickel and copper foil substrates, then transferred to flexible plastic substrates. Techniques for patterning and electrical contact formation were developed. The graphene thermoacoustic devices were characterized in an anechoic chamber. The sound output (in dB) was monitored as a function of the input electrical signal current and frequency, in the audible frequency range up to 10 KHz. A superimposed DC voltage bias is also important for low distortion sound output. The characterization also included simultaneous measurement of the average surface temperature of the device using an infrared pyrometer. Accurate sound reproduction was demonstrated with graphene based thermoacoustic devices, including voice and music. The efficiency of the graphene based thermoacoustic device is limited by the thermal quenching effect of the substrate. The maximum sound output is limited by degradation of the graphene film at high input power levels.

MECHANISMS OF HYDROGEN INTERCALATION IN EPITAXIAL GRAPHENE

Kevin M. Daniels[1], Anthony Boyd[2], Anindya Nath[3], Rachael Myers-Ward[2], Kurt Gaskill[2]

[1]National Research Council Postdoctoral Fellow residing at the US Naval Research Laboratory, DC, UNITED STATES OF AMERICA, [2]US Naval Research Laboratory, DC, UNITED STATES OF AMERICA, [3]George Mason University, VA, UNITED STATES OF AMERICA

Epitaxial growth of graphene via sublimation of silicon and graphitization of carbon atoms from silicon carbide (SiC) is ideal for large scale manufacturing. Covalent bonding, however, between the SiC (0001) substrate and the first carbon layer (6√3 buffer layer) significantly reduces the mobility to values lower than desired for many electronic and optoelectronic devices. This lowered mobility in epitaxial graphene (EG) is a consequence of (temperature dependent) SiC phonon scattering. The objective of this work is to clarify the mechanism of hydrogen intercalation, used to overcome phonon effects and improve the mobility where the interfacial Si dangling are passivated by hydrogen atoms. The 6√3 buffer layer is released from the SiC substrate where it is then promoted to a new Bernal staked layer of EG creating high mobility quasi-free standing epitaxial graphene. A systematic study of the hydrogen passivation of the Si dangling bonds is carried out, varying temperature, duration and substrate off-cut to observe how hydrogen is incorporated into the material. Nominally monolayer (ML) EG is synthesized from semi-insulating, (0001) 6H-SiC of three different offcuts in an Aixtron/Epigress VP508 horizontal hot-wall reactor. H-intercalation of EG was carried out in the same reactor, where the reactor is cooled to 950-1050°C with a flow of 80 slm of H_2 and a chamber pressure of 900 mbar for 60 minutes. Degree of intercalation is determined by Atomic Force Microscopy (AFM), Kelvin Probe Force Microscopy (KPFM), Hall, Raman and Scanning Electron Microscopy (SEM). SEM images of samples incompletely intercalated show constrasting regions down to a size scale comparable to the instrument resolution, ~20 nm. To elucidate the nature of these contrasting reigons, KPFM was performed. We assume samples with the highest mobility are fully intercalated, in these cases the KPFM variation was ~30 mV. For samples intercalated for shorter times and having lower Hall mobility, the local surface potential showed variation of ~180 mV. These measurements imply the formation domains having differing sheet charge density during the intercalation process with a size scale ~20 nm. We propose two intercalation mechanisms, the first is where hydryogen passivations of Si begins at the step edges and continues inward under the terraces. And the second is through defects which enable movement of hydrogen under the graphene. Mix of carriers in partially intercalated EG is of interest in applications such as linear p-n junctions.

FLOATING-ZONE CRYSTAL GROWTH AND CHARACTERIZATION OF THE SCINTILLATOR $MG_4TA_2O_9$

Dongsheng Yuan, Didier Perrodin, Tetiana Shalapska, Edith D. Bourret, Gregory A. Bizarri

Lawrence Berkeley National Laboratory, CA, UNITED STATES OF AMERICA

High-energy radiography is a strategic and critical technique for rapid detection of radioactive materials. $Mg_4Ta_2O_9$ was selected from a high-throughput search of tantalates and is now being developed for that application with the expectation to supersede the currently used tungstates in term of luminosity and cost and to top CsI in term of stopping power and afterglow. We report the synthesis, crystal growth, and characterization of $Mg_4Ta_2O_9$ and evaluate its intrinsic scintillation properties. $Mg_4Ta_2O_9$ has a trigonal crystal structure, and is observed to melt congruently at an unknown temperature but higher than 1800 ^{o}C. Single crystals were obtained by using floating-zone method at a pressure of 2 bar in air and with an excess of MgO (1 mol%) to compensate for an observed evaporation. Single crystal cylinders can be produced that are transparent and colorless. The light output and the energy resolution derived from pulse height spectra under γ-ray excitation of a ^{137}Cs source are 13000±2000 ph/MeV and 5.6 %, respectively. Time resolved X-ray luminescence shows 4.5 μs decay time and only around 15 % constant fraction. Furthermore, different growth parameters and a proper annealing process dramatically impact the light output and energy resolution, which is

used to investigate and understand the scintillation mechanism of $Mg_4Ta_2O_9$.

HYDROTHERMAL GROWTH AND CHARACTERIZATION OF UO2 SINGLE CRYSTALS GROWN ON NON-NATIVE SUBSTRATES

Martin Kimani[1], James M. Mann[2], Karl Rickert[3], James Petrosky[4], David Turner[2]

[1]KBRWyle Aerospace Group, CA, UNITED STATES OF AMERICA, [2]Air Force Research Laboratory, OH, UNITED STATES OF AMERICA, [3]Oak Ridge Institute for Science and Education, TN, UNITED STATES OF AMERICA, [4]Air Force Institute of Technology, OH, UNITED STATES OF AMERICA

There is growing interest in the growth and development of direct conversion, neutron sensitive solid-state radiation detector materials which efficiently discriminate between photon and neutron events. Single crystals of actinide materials such as uranium dioxide (UO_2) may be a suitable detection material due to the large amounts of energy (~185 MeV) released from a neutron induced fission event. Detectable electron hole pairs are produced by the energetic fission fragments on the order of 165 MeV resulting from the neutron induced fission event which is much greater than current detection schemes which rely on reaction energies between 2-6 MeV. The successful fabrication of UO_2 devices has been greatly hampered by the lack of high quality (semiconductor grade) single crystals of UO_2. Traditional melt growth techniques such as Czochralski are not applicable due to the high melting point of UO_2 (~2878°C). UO_2 single crystals have been successfully grown using melt growth techniques such as arc fusion, cold crucible, and solar furnace but their crystal quality is substandard due to thermal strain and oxygen non-stoichiometry. Crystal growth of UO_2 was investigated via a hydrothermal synthesis technique since this method has been successfully used in the synthesis of other refractory oxides such as Sc_2O_3, Lu_2O_3, and ThO_2. In this talk, we will present the hydrothermal growth of UO_2 single crystals using a variety of different non-native substrates such as yttrium stabilized zirconia (YSZ), Cu, Ge and lanthanum strontium aluminum tantalum oxide (LSAT) as seeds. The grown crystals were characterized using various techniques to determine their stoichiometry, crystallinity, conductivity, mobility and major carrier type.

GROWTH AND OPTICAL PROPERTIES OF CR-DOPED BETA-GA2O3 CRYSTALS AS RED AND INFRARED SCINTILLATOR BY THE FLOATING ZONE METHOD

Shunsuke Kurosawa[1], Toetsu Shishido[2], Akihiro Yamaji[2], Takahiko Horiai[2], Shohei Kodama[2], Takamasa Sugawara[2], Akiko Nomura[2], Kunio Yubuta[2], Yuji Ohashi[3], Yuui Yokota[4], Kei Kamada[3], Akira Yoshikawa[4], Akimasa Ohnishi[1], Mamoru Kitaura[1]

[1]Faculty of Science, Yamagata University, JAPAN, [2]Institute for Materials Research, Tohoku University, JAPAN, [3]NICHe, Tohoku University, JAPAN, [4]New Industry Creation Hatchery Center, Tohoku University, JAPAN

Radiation therapy has been widely used to treat the tumor. However, some medical accidents are reported due to over dose [1]. Thus, real-time dose-monitoring system is expected to save the accident, and Human body has an optical transparent area around near infra-red region (650 to 1200 nm). Using this “window”, a novel real-time dosimeter system can be developed with infra-red emission scintillators. From the knowledge of Laser material, Cr^{3+} doped oxide crystals can emit scintillation light in the infra-red region, and we investigated the luminescent properties of Cr^{3+}-doped crystals. In this paper, we investigated the luminescent properties of $Cr:Ga_2O_3$ and pure Ga_2O_3 prepared by sintering and the Floating Zone (FZ) method, as shown in Fig. from Cr_2O_3 and b-Ga_2O_3 powders as starting materials. $Cr:Ga_2O_3$ was found to have red and infra-red emission (around ~730 nm), and the light output of $Cr:Ga_2O_3$was larger than Cr-doped Gd3Ga5O12 as previous works.Moreover, the band gap energy was estimated to be approximately 4.9 eV using pure Ga_2O_3 crystal. We show the above results and discuss the feasibility for medical applications [1] “Lessons Learned from Accidental Exposures in Radiotherapy”, IAEA Safety Reports Series No. 17, IAEA, Vienna (2000).

Fig. Photograph of $Cr:Ga_2O_3$crystal grown by the Floating Zone method

HYDROTHERMAL GROWTH OF THO2, UXTH1-XO2 AND UO2 SINGLE CRYSTALS FOR NEUTRON DETECTION

James M. Mann[1], Martin Kimani[2], Christina L. Dugan[3], Christopher Young[4], Karl Rickert[5], James Petrosky[4]

[1]Air Force Research Laboratory, OH, UNITED STATES OF AMERICA, [2]KBRWyle Aerospace Group, CA, UNITED STATES OF AMERICA, [3]Air Force Institute of Technology, UNITED STATES OF AMERICA, [4]Air Force Institute of Technology, OH, UNITED STATES OF AMERICA, [5]Oak Ridge Institute for Science and Education, TN, UNITED STATES OF AMERICA

Single crystals incorporating fissionable actinide elements have been explored for neutron detection possibilities. The majority of the work has been aimed at developing a direct conversion detector from semiconductor grade UO_2 crystals. Uranium dioxide has many significant advantages which include a high density of neutron reactive uranium, potential to discriminate between neutrons and gamma radiation, an ability to observe both thermal and fast neutrons without the need for moderation, and a large 185MeV signal. Recently, successful growth of high quality crystals has been achieved by the hydrothermal synthesis technique. Crystals obtained by spontaneous nucleation and seeded growth resulted in UO_2 crystals too small for device fabrication ($<1mm^3$ and $3mm^3$ respectively). The potential of the hydrothermal technique to grow large area UO_2 crystals has been established, but the lack of large UO_2 substrates coupled with the relatively slow growth rates has thus far prevented significant sizes. In this talk we will discuss the hydrothermal growth of UO_2 on non-native seed crystals comprised of CaF_2, ThO_2 and $U_xTh_{1-x}O_2$. Given the lack of available ThO_2 and $U_xTh_{1-x}O_2$ substrates, a portion of the presentation will include the growth of these substrates before ultimately being utilized for growth of UO_2 single crystals. Characterization of the crystals by X-ray rocking curve, scanning electron microscope, energy dispersive X-ray, and X-ray fluorescence will also be presented.

SOLUTION GROWTH AND SCINTILLATION PROPERTIES OF 9-PHENYLCARBAZOLE

Edgar Van Loef, Gary Markosyan, Urmila Shirwadkar, Mickel Mcclish, Kanai S. Shah

RMD, MA, UNITED STATES OF AMERICA

In this paper we report on the crystal growth and characterization of 9-phenylcarbazole (PCz). Crystals of PCz were obtained by the solution growth technique. Several organic solvents were investigated including heptane, cyclohexane, toluene, p-xylene, methanol, ethanol, and acetone. The largest crystals of the highest quality were grown from acetone. Radioluminescence spectra of PCz crystals exhibit a broad emission band peaking at 450 nm. Single crystals of PCz show high light yields of up to 25,000 ph/MeV and a fast scintillation decay of less than 20 ns. Pulse shape discrimination with PCz crystals using neutron and gamma-rays from a ^{252}Cf source yields a Figure of Merit (FOM) of about 2.7 at 1.0 MeVee cut-off energy. As far as we are aware, phenylcarbazole is the brightest organic single crystal scintillator in existence and is a very promising organic neutron detector for a multitude of applications including homeland security, nuclear non-proliferation, nuclear physics, and non-destructive testing. *We would like to acknowledge the Defense Threat Reduction Agency of the United States for their financial support under contract # HDTRA1-14-C-0020.*

RECENTLY DEVELOPED UNIDIRECTIONAL ORGANIC SINGLE CRYSTAL CYLINDERS FOR SCINTILLATOR APPLICATION

Krishnasamy Sankaranarayanan

Alagappa University, INDIA

The well known organic scintillation materials namely t-stilbene and 1,3,5-triphenylbene were successfully grown unidirectionally with cylindrical dimension of 5cm x 2cm for t-stilbene and 10cm x 2.5cm for 1,3,5-triphenylbenzene. The growth along <001> in the case of t-stilbene and <110> for 1,3,5-triphenylbenzene and the obtained cylindrically morphology without any post growth machine lathing processes are the main features of the present study which may find commercial application as scintillation detectors. The selection of growth container facilitates the required cylindrical morphology and the temperature gradient assisted Sankaranarayanan-Ramasamy method offers crystals with acceptable merit. The grown crystals are investigated with PXRD, HRXRD, FT-IR, Micro-Raman, UV-Visible and Photoluminescence studies in order to establish phase purity, crystalline perfection, functional group identification, optical transparency and luminescence. The mechanical and thermal properties were also revealed by Vickers micro hardness test and TG/DTA analysis. The scintillation characteristics of the grown crystals under Gamma and Beta radiation sources resulted radioluminescence emissions at 365nm (t-stibene) and 355nm (1,3,5-triphenylbenzene). It is observed that the radioluminescence emission peaks are similar to that of their photoluminescence emission when t-stilbene was excited with 285nm and 1,3,5 triphenylbenzene by 275nm. The functionality of scintillation characteristics for both the materials on their crystallographic direction and on the absence of boundary between planes is in progress.

References: [1] M.M. Bourne. et. al., Nuclear Instruments and Methods in Physics Research A 806 **(2016)** 348-355. [2] Beatrice Fraboni. et. al., Advanced Functional Materials 26 **(2016)**2276-2291. [3] Natalia Zaitseva. et. al., Journal of Crystal Growth 314 **(2011)** 163-170. [4] Natalia Zaitseva. et. al., Nuclear Instruments and Methods in Physics Research A 789 **(2015)** 8-15.

IN-SITU OBSERVATION OF ICE CRYSTAL SURFACES AT THE MOLECULAR LEVEL BY ADVANCED OPTICAL MICROSCOPY

Gen Sazaki, Ken-Ichiro Murata, Masahiro Inomata, Jialu Chen, Ken Nagashima, Yoshinori Furukawa

Institute of Low Temperature Science, Hokkaido University, JAPAN

Ice is one of the most abundant and ubiquitous materials on the earth. Hence, its phase transition governs wide variety of phenomena in nature. To reveal the surface structure and growth kinetics of ice crystals, we developed our advanced optical microscopy, which can visualize individual elementary steps (0.37 nm in height) on ice surfaces. In the conference, we will show our recent two topics: the thermodynamic origin of quasi-liquid layers and the growth kinetics of elementary steps on ice crystal surfaces. Surface melting is one of the phase transitions of ice crystals, and it dominates the surface properties of ice crystals at temperature near the melting point. By our advanced optical microscopy, we recently found that two-types of quasi-liquid layers (QLLs), which show different morphologies (thin layers and drops) [1], appear kinetically only at water vapor pressure higher than a certain critical value [2]. From this result, we came up with the idea that interface free energies at QLL-ice interfaces may change with water vapor pressure. To probe this idea, we measured wetting angles of QLLs at ice crystal surfaces by Michelson interferometry, and found that with increasing water vapor pressure, the wetting becomes better [3]. From this finding, we can phenomenologically explain the emergences of the two-types of QLLs as follows. At an equilibrium condition, no QLL appear. But with increasing water vapor pressure, the drop-type QLLs appear first, then the thin-layer-type QLLs finally appear because of the better wettability. It is well-known that with decreasing temperature, the habit of snow crystals changes from plates (0~-4°C), to columns (-4~-10°C), to plates (-10~-22°C), and finally to columns (<-22°C) repeatedly. However, the cause of this habit change has been a mystery for long years. To solve this problem, we measured the growth kinetics of elementary steps on ice basal faces, and determined a step kinetic coefficient as a function of temperature. Then we found that the step kinetic coefficient does not decrease monotonically with decreasing temperature. The coefficient shows a minimum at -5°C and a maximum at -15°C. In the conference, we will discuss the causes of the non-monotonic changes in the step kinetic coefficient. 1) G. Sazaki, et al., *Proc. Nat. Acad. Sci. USA.*, **109**, 1052-1055 (2012). 2) H. Asakawa, et al., *Proc. Nat. Acad. Sci. USA.*, **113**, 1749-1753 (2016). 3) K. Murata, et al., *Proc. Nat. Acad. Sci. USA.*, **113**, E6741-E6748 (2016).

FORMATION AND PROPOGATION OF MACROSTEPS IN THE PRESENCE OF IMPURITIES

James F. Lutsko[1], Mike Sleutel[2], Alexander E..S. Van Driessche[3]

[1]Universite Libre de Bruxelles, BELGIUM, [2]Vrije Universiteit Brussel, BELGIUM, [3]Univ. Grenoble Alpes, FRANCE

We report on kinetic Monte Carlo computer simulations of the formation of macrosteps on a crystal growing in an impure environment. Our simulation method includes an explicit representation of the solution above the crystal surface and the transport of material in solution, including impurity species which are fully dynamic. We demonstrate the spontaneous formation of macrosteps – i.e. step trains compressed into a small region – due to the effect of fluctuations in the concentration of impurities adsorbed onto the crystal surface. Once formed, macrosteps are found to be mobile even when the adsorbed impurity concentration is sufficiently high as to pin individual steps – a phenomenon observed in the potassium dihydrogen phosphate/Fe3+ system. Our results are relevant to mineral formation in geologic conditions where low supersaturation and high impurity concentration are the norm.

NUCLEATION AND GROWTH OF TWO-DIMENSIONAL ISLANDS OF COLLOIDAL CRYSTALS

Jun Nozawa, Satoshi Uda, Suxia Guo, Junpei Okada, Haruhiko Koizumi

Institute for Materials Research, Tohoku University, JAPAN

Colloidal crystals—periodic array of colloidal particles—attract great interests in broad fields because of their potential application to the novel functional device such as photonic crystals and chemical sensors. In the meantime, since colloidal crystal shows similar phase transition to that of atomic system, it has been employed as a model to reveal detailed mechanism of diverse basic physical phenomena. We focus on the nucleation and growth of two-dimensional (2D) islands on the terrace of colloidal crystals with the attractive system, in which polymer is added to generate depletion attractive interaction. According to our investigations, important characteristics of the attractive system are revealed; density of the environment is quite smaller than that of the crystallized solid phase which results in generating smooth interface. The 2D nucleation is found to be predominant growth mechanism in those situation. In-situ observation has been conducted to measure nucleation rate, J, and critical radius, r^*, and to observe further growth of 2D islands. In the initial stage of the crystallization, nucleation of monolayer colloidal crystals takes place on a bottom of the cell. Then, 2D nucleation occurs on the surface of colloidal crystals. We recognized important features about the nucleation process. Smaller embryos shrink and then disappear, whereas larger embryos keep growing. This means that there is a critical size, which is in accordance with framework of the classical nucleation theory (CNT). The J and r^* were measured by in situ observation at various f_{area}. The data are well fitted linearly with $1/\ln(f_{\mathrm{area}}/f_{\mathrm{eq}})$, suggesting that nucleation process of colloidal crystals added with polymer basically follow framework of CNT. Based on the CNT, J and r^* have line relation to the $1/\ln(C/ C_{\mathrm{eq}})$. Here, equilibrium area fraction, f_{eq}, was determined experimentally as the f_{area} that dissolution of islands starts. The step free energy, g, is obtained from the gradient of the slopes in those figures, and the g values agreed well with each other although they are obtained from independent observation objects. These facts suggest that the nucleation process of colloidal crystals with added polymer agrees with framework of the CNT. We also investigated the effect of the substrate on the nucleation rate, and growth mechanism of 2D islands. These fundamental studies contribute well to grow high quality 2D colloidal crystals, which has versatile potential application for the functional devices such as photonic or sensor devices.

HERRING'S SCALING LAW OF DIFFUSION REVISITED

Marek Petrik

Philipps University, GERMANY

Coarsening in nanocrystalline (nc) solids – the sacrificial growth of the larger members of an ensemble of nanocrystals at the expense of the smaller ones – is well understood in the case of Ostwald ripening, i.e. in biphasic systems where mass transport takes place by dissolution and reprecipitation. Precipitation-hardened alloys provide an example. Analytical expressions describing the growth kinetics under various conditions (diffusion- or reaction-rate-limited) in such systems were derived many decades ago by Carl Wagner and others. The situation is much less clear-cut for single phase nc-solids which are more common than the ideal Ostwald-type systems. Aside from the classical curvature-driven coarsening observed at the macroscale in polycrystals, the mechanism of growth and the numerical value of the scaling exponent for nc-systems remain subject to controversy. In particular, the possibility of non-classical coarsening at the nanoscale due to additional (rotational) degrees of freedom of the nanocrystals complicates the picture. In addition, the reproducibility of quantitative experimental data tends to be poor for nc samples. Recently, we proposed to have recourse to a classical elementary atomistic model in order to explain an unexpected substantial increase of the rate of dissolution of NiO crystals at the nanoscale, surpassing that predicted from surface energy considerations alone [1]. Similarly, regarding crystal growth, we have now revisited the elementary scaling relationships for diffusive mass transport deduced from a simple dimensional analysis long ago (Conyers Herring, 1950). A systematic evaluation of experimental growth isotherms (crystal size as a function of time) for a large number of samples – no less than 159 isotherms, for both nano- and macrocrystalline specimens, partly from the literature and partly from our laboratory – reveals, according to Herring's classification, a particular mode of thermally induced growth at the nanoscale, different from that observed in macroscale polycrystals. This growth mode is rationalized in terms of a predominance of pipe-diffusion, as opposed to surface diffusion which becomes dominant when an intermediate crystal size is reached, and is in turn superseded by volume diffusion as soon as macroscopic dimensions prevail. Thus, a unique scaling exponent, characteristic of the growth kinetics of nanocrystals, is derived for the first time. The results are shown to be self-consistent by collating all the measurements in a renormalized master plot covering several orders of magnitude, whereby the above-mentioned inherent variability of the experimental data averages out.

[1] M. Petrik, B. Harbrecht, *ChemPhysChem* **2013**, *14*, 2403-2406.

NEW STRAIN STATES IN EPITAXIAL COMPLEX OXIDES

Judith L. Macmanus-Driscoll[1], Ady Suwardi[1], Haiyan Wang[2], Aiping Chen[3], Quanxi Jia[4]

[1]University of Cambridge, UNITED KINGDOM, [2]Purdue University, UNITED STATES OF AMERICA, [3]CINT, Los Alamos, NM, UNITED STATES OF AMERICA, [4]Univ. at Buffalo, SUNY, Department of Materials Design and Innovation, NY, UNITED STATES OF AMERICA

Most complex oxides have strongly correlated properties. In particular, the properties are highly sensitive to strain states in the films. Currently, strain is controlled via epitaxial growth on single crystal oxide substrates, but elastic effects means that overall cell volume is conserved, i.e. if the film is tensed in-plane, it will be compressed out-of-plane. In addition, the epitaxial strain is only maintained uniformally to a few nm before relaxation occurs. In order to precisely engineer the huge potential range of functional properties that oxide films possess, another route to explore for strain control is growth of heteroepitaxial vertically aligned nanostructured (VAN) films. Here, a new range of strain states can be induced, including 'auxetic-like' states where the lattice is expanded in 3D. In addition, strain is very uniform which is extremely important for giving highly cyrsyalline materials with less defects. The mechanisms for inducing the new strain states will be explained, and examples of resulting strongly enhanced properties which have come about in a number of systems will be discussed, e.g. in magnetics, ionics, and ferroelectrics.

DOPANT SITE STRUCTURE ANALYSIS IN PEROVSKITES

Mikk Lippmaa

Institute for Solid State Physics, University of Tokyo, JAPAN

Band gap tuning by doping is a common approach for developing oxide materials for optical energy conversion applications such as photovoltaics or photocatalysts. Our work is directed at designing titanate-based materials for photoelectrochemical water splitting that can be used to harness sunlight to produce hydrogen gas from water. Titanates are suitable materials due to the excellent chemical stability in water. However, materials such as TiO_2 or $SrTiO_3$ have band gaps that are too wide to absorb visible sunlight. It is therefore necessary to reduce bandgap without compromising the chemical stability. As a model system, we use noble metal doping of $SrTiO_3$. In this particular case, additional dopant–related states form in the band gap of the host material, effectively reducing the optical band gap. It is known that Rh and Ir are particularly effective in this regard due to a suitable alignment of the 4*d* or 5*d* states of the dopants with the band edges of $SrTiO_3$. Our thin film work has shown that Rh:$SrTiO_3$ and Ir:$SrTiO_3$ are indeed effective photocatalysts that can be used for hydrogen and oxygen evolution from water, respectively. However, the carrier mobility in these materials is unexpectedly low, reducing the efficiency of extracting photogenerated carriers. Transient THz and infrared absorption measurements have shown that photocarriers are lost in Rh:$SrTiO_3$ to trapping and recombination on a picosecond timescale. This indicates that unexpected in-gap trap states exist in the doped material. We have studied the dopant site structure by element-specific x-ray fluorescence holography, which can be used to determine the real-space 3-dimensional structure of the crystal lattice surrounding a dopant atom. The measurements show that several metal dopants in $SrTiO_3$ tend to form local clusters with oxygen vacancies or due to metal substitution at the oxygen site. Such nanoscale clusters cannot be detected by normal diffraction or surface analysis results but have a dramatic effect on photoconductivity and photocarrier mobility. The local symmetry reduction of the dopant site modifies the usual octahedral crystal field splitting of the d-electron manifolds, leading to additional in-gap energy levels that can lead to rapid carrier trapping or recombination.

PROBING INTERFACIAL SUPERCONDUCTIVITY IN FE-BASED SUPERCONDUCTORS BY IN-SITU ARPES

Hong Ding

Institute of Physics, Chinese Academy of Sciences, CHINA

In this talk I will report our recent in-situ ARPES results on MBE-grown monolayer films of Fe-based and Cu-based superconductors, including 1. Observation of high-Tc superconductivity in rectangular FeSe/STO(110) monolayer; 2. Enhanced superconductivity accompanying a Lifshitz transition in electron-doped FeSe monolayer; 3. Experimental indication of possible high-Tc topological superconductivity in Fe(Te,Se)/STO monolayer.

GRAPHENE QUANTUM RESISTANCE STANDARD

Alexander Tzalenchuk

National Physical Laboratory, UNITED KINGDOM

Graphene has potential to supersede conventional semiconductors as the material of choice for quantum electrical metrology. The combination of large inter-Landau level spacing, extremely fast hot electron relaxation [1] and anomalously strong pinning of the filling factor v = 2 in epitaxial graphene on SiC [2] result in exceptionally wide QHE plateaus extending over 50 T in recent measurements [3], large QHE breakdown current, and hence a superior signal-to-noise ratio compared to measurements on conventional semiconductors. Resistance metrology using graphene has seen a rapid progress from the first precision measurement on graphene [4] and culminating in the most precise ever demonstration of equivalence of the quantised values of the Hall resistance in graphene on SiC compared directly with GaAs [5]. Important as they are these results were obtained using the same expensive cryo-magnetic equipment (<300 mK, up to 14 T) as needed to realise the resistance scale using conventional semiconductors. Can graphene do any better? The aspiration of the modern-day metrology is to provide quantum standards at the fingertips of the end users, shortening the calibration chain from primary standards to the final product. As a step towards realisation of this objective we have recently demonstrated measurements of the QHE with part-per-billion accuracy in a small table-top cryogen-free pulse-tube system operating at around 4 K and magnetic field up to 5 T [6]. In my talk I will review the fundamentals of the graphene technology behind this development. [1] A. M. R. Baker *et al., Phys. Rev. B* **87**, 045414 (2013). [2] T. J. B. M. Janssen *et al.*, *Phys. Rev. B* **83**, 233402 (2011). [3] J. A. Alexander-Webber *et al., Sci. Rep.* **6**, 30296 (2016). [4] A. Tzalenchuk *et al., Nat. Nanotech.* **5**, 186-189 (2010). [5] T. J. B. M. Janssen *et al., New J. Phys.* **13**, 093026 (2011). [6] T. J. B. M. Janssen *et al.*, *2D Mater.*, **2**, 035015 (2015).

POLYMER ASSISTED SUBLIMATION GROWTH OF EPITAXIAL GRAPHENE FOR QUANTUM RESISTANCE METROLOGY

Mattias Kruskopf[1], Davood Momeni Pakdehi[1], Klaus Pierz[1], Stefan Wundrack[1], Rainer Stosch[1], Thorsten Dziomba[1], Martin Götz[1], Jens Baringhaus[2], Johannes Aprojanz[2], Christoph Tegenkamp[2], Jakob Lidzba[3], Thomas Seyller[3], Frank Hohls[1], Franz J. Ahlers[1], Hans W. Schumacher[1]

[1]Physikalisch-Technische Bundesanstalt, GERMANY, [2]Institute of Solid State Physics of Leibniz Universität Hannover, GERMANY, [3]Institute of Physics of Technische Universität Chemnitz, GERMANY

A new generation of quantum standards for the realization of the unit Ohm based on graphene is investigated by national metrology institutes. Such a graphene-based resistance standard promises highest precision under relaxed measurement conditions by enabling the use of compact measurement setups. The requirements of this and other electronic device applications in general imply high demands on the graphene properties and homogeneity over large areas. The main challenge of the epitaxial growth of graphene on silicon carbide (SiC) substrates is to suppress the formation of high step edges and bilayer/multilayer graphene domains since both drastically degenerate the electrical properties of the graphene monolayer. This work presents significant improvements by means of a new polymer assisted sublimation growth (PASG) process [1]. The thermal decomposition of a deposited polymer provides additional carbon and a high number of nucleation sites which accelerates the buffer layer growth and stabilizes the SiC surface. Large-area Raman mappings and investigations by atomic force microscopy prove that a closed graphene monolayer without bilayer inclusions is obtained on the centimeter scale with structure heights ≤ 0.75 nm. Microscopic four-point probe and precision magneto-transport measurements demonstrate the remarkable electronic properties of this material. The analysis of the experimental results extends the current understanding of the graphene growth process by emphasizing the importance of nucleation and the amount of available carbon.

Figure 1 AFM topography (50 μm x 50 μm) of a PASG graphene sample grown at 1750 °C on a 6H-SiC (0001) substrate with step heights ≤ 0.75 nm. The representative Raman mapping (30 μm x 30 μm) of the 2D-peak FWHM shows the outstanding homogeneity of the graphene monolayer with a mean value of 32.9 ±1.8 cm^{-1} (green/blue). Reference: [1] Kruskopf et al. “Comeback of epitaxial graphene for electronics: large-area growth of bilayer-free graphene on SiC”, 2D Materials 3.4 (Oct. 2016), p. 041002

IMPACT OF QUASI-FREE STANDING GRAPHENE EPITAXIAL GRAPHENE ON TERAHERTZ OPTOELECTRONICS

D. K. Gaskill[1], Kevin M. Daniels[2], M. Jadidi[3], A. Shuskov[3], A. Boyd[1], A. Nath[4], R.L. Myers-Ward[1], T. Murphy[3], H.D. Drew[3]

[1]Naval Research Laboratory, DC, UNITED STATES OF AMERICA, [2]U.S. Naval Research Laboratory, UNITED STATES OF AMERICA, [3]University of Maryland, MD, UNITED STATES OF AMERICA, [4]George Mason University, VA, UNITED STATES OF AMERICA

Large area, single crystal epitaxial graphene (EG) is attractive for optoelectronic applications ranging from many terahertz down to the sub-terahertz. We review the utility of graphene ribbons, having resonant frequencies dependent upon the graphene sheet density and the (subwavelength) patterned width and period, to enhance absorption or transmission. In addition, we discuss the impact of quasi-free standing (QFS) graphene on the resonant frequencies of graphene. Because QFS graphene results in mobility improvement by ~4-fold, unprecedented narrow resonances are achieved, implying the potential for high performance THz optoelectronics. In addition, improved mobility should translate into increased detection efficiency in the sub-terahertz domain using resonance enhanced field effect transistor or photothermoelectric detectors.

FORMATION OF GRAPHENE NANORIBBONS AND SHEETS BY DIFFUSION OF CARBON IN LIQUID METALS INDUCED BY ELECTROCHARGING ASSISTED PROCESS

Lourdes G. Salamanca-Riba[1], Xiaoxiao Ge[2], Liangbing Hu[2], Oded Rabin[2], Manfred Wuttig[2], Balu Balachandran[3], Daniel P. Cole[4]

[1]University of Maryland, UNITED STATES OF AMERICA, [2]University of Maryland, MD, UNITED STATES OF AMERICA, [3]Argonne National Laboratory, IL, UNITED STATES OF AMERICA, [4]Army Research Laboratory, MD, UNITED STATES OF AMERICA

Graphene nano-ribbons and nano-sheets are produced in the crystal lattice of metals by a process we call “electrocharging assisted process” (EAP) at high temperatures. In this process the metal is heated above its melting temperature together with particles of activated carbon. The mixture is stirred, and a high current is applied between a graphite electrode inserted into the metal and the crucible containing the mixture. The current is believed to induce ionization of the carbon from the particles followed by polymerization with other C ions and bonding to metal atoms forming ribbons and chains. Raman scattering, X-ray photoelectron spectroscopy (XPS) and electron energy loss spectroscopy (EELS) of the resulting materials, called covetics, reveal the presence of graphitic carbon with mostly *sp2* bonding and small amounts of *sp3* bonding. Transmission electron microscopy (TEM), in combination with EELS spectrum imaging, indicate that the graphitic regions form graphene nanoribbons and nanosheets which have a preferred orientation with the lattice of the metal. The graphitic nanostructures give rise to an increase in the ultimate tensile strength and changes in the electrical and thermal conductivity of the metal. Films of copper with carbon deposited by e-beam evaporation and pulsed laser deposition (PLD) using bulk copper covetic as target show that under certain deposition conditions the carbon is transferred into the film. The films that contain carbon show higher transmittance than pure copper films of the same thickness and in some instances higher conductivity and resistance to oxidation under ambient conditions. Density functional theory and first principles calculations of the phonon density of states indicate strong C-metal covalent bonding at edges of graphene nanoribbons and sheets. The C-metal bonds are Raman active and produce weak signals in the Raman spectra. We will present structural characterization and electrical measurements of bulk Cu, Al and Ag covetics as well as transmittance and resistance Cu covetic films grown by e-beam deposition and PLD.

* Funded by ONR Award No N000141410042, and ANL/DOE subcontract No. 6F-30062

COLLOIDAL NANOSTRUCTURES: IN-SITU ELECTRON MICROSCOPY OF PLASMON-MEDIATED SYNTHESIS, CHEMISTRY AND SELF-ASSEMBLY

Eli Sutter

University of Nebraska-Lincoln, UNITED STATES OF AMERICA

In-situ transmission electron microscopy (TEM) can be used to follow the behavior and measure the properties of nanostructures over a wide range of environmental conditions with resolution down to the atomic scale. Liquid-cell electron microscopy (LCEM), in particular, is the only technique that allows direct imaging of nanometer-scale processes in liquids. It has been successfully applied to imaging various processes in liquids, solutions, and colloidal suspensions that were typically investigated ex-situ on samples taken at different process stages, or in some cases in-situ using reciprocal space techniques. Here I will demonstrate the power of LCEM to probe complex solution-phase processes in real space, including plasmon-mediated colloidal synthesis of nanostructures, galvanic replacement reactions, and the self-assembly of nanocrystal superstructures in solution. Our results demonstrate that real-time electron microscopy can substantially advance our understanding of a wide range of processes involving nanoscale objects in bulk liquids.

STEP MORPHOLOGY OF 2D ISLANDS ON THE (110) FACE OF LYSOZYME CRSYTALS GROWN IN SPACE

Katsuo Tsukamoto[1], Hitoshi Miura[2], Hironori Hondoh[3]

[1]Osaka University, JAPAN, [2]Nagoya City University, JAPAN, [3]Hiroshima University, JAPAN

The step morphology of 2D islands nucleated on the surface of crystals has not always been understood based on the 3D morphology or the crystal structure. Sometimes 2D nuclei are twinned like on YIG. The 2D step morphology on the (110) face of tetragonal lysozyme crystals is also interesting in another sense. When the crystal grows from impure solution, the form of 2D islands show ellipse that elongates normal to the c-axis. When the crystal grows from very pure solution, the morphology shows rhombus or parallelogram that elongated also normal to the c-axis. However even from the purest solutions, all edges of the 2D islands are not parallel to the edge of the crystals. In order to understand these phenomena, macrobond analysis [1] has bee applied to the structure of tetragonal lysozyme crystals, though the experimental 2D morphology still could not be understood well. This situation was the same also for spiral steps. Exact growth rate *vs* supersaturation and step morphology have been measured by laser interferometer at the international station from three-level of impurity contents [2, 3]. In that experiment, we for the first time observed ideal morphology of spiral steps at higher supersaturation, which was predicted from the macrobond analysis. The 2D and spiral step morphologies are then interpreted based on the selective adsorption of dimer-molecules (impurity) at one set of step fronts. This result strongly supports the reduction of impurity adsorption to the crystals under microgravity, which was concluded from the growth rateor step

velocity *vs* supersaturation measurement done from the same crystals.

[1] Y. Matsuura, A.A. Chernov, Acta crystallographica. Section D, Biological crystallography, 59 (2003) 1347-1356. [2] I. Yoshizaki, K. Tsukamoto, T. Yamazaki, K. Murayama, K. Oshi, S. Fukuyama, T. Shimaoka, Y. Suzuki, M. Tachibana, Review of Scientific Instruments, 84 (2013). [3] Y. Suzuki, K. Tsukamoto, I. Yoshizaki, H. Miura, T. Fujiwara, Crystal Growth & Design, 15 (2015) 4787-4794.

ADVANCES IN SINGLE-CRYSTAL FIBERS AND THIN RODS GROWN BY LASER HEATED PEDESTAL GROWTH

Gisele Maxwell

shasta crystals inc., UNITED STATES OF AMERICA

Single-crystal fibers are an intermediate between laser crystals and doped glass fibers. They have the advantages of both guiding laser light and matching the efficiencies found in bulk crystals, which is making them ideal candidates for high-power laser and fiber laser applications. This work focuses on the growth of a flexible fiber with a core of dopant (Er, Nd, Yb, etc.) and a polycrystalline clad of yttrium aluminum garnet (YAG) that will exhibit good wave guiding properties. Direct growth or a combination of growth and cladding experiments are described. New processes to manufacture and clad longer than a meter lengths are explained. For single-pass amplification in small rods (0.5mm in diameter), a single-pass linear gain of 7.4 was obtained for 29 nJ pulses of 5 ns duration at 1 MHz repetition rate. We also obtained in thin fibers (diameter 50 microns) a laser efficiency of over 58% in a diode-pumped configuration. These results confirm the potential for single-crystal fibers to overcome the limitations of the glass fibers commonly used in fiber lasers, making them prime candidates for high-power compact fiber lasers and amplifiers.

MARKET TREND IN THE SAPPHIRE INDUSTRY AND A DISCUSSION FOR DEVELOPMENT DIRECTION

Jongkwan Park, Matthew Jensen, Ryan Loquist, Clark Blockburger, Matthew Montgomery

Rubicon Technology, IL, UNITED STATES OF AMERICA

Owing to the shortage of sapphire in late 2009, there was astronomical investment and optimistic expectations in the sapphire industry due to surging demand for LED substrates. Soon or later, the market plunged, and became over-supplied because of excessive investment from Eastern Asia. In past 2-3 years, it has been consequently exacerbated by the trials of cell phone companies applying for the display cover. Although there are outstanding physical properties as a display cover, brittleness of crystal and difficulties for fabrication limited the concept to model and planning stages. It estimated that about 30% of sapphire manufacturers have stopped running in 2016 while the price dropped up to 70% of its value over the last two years[1]. Technological trends have severely affected the industrial movement, too. Both EFG and Kyropoulos (KY) are well known as decent methods to produce sapphire for many years. Responding to the demand, graphite based Cz and CHES competed for mass-production market share although they were short of success. Since the market requires not only the quantity but also the quality, KY eventually remains as the most dominant supplying method. However, even KY furnace has adopted graphite for an insulating materials. As a KY sapphire supplier, Rubicon Technology has played a substantial role for developing sapphire in a large size. However, we can’t bear out an over supplied market for LED substrate. Through a significant reduction of its size, we have learned and focused on exclusively designed sapphire[2]. Rubicon Technology are selectively deepening our strength for the limited customers with a specialized technology.

SINGLE CRYSTAL GROWTH OF SUBMILLIMETRE DIAMETER SAPPHIRE TUBE BY THE MICRO-PULLING DOWN METHOD FOR ULTRASOUND-FACILITATED DRUG DELIVERY SYSTEM

Kei Kamada[1], Vladimir V. Kochurikhin[2], Gushchina Liudmila[2], Mikhail Ivanov[2], Yasuhiro Shoji[3], Shunsuke Kurosawa[4], Yuji Ohashi[5], Yuui Yokota[6], Akira Yoshikawa[3]

[1]C&A, JAPAN, [2]General Physics Institute, Russian Academy of Sciences, RUSSIAN FEDERATION, [3]Institute for Materials Research, Tohoku University, JAPAN, [4]Faculty of Science, Yamagata University, JAPAN, [5]NICHe, Tohoku University, JAPAN, [6]New Industry Creation Hatchery Center, Tohoku University, JAPAN

Convection-enhanced delivery (CED) is an effective drug delivery method that delivers high concentration of drugs directly into the targeted lesion beyond the blood-brain barrier. The efficacy of this local infusion technique for treating focal central nervous system diseases such as brain tumors, neurodegenerative diseases, and spinal cord injury has recently been demonstrated. Recently, the efficacy of ultrasound assistance for CED was reported for

various drug delivery applications. Y. Mono et al. developed a new ultrasound-facilitated drug delivery (UFD) system that enables the application of ultrasound at the infusion site [1]. In this system, steel bar with 4-15cm length and 0.65mm diameter with a 0.2mm x 0.19mm groove along this bar was used as a guide. A 0.2 mm outer diameter (OD) and 0.1mm inner diameter (ID) silicone tube was connected to the guide and the drug is delivered though this tube into a brain. However, the drug transportation is limited because ultrasound vibration does not propagate in the tube effectively and the inner diameter is so narrow. MRI simultaneous imaging was impossible due to the presence of metal steel bar. Additional treatment due to the metal biocompatibility also was difficult. On the other hand, sapphire is biocompatible, antimagnetic material with enough strength, hardness and transparency for UFD. Sapphire is thought as the most promising material for UFD at the point view of not only physical properties but also low material cost and mass productivity. Up to now, shaped crystal growth technique of sapphire single crystals with the shapes of tube, plate, and fiber was commercially developed mainly by the Edge defined Film Fed Growth (*EFG*) method [2]. However, there are no detailed reports about realized growth technology for obtaining submillimetre diameter sapphire tubes. In this work we developed the growth technology for the OD:0.65mm and ID:0.25mm sapphire tube by using the micro-pulling down (m-PD) method. The Ir crucible with a die composed of a equivalent hole and Ir wire was heated by RF coil in N_2 atmosphere. Example photograph of the grown tube is shown in Fig. 1. In our presentation, details about crucible and insulator design, growth conditions and evaluation of the strength will be reported. Furthermore, examination of UFD using the grown tube also will be introduced. [1] Y Mano, et al., J. Neurosurgery 124(2016) 1490-150 [2] , J. Cryst. Growth 50(1980) 8-17

UNIDIRECTIONAL SOLIDIFICATION OF IR/IR-RH FIBER CRYSTALS FOR THERMOCOUPLE BY ALLOY-MICRO-PULLING DOWN METHOD

Rikito Murakami[1], Yuui Yokota[2], Kei Kamada[3], Yasuhiro Shoji[3], Shunsuke Kurosawa[4], Yuji Ohashi[3], Akihiro Yamaji[3], Akira Yoshikawa[3]

[1]C&A Corporation, JAPAN, [2]New Industry Creation Hatchery Center, Tohoku University, JAPAN, [3]Institute for Materials Research, Tohoku University, JAPAN, [4]Department of Physics, Yamagata University, JAPAN

Thermocouples are used in many fields including crystal growth. For example, in the case of oxide crystal growth whose melting temperature are high (~2000°C) in sparse oxygen mixed atmosphere, Ir/Ir-Rh thermocouple is used. In general, it is preferable that thermocouples are flexible enough to set them freely to samples (crucible, insulators and so on), however, present Ir/Ir-Rh thermocouples are brittle and easily rapture by deformation. Our group have studied an alloy wire synthesis process by micro-pulling down method (Alloy-micro-pulling down method, A-μ-PD method) with alumina crucible, and succeeded in growing Pd-In-Fe and NiFeCoGa wires. Recently, we also succeeded in growing Ir were (Tm=~2447°C) with diameter of 1 mm and with length of more than 10 m by developing the zirconia crucible which can be used at over 2500°C. The grown wires have shown excellent flexibility due the elongated coarse grains along growth direction, therefore, it is highly expected to apply A-μ-PD method to produce thermocouples. For practical application, there are some problems to be solved in: (i) to make wires with diameter as thin as 0.5 mm, which is equivalent to existing commercial thermocouples, (ii) to evaluate thermoelectromotive force (EMF) at high temperature. In this research, we aimed to fabricate deformable Ir/Ir-Rh thermocouple by A-μ-PD method and measure the EMF. Ir and Rh powders (99.9% purity) were used as raw materials. Pure Ir and Ir-40 wt.% Rh were pelletized by arc melting, and then wires with diameter of 0.5 mm were produced in an A-μ-PD furnace (Micropuller A-01, C&A corp.) using zirconia crucibles. In order to observe the structure by scanning electron microscope (SEM, J-7800F, JEOL), after mechanical polishing, cross section polishing (CP) treatments with argon ion beam were performed to remove surface strain. The crystal grain size and crystal orientation were evaluated by the electron back scatter diffraction (EBSD) technique. Fig. 1 (a) and (b) shows a band contrast image and a crystal orientation map for normal direction of the Ir-40Rh wire. From these images, the grown wire consists of several large and oriented crystal grains. In addition, the EMF was evaluated using a tubular furnace and a commercially available thermocouple. At this time, the reference junction was kept at 0 °C. The EMF curve showed good correspondence with that of existing thermocouple. In the presentation, mechanical

properties will be also reported.

CRYSTALLIZATION OF ALPHA-LACTOSE MONOHYDRATE (α-LM) FROM AQUEOUS SOLUTION USING DIFFERENT ORGANIC SOLVENTS

P Parimaladevi, K Vinodhini, **Srinivasan Karuppannan**

Bharathiar University, INDIA

The crystal purity, size, size distribution, morphology and polymorphism are the specific target characteristics which have the potential to impact drug delivery, bio-performance of the pharmaceutical products and texture, functionality, consumer perception of the food products. Alpha-lactose monohydrate (α-LM) is an important disaccharide and is widely used as a carrier in dry powder inhaler (DPI) and also used as a main ingredient in most of the dairy products. The quality, shelf-life and bio-pharmaceutical performance of the DPI and dairy products depends on the size, size distribution and morphology of α-LM. To produce α-LM with preferred qualities, it is essential to control the crystallization conditions. Crystallization of α-LM is an important purification step in refining lactose from whey solutions. Nucleation of α-LM occurred only after a very long time ~134 h and this is a major drawback leading to the uneven distribution and growth of larger crystals. To overcome these problems, we employed gas-phase diffusion and anti-solvent crystallization to reduce the nucleation time and to control the size and morphology of α-LM. The aqueous solution of α-LM was mixed with different volumes of organic solvents like, DMSO, ethanol and acetone. The solubility of α-LM in aqueous solution was decreased by the addition of DMSO in the ratio 10-50% v/v and it increases by further addition of DMSO (i.e., 50-95 %). The different levels of supersaturation generated through gas-phase diffusion and anti-solvent crystallization leads variation in the nucleation time of the solution, size and morphology of the nucleated crystals. The level of supersaturation generated through anti-solvent crystallization process is greater than that of gas-phase diffusion process. The nucleation time of lactose was greatly reduced and the size of the nucleated crystals was very small in anti-solvent process compared to the gas-phase diffusion. The variation in size and morphology of the crystals grown by these two methods were analyzed by optical microscope and the physical properties were analyzed by PXRD and DSC. The obtained results reveal that, crystals grown by anti-solvent process having different morphologies and contain the mixture of α-LM and anhydrate forms of lactose, but the crystals grown by gas-phase diffusion having tomahawk morphology and contain only α-LM. By employing gas-phase diffusion crystallization process we could able to crystallize α-LM crystals within shorter induction time when compared to conventional crystallization method and also adopting this method we could achieve α-LM crystals with high purity when compared to anti-solvent crystallization method.

ADVANCED PULSED LASER DEPOSITION

Gertjan Koster

University of Twente, NETHERLANDS

Advances in thin film synthesis and characterisation of complex oxide perovskites have shown that physical properties are highly sensitive to slight deviations from ideal crystal stoichiometry. An example is the lanthanum aluminate ($LaAlO_3$) on strontium titanium oxide ($SrTiO_3$) hetero structure, where at the interface between these insulating materials a two-dimensional electron liquid (2-DEL) forms, showing interesting phenomena, such as superconductivity and magnetism. Small variations in the composition of the $LaAlO_3$ layer eventually determine the conductive state measured at the hetero-interface. More generally, the main goal and challenge in the synthesis of complex oxide thin films is to control stoichiometry and herewith control thin film properties. This challenge in obtaining high purity thin films has driven the development and understanding of thin film deposition techniques. Regarding the growth of complex metal oxides, Molecular Beam Epitaxy (MBE) and Pulsed Laser Deposition (PLD) are the most widely mentioned for their capability of growing near stoichiometric thin films. In PLD, the congruent ablation of a target material using a high intensity pulsed laser results in a plasma plume which expands towards a substrate. Species subsequently condense on the substrate, where due to high supersaturation a high-density nucleation of small two-dimensional islands is promoted, enhancing near stoichiometric growth. The breakthrough for PLD came in 1987 with the synthesis of the high Tc superconducting $YBa_2Cu_3O_7$ thin films, which was of superior quality to that of films deposited with alternative techniques, stressing the importance of stoichiometry control. However, a mechanistic understanding is still lacking, in particular regarding processes that take place in the plasma plume. Here we report on the research that has been carried out in understanding the element specific composition of the plume in relation to the quality of the films. By applying two-dimensional laser induced fluorescence (LIF) and self-emission spectroscopy (SES) on multiple plasma constituents, we are able to directly link the oxidation of plasma species in complex oxide PLD plasmas for the stoichiometry and crystalline quality of the thin films grown, applied to various oxide model systems. Spatiotemporal LIF mapping of the plasma species in different background gas compositions give new input for modelling surface growth, as well as provides additional control over the exact degree of stoichiometry of thin films.

SYNTHESIS OF FREESTANDING SINGLE-CRYSTAL OXIDE THIN FILMS AND HETEROSTRUCTURES

Yasuyuki Hikita

SLAC National Accelerator Laboratory, UNITED STATES OF AMERICA

Epitaxial complex oxide thin films and heterostructures provide an ideal platform to develop novel physical and chemical properties for applications ranging from quantum transport [1] to catalysts for renewable energy resources [2]. This owes to the flexibility in the control of their physicochemical properties by chemical composition as well as external perturbations such as strain and electric fields. In parallel, there have been efforts to make oxide thin films and heterostructures freestanding from the substrate [3] or the underlying sacrificial buffer layer [4, 5] by selective etching allowing mechanical manipulation of these functionalities. One of the main challenges to this end has been the establishment of a versatile method applicable to a wider range of functional oxides with fewer restrictions on the combination of the buffer material and the etchant, often requiring strong acids due to the robust nature of the oxide buffers. We have recently developed a technique to synthesize millimeter-size single crystalline oxide thin films freestanding from the substrate by employing a water-soluble buffer layer ($Sr_3Al_2O_6$) [6]. This method involves growth of thin films on an epitaxial $Sr_3Al_2O_6$ stabilized on an oxide substrate, followed by selective etching using pH-neutral water to detach the thin film from the substrate. In this presentation, I will introduce this technique with emphasis on the challenges encountered in the epitaxial growth of the heterostructures and the etching processes. We believe that the successful fabrication and characterization of freestanding complex oxide thin films could bring many opportunities both in the field of fundamental scientific research and device applications. [1] Y. Matsubara, K. S. Takahashi, M. S. Bahramy, Y. Kozuka, D. Maryenko, J. Falson, A. Tsukazaki, Y. Tokura, and M. Kawasaki, Nature Commun. **7**, 11631 (2016). [2] L. C. Seitz, C. F. Dickens, K. Nishio, Y. Hikita, J. Montoya, A. Doyle, C. Kirk, A. Vojvodic, H. Y. Hwang, J. K. Nørskov, and T. F. Jaramillo, Science **353**, 1011 (2016). [3] D. M. Paskiewicz, R. Sichel-Tissot, E. Karapetrova, L. Stan, and D. D. Fong, Nano Lett. **16**, 534 (2016). [4] H. Ohta, A. Mizutani, K. Sugiura, M. Hirano, H. Hosono, and K. Koumoto, Adv. Mater. **18**, 1649 (2006). [5] L. Pellegrino,M. Biasotti, E. Bellingeri, C. Bernini, A. S. Siri, and D. Marré, Adv. Mater. **21**, 2377 (2009). [6] D. Lu, D. J. Baek, S. S. Hong, L. F. Kourkoutis, Y. Hikita, and H. Y. Hwang, Nature Mater. **15**, 1255 (2016).

NON-EQUILIBRIUM SYNTHESIS OF HIGHLY POROUS SINGLE-CRYSTALLINE OXIDE NANOSTRUCTURES

Dongkyu Lee, Xiang Gao, Lisah Fan, Erjia Guo, Thomas O. Farmer, William T. Heller, Michael R. Fitzsimmons, Matthew F. Chisholm, Ho Nyung Lee

Oak Ridge National Laboratory, TN, UNITED STATES OF AMERICA

Nanoscale structures and materials have attracted great interest over the last two decades owing to their physical properties or behaviors, which differ completely from those of their bulk counterparts. The fabrication of nanostructured materials requires using specialized methods and understanding growth mechanisms, and demand is growing for developing materials with vertically aligned geometries. As vertically aligned material systems offer many advantages, such as large length-to-width aspect ratio, high surface-to-volume ratio, and high density interfaces, a great number of opportunities can be realized by vertically aligned single crystalline nanomaterials. However, directed synthesis of such vertically aligned single crystalline nanostructures has been virtually unexplored. One of the main reasons is that while the formation of single crystalline phases requires a lot of heat to stabilize defect-free lattice structures, synthesis at a high temperature, close to or above the crystallization temperature of most oxide materials, usually promotes the surface diffusion of adatoms, forming a flat film. Therefore, achieving the ultimate control of this 2D oxide growth to construct 3D architectures has been extremely difficult, despite the enormous potential for technological breakthroughs. In this presentation, we will present a completely new synthesis route to the formation of micron-long single-crystalline oxide nanobristles.[1] Single crystalline nanostructures of either CeO_2 or Y_2O_3, with a large porosity (up to ~50 %), were fabricated by pulsed laser epitaxy enabling a direct and template-free synthesis. This directed synthesis was made possible by growing oxide nanostructures under kinetically and thermodynamically balanced non-equilibrium conditions, far from the conventional growth conditions optimized for 2D thin films. This discovery suggests the great potential of the pulsed laser epitaxy technique for design of functional oxide materials with precisely controlled morphologies and dimensions. In addition, due to the extremely large surface area offered in these oxide nanostructures, many technological applications can be envisioned, including chemical sensors, fuel cells, membranes, and photovoltaic and electronic devices, in which a large contact area is critical for obtaining high efficiency and capacity. 1. D. Lee, X. Gao, L. Fan, E. Guo, T. O. Farmer, M. R. Fitzsimmons, M. F. Chisholm, and H. N. Lee, *Adv. Mater. Interfaces* **4**, 1601034 (2017). * This work was supported by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy.

TUNING FUNCTIONAL PROPERTIES IN OXIDE NANOCOMPOSITES

Aiping Chen[1], Erik Enriquez[1], Haiyan Wang[2], Judith L. Macmanus-Driscoll[3], Quanxi Jia[4]

[1]CINT, Los Alamos, NM, UNITED STATES OF AMERICA, [2]Purdue University, UNITED STATES OF AMERICA, [3]University of Cambridge, UNITED KINGDOM, [4]Univ. at Buffalo, SUNY, Department of Materials Design and Innovation, NY, UNITED STATES OF AMERICA

Oxide nanocomposites have attracted great attention due to the tunable lattice strain, large vertical interfacial area and emergent phenomena. The flexibility of design multifunctional properties in nanocomposites has opened new averneu for device applications. In this talk, I will focus on our efforts on the design, synthsis and characterization of different vertical heteroepitaxial nanocomposites. From a design point of view, we summarize the optimized flow for the strain design in oxide nanocomposites. Via advanced growth design, we are able to manipulate the nanoscale thin films growth and the strain status in nanocomposites. We can further control the functional properties at heterointerfaces in a variety of materials systems by using the lattice strain.

CATION STOICHIOMETRY CONTROL FOR HIGH-QUALITY EPITAXY OF COMPLEX OXIDES BY PULSED LASER DEPOSITION

Tsuyoshi Ohnishi

National Institute for Materials Science, JAPAN

Epitaxial oxide thin films are at the heart of new oxide electronics and ionics applications including solid-state batteries. Complex oxide films are often grown by pulsed laser deposition (PLD) because the technique is believed to be material-agnostic. Here we show that one of the fundamental premises to justify the use of PLD, that material is transferred from a sintered or a single crystal target to the film without stoichiometry deviations, is incorrect even when no volatile elements are involved. The commonly-used solution of increasing the laser energy density (fluence) above a material-specific threshold value to obtain stoichiometric films does not work. Lattice volume expansion in oxide thin films, which are often incorrectly ascribed to oxygen deficiency, correlate with cation nonstoichiometry in case of $SrTiO_3$ leastwise. We show that adequate choice of ablation laser conditions is essential and often more important than the growth temperature and oxygen pressure for obtaining bulk-like properties in oxide epitaxial thin films. This idea is expanded not only to the (Nb:)$SrTiO_3$ homoepitaxy, but also to a Ru-volatile $SrRuO_3$, a Li-volatile/light-element $LiCoO_2$, and a 3-cation $Li_{3x}La_{2/3-x}TiO_3$ heteroepitaxy in order to reacknowledge the importance of growth temperature and oxygen pressure, in addition to the laser ablation conditions in terms of cation stoichiometry control.

SUBMILLIMETER-SIZED NATAO3 SINGLE CRYSTALS GROWN VIA COOLING OF NA_2MOO_4 FLUX

Sayaka Suzuki[1], Haruka Saito[2], Tetsuya Yamada[3], Katsuya Teshima[3]

[1]Faculty of Engineering, Shinshu University, JAPAN, [2]Graduate School of Science and Technology, Shinshu University, JAPAN, [3]Center for Energy and Environmental Science, Shinshu University, JAPAN

$NaTaO_3$, which has a perovskite structure, is especially known as a semiconductor photocatalyst for overall water splitting under ultraviolet light irradiation. $NaTaO_3$ particles have been synthesized by solid-state reaction, sol-gel, hydrothermal, solvothermal, and flux methods. However, large-sized crystals exceeding several hundred micrometers have not been reported. Here, we report the growth of submillimeter-sized $NaTaO_3$ crystals by the cooling of a Na_2MoO_4 flux. Flux method is one of the crystal growth technique from high-temperature solution. It can produce high-quality crystals at temperatures below the melting points of the solutes. The crystal size and shape can be controlled by varying the growth conditions, such as flux, solute concentration, cooling rate, etc. A stoichiometric mixture of Na_2CO_3 and Ta_2O_5 powders was used as a solute, and $Na_2MoO_4 \cdot 2H_2O$ powder was chosen as the flux. The solute concentration was varied from 1 to 50 mol%. The platinum crucibles containing each mixture were heated to 1000-1500 °C and held at each temperature for 10 h. They were then cooled at a rate of 150 or 5 $°C \cdot h^{-1}$. After cooling to room temperature, the crystal products were separated from the remaining flux in warm water. The obtained crystals were observed by scanning electron microscope. Phases and elongated directions of the crystals were studied by X-ray diffraction. Well-formed, cube-like $NaTaO_3$ crystals were successfully grown from a Na_2MoO_4 flux. The crystals were grown by cooling of the Na_2MoO_4 flux, because the flux evaporation rate was less than 1wt% at any solute concentration and holding temperature. In addition, the crystal size was dependent on cooling rate and solute concentration. When the $NaTaO_3$ crystals were grown at a solute concentration of 1 mol% and a holding temperature of 1500°C, submillimeter, plate-like crystals were grown in addition to cube-like crystals of several tens of micrometers. Acknowledgements: This research was partially supported by JSPS Grant-in-Aid for Scientific Research (A) 25249089.

GROWTH ANGLE - A MICROSCOPIC VIEW

Konstantin Mazuruk[1], Martin Volz[2], Arnold Croll[1]

[1]University of Alabama in Huntsville, AL, UNITED STATES OF AMERICA, [2]NASA Marshall Space Flight Center, AL, UNITED STATES OF AMERICA

The growth angle that is formed between the side of the growing crystal and the melt meniscus is an important parameter in the detached Bridgman crystal growth method, where it determines the extent of the crystal-crucible wall gap, and in the Czochralski and float zone methods, where it influences the size and stability of the crystals. The growth angle is a non-equilibrium parameter, defined for the crystal growth process only. For a melt-crystal interface translating towards the crystal (melting), there is no specific angle defined between the melt and the sidewall of the solid. In this case, the corner at the triple line becomes rounded, and the angle between the sidewall and the incipience of meniscus can take a number of values, depending on the position of the triple line. In this work, a microscopic model is developed in which the fluid interacts with the solid surface through long range van der Waals or Casimir dispersive forces. This growth angle model is applied to Si and Ge and compared with the macroscopic approach of Herring. In the limit of a rounded corner with a large radius of curvature, the wetting of the melt on the crystal is defined by the contact angle. The proposed microscopic approach addresses the interesting issue of the transition from a contact angle to a growth angle as the radius of curvature decreases.

POTASSIUM-COBALT SULFIDE CRYSTAL GROWTH ASSISTED BY LOW FREQUENCY VIBRATIONS

Andrey Sadovskiy[1], Ivan Ermochenkov[2], Evgeniya Dubovenko[2], Marina Zykova[2], Ekaterina Sukhanova[2], Igor Avetissov[2]

[1]IPG IRE-Polus, RUSSIAN FEDERATION, [2]Dmitry Mendeleev Univeristy of Chemical Technology of Russia, RUSSIAN FEDERATION

The spectral feature of light on the Earth's surface is the presence of a gap in the range of 200-300 nm. This is a consequence of the absorption by the ozone layer. This effect allows detecting , with high accuracy, UV radiation sources in this range, such as electrical discharges, flames, etc. Therefore, optical filters that are transparent in the required range and opaque in the rest of the wavelength range are of great interest. The most effective filters are elements cut from crystals of sulfates Since these crystals are colored and transparent in some part of the visible spectrum, a circuit is used of two successively mounted filters, selected so that the resulting optical element is transparent only in the UV range. One of the crystals often used for such purposes is cobalt potassium sulfate crystal. Single crystals of $K_2Co(SO_4)_2{\cdot}6H_2O$ are commonly grown from solution, using the temperature reduction method [1]. But the growth rate is very low and the process is very sensitive to the purity of raw materials. In the research we made an attempt to enhance the process by application of the axial low frequency vibration control technique (AVC-technique) which is referred as a powerful tool for liquid structure control as well as heat mass-transfer control [2]. Numerical modeling of heat-mass transfer in liquid under the AVC action was fulfilled. The liquid structure was experimentally analyzed depending on AVC activation by Raman spectroscopy and corresponding AVC-regimes have been chosen for the crystal growth. The grwoth rate at the AVC application was ~2 times more and the AVC-grown crystal faceted by other planes comparing with traditionaly grown crystal (Fig 1). We observed the significant enchancement of structural quality and spectral propeties of the AVC-grown crystal compared with traditionaly grown crysta. The dislocation density was in in one order less. Transparensy in 200-380 nm range was in 10% higher.

Fig.1 Facetting of $K_2Co(SO_4)_2{\cdot}6H_2O$ crystals grown from AVC activated (right) and non-activated water solutions. [1] A.A. Zhokhov et al. Crystallography Reports, 2016 (61) 6 1027–1030 [2] A. Sadovskiy et.al, JCG, 2014 (417) 16

INVESTIGATION OF ENHANCED ROOM TEMPERATURE FERROMAGNETISM IN CO DOPED SNO_2 NANOPARTICLES

Rajan Renu[1], R Ezhil Vizhi[1], D Rajan Babu[1], **H Arul**[2]

[1]VIT University, INDIA, [2]Kumaraguru Institute of Technology, INDIA

The citrate gel combustion technique was used to synthesize polycrystalline Cobalt doped SnO_2 diluted magnetic semiconductors with dopant concentrations of 0, 1, 5, 10 and 15%. We present the results of a detailed investigation of the structural, optical, and magnetic properties of chemically synthesized pure and Co-doped SnO_2 powders using x-ray diffraction (XRD), diffuse reflectance spectroscopy, FTIR spectroscopy and magnetometry. . The structures of all the samples were confirmed to be tetragonal from the x-ray diffraction analysis. The crystallite sizes of all the samples were in nanoscale range, which increases with an increase in dopant concentration; whereas a reduction in lattice parameters were observed with increase in doping. The diffuse reflectance spectroscopy data reveals that the absorption edge transfers to upper wavelengths and energy bandgap was found to be decreasing with an increase of Co concentration. Vibrational spectroscopy shows the characteristic absorption peaks of Sn–O and confirms the incorporation of Co ions in SnO_2 lattice. The presence of room temperature ferromagnetism has been confirmed by the magnetization studies even for the undoped sample. The magnetization loop obtained for pure SnO_2 alone was a distorted one. As there were no magnetic impurities present in the undoped sample, we assume that the origin of ferromagnetism may be the exchange interactions between localized electron spin moments resulting from oxygen vacancies at the surfaces of nanoparticles. The magnetic moment was found to increase with increasing Co content. Increasing the Co doping to 15% leads to a rapid increase in saturation magnetization which is contradictory to the existing literature results, were a reduction in ferromagnetism was reported for higher doping concentrations. Even though Ms increases, the higher coercivity of 430 G remains same for both 10% and 15% of the dopant. Magnetic hysteresis loops were observed at room temperature with high coercivity Hc of 430 G and remanent magnetization Mr of 204 memu/g for 15 wt% Co doped sample. The striking similarity between the changes in the lattice parameters and the magnetic properties of $Sn_{1-x}Co_xO_2$ indicates a structure-magnetic property relationship. Finally, it has been concluded that the ferromagnetic properties depend not only on the surface diffusion of Co ions and the distribution of defects such as oxygen vacancies or vacancy clusters but also on nanometric size of the materials and the dopant. This study demonstrates that the Co doped SnO_2 materials can be used for applications in optoelectronics and spintronics.

CALCIUM CARBONATE IN THE SUGAR TECHNOLOGY

Evzen Sarka, Zdenek Bubnik

University of Chemistry and Technology, Prague, CZECH REPUBLIC

Classical juice purification in the sugar industry is based on lime addition and application of carbon dioxide. The main role of the formed calcium carbonate in the sugar industry is an adsorbent of impurities (non-sugars) contained in sugar juices. The resulted precipitate is a significant by-product called carbonation mud (sludge). The paper deals with polymorphism of calcium carbonate, which has three common polymorphs - calcite, aragonite, and vaterite. The further natural forms are hydrates such as monohydrocalcite, ikaite - hexahydrate of calcium carbonate[1], hydrate of aragonite and vaterit[2], or amorphous $CaCO_3$. Kantiranis[3] and Šárka[4] found that the calcium carbonate sediment from sugar factories is mainly consisting of calcite. On the other hand needle aragonite precipitates were revealed for carbonation sludge precipitated in laboratory from frozen raw juice (purity 86.6%)[5]. Size of aggregates of the carbonation precipitate is an important property to have good filtration possibility of the carbonation juice. For increasing the particle size it is necessary:

- high-quality progressive pre-liming
- recycling of 1st carbonation precipitate to prelimer
- optimal alkalinity (pH) of the 1st carbonation
- sufficient lime addition
- addition of flocculants

The mechanism of the calcium carbonate formation during carbonation is described. Carbonic system is derived from the dissolution of carbon dioxide which is intimately involved in the control of the pH. The first step is dissolving of carbon dioxide from bubbles with follow-up hydration in two ways – to ion HCO_3^- or H_2CO_3. Many scientific publications inform about calcium-sugar complexes which can influence the balances inclusive the $CaCO_3$ precipitation because they would increase the solubility. But the complex formation is probably not so significant at carbonation temperature (» 85 °C). The analytical methods to characterize the chemical composition and crystallinity of calcium carbonate are designated. Aspects of new industrial application of carbonation mud are given. 1. Shaikh A.M.: A new crystal-growth form of vaterite, CaCO3. J. Appl. Crystallogr. 23, 1990, 263-265. 2. de Leeuw N., Parker S.C.: Surface structure and morphology of calcium carbonate polymorphs calcite, aragonite, and vaterite: an atomistic approach. J. Phys. Chem. B 102, 1998, 2914-2922. 3. Kantiranis N.: Re-cycling of sugar-ash: a raw feed material for rotary kilns. Waste Management 24, 2004, 999-1004. 4. Šárka E.: Vedlejší produkty cukrovarnického a škrobárenského průmyslu – vznik, využití a optimalizace parametrů. Listy cukrov. a řep. 128, 2012, 307-312. 5. Šárka E.: Activation of carbonation slurry concentrate - A method of saving limestone. Zuckerind. 124, 1999, 406-410.

ANALYSIS OF VERTICAL GRADIENT FREEZE (VGF) PROCESS SCALE-UP FOR THE GROWTH OF CADMIUM ZINC TELLURIDE (CZT) SINGLE-CRYSTAL, LARGE-AREA SUBSTRATES

John Roerig[1], Nathan T. Morgan[1], Kelly Jones[2], Scott Johnson[2], Jeffrey J. Derby[1]

[1]University of Minnesota, MN, UNITED STATES OF AMERICA, [2]Raytheon Vision Systems, CA, UNITED STATES OF AMERICA

Computational models are being developed by the University of Minnesota to provide insight for the scaling of a vertical gradient freeze (VGF) process employed by Raytheon Vision Systems (RVS) for the growth of cadmium zinc telluride (CZT). The baseline process currently produces 92-mm diameter boules toward the production of large-area substrates, with an initial scale-up goal of 125-mm diameter boules and a target scale-up to 150-mm diameter. The goal of the University of Minnesota effort is to cooperatively work with RVS to develop, validate, and employ coupled, multi-scale computational models to optimize the CZT crystal growth processes This poster will present initial results on this collaborative project. Computations of heat transfer, obtained using CrysMAS, a code developed by the Crystal Growth Laboratory, Fraunhofer IISB, will be compared to measured thermal profiles through the VGF furnace. Preliminary computations using our finite element code, Cats2D, will be presented to highlight the growth characteristics of this process. Of particular interest are prospects for model-directed process scaling to larger boule diameter and furnace design toward improving single-crystal yield. --------------- This work has been supported by the USDOD/Air Force, Defense Production Act (DPA) Title III Cadmium Zinc Telluride (CdZnTe) Substrate Program, under Raytheon Vision Systems Award 4201198079.

POCESSING OF CONCENTRATED SOLAR RADIATION PV MODULES ON THE BASIS OF ALGAAS-GAAS HETEROSTRUCTURES

Ia Trapaidze[1], Gela Goderdzishvili[1], Lia Trapaidze[2], Rafiel Chikovani[1]

[1]Dep. of Physics, Georgian Technical University, GEORGIA, [2]Dep. orf Physics, Tbilisi State Univeristy, GEORGIA

Among the alternative and renewable sources of energy the transformation of solar energy directly into electric energy attracts more growing attention. Till present the photoelectric transformers of solar radiation practically have been prepared only on crystalline silicon. The goal of researchers is to increase efficiency of photoelectric transforming systems and to lower the cost. These actual problems have defined goal of our research. In the present work for fabrication of hetero-structures of AlGaAs-GaAs we have used the low-temperature liquid-phase epitaxial method to develop the technology and construction of preparation of photoelectric transforming elements of solar concentrated radiation, study of their electro-physical properties. On the basis of multilayer hetero-structure we have labored out the design and technology fabrication of photoelectric transforming element and module of solar concentrated radiation. On the basis of p-n hetero-structures prepared by the low-temperature technological methods we have created a laboratory version of solar cells and module. We have worked out the methods of testing modules and lenses in the field conditions and have carried out the testing. On the basis of analysis of the received results we have labored out a recommendation about the industrial version of solar concentrated radiation. In the low-temperature liquid-phase epitaxial method we introduced the changes and identified: a chemical composition of solid solutions of separate layers of multilayer hetero-structures; the optimal thicknesses; type and concentration of doping material; the temperature-time modes of the growing processes. As a result in the obtained hetero-structures the high value of efficiency coefficient of solar concentrated radiation up to 23,4% (K=100-500) and stability of technological process have been achieved. On basis of obtained hetero-structures for module of concentrated module we have developed the topology of the crystals of solar cells and on their basis we have created the design of module by using the panel of Frenkel lenses. By using of testing methods of elements and modules we have studied the main parameters both in laboratory and field conditions. On the basis of results obtained from field testing carried out in the mentioned regions which have been reflected on the parameters of transforming system and on its loading characteristics, it is shown that there exists the definite correlation between the transformation efficiency and two main parameters – thickness of atmospheric layer (AM) and state of the atmosphere in a given region. We developed design and fabricated a pilot model of low power tourist mobile photoelectric system.

AXIAL VIBRATION CONTROL TECHNIQUE FOR CRYSTAL GROWTH FROM LIQIUD

Andrey Sadovskiy[1], Vladimir Kostikov[2], Ekaterina Sukhanova[2], Igor Avetissov[2]

[1]IPG IRE-Polus, RUSSIAN FEDERATION, [2]Dmitry Mendeleev Univeristy of Chemical Technology of Russia, RUSSIAN FEDERATION

To date the axial low-frequency vibration control technique (AVC) has already been experienced on a number of crystal growth processes [1,2]. However, the problem of the general regularities between AVC parameters and vibrational flows' characteristics has still remained open. To understand the nature of the vibratory flow formation and properties we have conducted the system analysis of flows' behavior in Bridgman configuration. ANSYS 14.5 Fluent was used for numerucal simulation and Ge melt was considered as a model substance. The AVC technique was realized by harmonic oscillations of a cylindrical disk submerged into melt (Fig.1). The disk is specified by three critical parameters: 1) diameter (***d)***, 2) thickness (***l)***, and 3) radius of the edge curvature (***r***) between a cylindrical generatrix and a faceplate, which sufficiently influenced on flows' generation [1]. We carried out an analysis of ***d, l, r*** influence on parameters of steady vibrational flows and on viscous dissipation energy (P_w). At crystal growth the average vibrational flows are responsible for heat-mass-transfer, while P_w determines liquid structure characteristics [3]. We establised that the mean velocity of vibrational flows was inversely to ***r*** and demonstrated non-linear increase with AVC amplitude (***A***). An integral P_w for the whole melt volume demonstrated $P_w \sim v_{osc}^3$, dependence, here $v_{osc} = 2 \pi f A$ (Table 1). The maximum P_w close to the disc edge is proportional to oscillating velocity v_{osc}, but it increases faster with 3.8 number exponent.

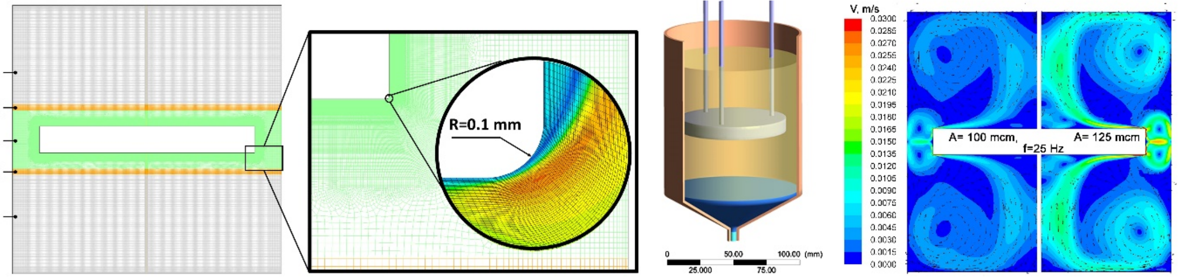


Fig.1. Grid of calculation area (left) and scheme of the AVC-Bridgman technique (center): 1—stationary zones, 2—stress–strain zones, 3—disk zone. Velocity vectors of flows (right) and integral viscous dissipation near the oscillating disk edge (right) at AVC impact on Ge melt

Table 1. Regression equations of different parameters *vs* AVC intensity $\boldsymbol{I}_{AVC} = \boldsymbol{A}^m \boldsymbol{f}^n$ (***A*** in micrometer, ***f*** in Hz and scaling of 10^{-9} applied to the I_{vib} value)

Parameter	Regression	Determination coef.	Vibrational Intensity
V_{avg}, mm/s	$7.6126\ I_{vib} - 1.4593$	$R^2=0.9976$	$I_{vib} = A^3 f^{2.05} \times 10^{-9}$
F_{disk}, N	$0.2008\ I_{vib} + 0.876$	$R^2=0.9965$	$I_{vib} = A^{1.3} f^{2.6} \times 10^{-9}$
P_{int}, W	$(1.989\ I_{vib} + 3.756) \times 10^{-5}$	$R^2=0.9993$	$I_{vib} = A^3 f^3 \times 10^{-9}$
P_{max}, W/m^3	$9403.8\ I_{vib} - 37718$	$R^2=0.9965$	$I_{vib} = A^3 f^{3.3} \times 10^{-9}$

[1] I.Ch. Avetissov et al., JCG **360**, 167 (2012) [2] I. Kh. Avetisov et al., Crystallography Reports **50(1)** S124 (2005). [3] A. Sadovskiy et al., JCG **417**, 6 (2015)

MONTE CARLO STUDY OF THE GROWTH KINETICS DURING MBE OF GAAS ON THE SUBSTRATES WITH DIFFERENT ORIENTATIONS

Maxim S. Solodovnik, Sergey V. Balakirev, Oleg A. Ageev, Ilya A. Mikhaylin, Mikhail M. Eremenko

Southern Federal University, RUSSIAN FEDERATION

A great interest to the diffusion and nucleation processes during GaAs epitaxial growth has still been apparent. The crystal structure, energy barriers for relevant microscopic processes and the temperature influence on the island and adatom characteristics are actively investigated, particularly for the GaAs(001) surface. However, in recent years there has developed an interest to the deposition of material on non-(001) oriented substrates due to their specific advantages. Many experimental works in this field have enabled a big progress, but theoretical studies of the MBE growth on non-(001) oriented substrates are rare or even not carried out at all. In the present work, the kinetic Monte Carlo method is used to study kinetic processes during MBE growth of GaAs on the (001), (111)A and (110) surfaces. The model takes in account the most relevant steps of the growth such as surface diffusion of Ga and As_2, chemisorption and physisorption of Ga and As_2, desorption and readsorption of As_2. Each event is implemented sequentially with a probability determined by the Arrhenius equation. The crystal is considered to be two-dimensional with zinc blende lattice structure and reconstructed surface according to the phase diagram. The simulations show that the surface diffusion of Ga adatoms on the GaAs(111)A surface is isotropic, whereas the (001) and (110) surfaces provide anisotropic diffusion. As a result, nuclei are elongated along the dimer rows of the (2×4) reconstruction on the (001) surface and along the [1-11] direction on the (110), whereas islands on the (111) surface are chaotic in shape. The triangular shape of the (110) islands is due to the crystallographic features of the (1×1) reconstruction observed in a wide range of technological parameters. The growth rate v and As_2/Ga flux ratio $R_{As/Ga}$ are observed to have an influence on the diffusion parameters of Ga adatoms. However, these dependences are much stronger for the GaAs(111) and GaAs(110) surfaces. The diffusion length is found to be larger for the (111) and (110) surfaces in a wide range of the kinetic growth parameters, in good agreement with previous works, but with increasing both growth rate and V/III flux ratio the diffusion lengths for both surfaces tend to become equal. The reason of this behavior is an excess of arsenic species suppressing Ga surface diffusion. The reported study was funded by Grant of the President of the Russian Federation, project No. MK-2629.2017.8.

MODELING THE DEFECT STRUCTURE OF GROWING CRYSTAL USING THE VLASOV MODEL FOR SOLIDS

Vitalyi Igorevich Talanin, Igor Evgenievich Talanin, **Vladislav Igorevich Lashko**

Department of Computer Science & Software Engineering, Institute of Economics & Information Technology, UKRAINE

With the help of classical theory of nucleation and growth of second-phase particles in solids we can describe the formation and transformation of the defect structure of solid, both in the process of its growth, and as result of various technological impacts [1]. The Vlasov approach is based on the solution of the Vlasov kinetic equation. Vlasov equation represents a system of equations that describe the evolution of the particle continuum with potential of the pair interaction. For the first time a solution for ideal solid state was conducted Vlasov. Vlasov showed that the spatial periodic distribution is one of the particular conditions of particle motion [2]. We have considered the complex formation in the semiconductor silicon in accordance with the Vlasov model for solid [3]. It was demonstrated that the Vlasov model for solid state can be applied for the research not only the hypothetical ideal crystals, but also for description of formation of structure of real crystal. The formation of silicon-carbon and silicon-oxygen complexes during cooling after the growth of dislocation-free silicon single crystals has been calculated using the Vlasov model of crystal formation. It has been confirmed that the complex formation begins in the vicinity of the crystallization front. The Vlasov model for solid state describes the processes of complexation during the growth of real crystals adequately classical theory of nucleation and growth of second-phase particles in solids. Method of calculation of the initial defect structure of crystals was proposed. This method includes the Vlasov model for solid state and the classical theory of nucleation and growth of second-phase particles in solids. Using the Vlasov model for solids, it has been shown that complex formation is unlikely in low-temperature crystal treatments. In this case, the processes of growth and transformation of growth defects occur. A software package was developed for analyzing and calculating the defect structure, which is formed during crystal growth. [1]. Talanin V.I., Talanin I.E. Physics of the Solid State. 2016, **58**, 427-437. [2]. Vlasov A.A. Journal of Physics. 1945, **9**, 130-139 (in USSR). [3]. Talanin V.I, Talanin I.E. Physics of the Solid State. 2016, **58**, 2050-2054.

GROWTH OF ZNO NANOROD ARRAYS ON PATTERNED SUBSTRATES

Jan Grym, Ondřej Černohorský, Roman Yatskiv, Šárka Chlupová, Antonín Schenk, Nikola Bašinová, David Roesel, Jan Vaniš, Stanislav Tiagulskyi

Institute of Photonics and Electronics of the CAS, CZECH REPUBLIC

A great deal of interest has been recently directed towards the design of new devices using one-dimensional semiconductor nanostructures. Despite a large number of applications, the anisotropic growth of ZnO from solutions is not well understood and the growth technology mostly relies on empirical results. We investigated the growth mechanisms of hydrothermally prepared ZnO vertical nanorod arrays on patterned substrates and seed layers in continuous-flow reactors (Fig. 1). Unlike conventional batch reactors, in the continuous-flow reactors the solution supersaturation can be accurately controlled, which enables to compare experimental results with fundamental crystal growth theories [1]. ZnO is a direct wide bandgap semiconductor crystallizing in the wurtzite structure with a series of unique properties: a large exciton binding energy; good optical transmittance in the visible region; high optical gain; piezoelectricity; room temperature ferromagnetism; mechanical stability given by the high melting point and large cohesive energy; radiation hardness; or biological compatibility. These properties allow for applications of ZnO in UV light-emitting devices and detectors, field-effect transistors, solar cells, piezoelectric nanogenerators, or chemical sensors [2]. For the majority of these applications, upright standing arrays with controlled positioning, sizes, and physical properties are preferred. The upright standing arrays of ZnO nanorods were prepared by hydrothermal growth on Si substrates with textured and randomly oriented ZnO seed layers and on GaN epitaxial layers patterned by electron and ion beam lithography. To study the electric charge transport in the nanorods, electrical contacts were formed by the deposition of colloidal graphite [3], by metal evaporation and by the deposition of Pt using the gas injection system in the SEM. The transport properties were correlated with the structural and optical

properties investigated by x-ray diffraction and photoluminescence spectroscopy. *This work was supported by the Czech Science Foundation projects: 17-00355S, 15-17044S, and 17-00546S.* [1] S.A. Morin, M.J. Bierman, J. Tong and S. Jin, Mechanism and Kinetics of Spontaneous Nanotube Growth Driven by Screw Dislocations. Science, 328(5977): p. 476-480. 2010. [2] U. Ozgur, Y.I. et al, A comprehensive review of ZnO materials and devices. Journal of Applied Physics, 98(4): p. 041301. 2005. [3] R. Yatskiv, V.V. Brus, M. Verde, J. Grym and P. Gladkov, Electrical and optical properties of graphite/ZnO nanorods heterojunctions. Carbon, 77(0): p. 1011-1019. 2014.

KINETIC MONTE CARLO MODEL OF DROPLET EPITAXY FOR IN/GAAS(001) NANOSTRUCTURES: EXPERIMENTS AND THEORY

Sergey V. Balakirev, Maxim S. Solodovnik, Oleg A. Ageev, Mikhail M. Eremenko, Ilya A. Mikhaylin

Southern Federal University, RUSSIAN FEDERATION

Droplet epitaxy is a promising growth method which allows producing dislocation-free and coherent nanocrystals. Although several experimental works concerned the growth of InAs/GaAs quantum dots by these technique, a lot of processes still need to be clarified, especially during the nucleation stage. In this work, a hybrid kinetic Monte Carlo model in combination with the classical nucleation theory is used to investigate the formation of In/GaAs(001) nanostructures during MBE. To validate the model, experiments under simulated growth conditions are carried out. Within the framework of a lattice model the crystal is represented as a 1+1 dimensional zinc blende lattice. An indium atom can occupy each lattice site having a tetragonal face-centered lattice as the most favorable. Atoms are bound with neighboring atoms of the first 7 coordination spheres. The diffusion hops are allowed in empty lattice sites with a probability expressed by the Arrhenius equation. In search of the most energetically favorable positions, atoms form islands. As a nucleus reaches critical size, the binding energies of atoms increase, according to the classical nucleation theory. Using this model, the growth rate and temperature influence on the characteristics of In nanostructure arrays is investigated. An increase of the droplet density is observed both with increasing growth rate and decreasing substrate temperature. This behavior is attributed to the suppression and enhancement of the surface diffusion of In adatoms, respectively. Since the critical island size falls with increasing supersaturation, the average island size is observed to decrease at the same time. The possibility to control island characteristics by altering the deposition thickness is also found. In this case, the island density remains almost steady whereas the average size can be adjusted. The simulation results demonstrate good agreement with experiments. According to SEM and AFM images, droplet surface density, average diameter and height correlate with the simulation values very well. Thus, the model is applicable to the description of the initial stage of the nanostructure formation and is intended to be developed to consider the processes of the droplet crystallization and formation of nanostructures on modified surfaces with complicated morphology. This work was supported by the Russian Science Foundation Grant No. 15-19-10006. The results were obtained using the equipment of the Research and Education Center and Center for Collective Use "Nanotechnologies" of Southern Federal University.

SYNTHESIS OF WATER SOLUBLE, LUMINESCENT LFNH NANOCRYSTALS FOR BIOLOGICAL APPLICATIONS

Mahendra M. Khandpekar[1], Tarannum W. Attar[2]

[1]Birla College of Arts, Science & Commerce, INDIA, [2]G M Momins College of ASC, INDIA

The recent interest in doped LaF_3 nanocrystals is due to its antimicrobial and antibacterial properties. $LaF_3:Nd^{3+},Ho^{3+}$ nanocrystals having spherical and hexagonal geometry with near uniform particle size of about 15nm have been successfully synthesized using chlorides of La, Nd and Ho with NH_4F in deionized water under clean conditions. Presence of elements was confirmed from EDAX analysis. The XRD analysis shows hexagonal crystal structure with $a = b = 7.098\ A^0$ and $c = 7.230\ A^0$, Space group: P3c1 (165) ($\alpha = \beta = 90^0$ and $\gamma = 120^0$. The c/a ratio is found to be 1.018 and the cell volume was found to be $364.26(A^0)$. SEAD pattern shows formation of strong diffraction rings corresponding to the (221), (113), (111), (110), (006), (223) reflections, and are in agreement with the hexagonal LaF_3 structure. The FTIR spectrum shows presence of surface groups like O-H, C-H and C-N which makes it water soluble. Multiple absorption edges in UV-Visible spectrum representing quantum dots with energies lying between 3.686 eV- 4.838 eV. Wide transparent region beyond 400nm further suggests its use in optoelectronic devices. Red coloured emission (629nm) is observed in PL spectra with excitation wavelength of 330 nm. SHG efficiency of 0.735 times that of KDP was confirmed by the emission of green radiation (532nm) from the sample. The dielectric constant and dielectric loss shows normal behaviour of dielectric materials. Dc conduction is dominant due to space charge effect and doping is seen to enhance the ionic conductivity of the sample.

HOT-PRESSED PRODUCTION AND LASER PROPERTIES OF FE^{2+}:ZNS AND FE^{2+}:ZNSE

Roman Avetisov[1], Stanislav Balabanov[1], Konstantin Firsov[2], Evgenii Gavrishchuk[1], Andrey Gladilin[2], Vladimir Ikonnikov[1], Viktor Kalinushkin[2], Igor Kononov[2], Oleg Uvarov[2], Marina Zykova[3], Elena Mozhevitina[3], Dmitry Savin[1], Natalia Timofeeva[1], Igor Avetissov[3]

[1]G.G. Devyatykh Institute of Chemistry of High-Purity Substances of the RAS, RUSSIAN FEDERATION, [2]Prokhorov General Physics Institute, Russian Academy of Sciences, RUSSIAN FEDERATION, [3]Dmitry Mendeleev Univeristy of Chemical Technology of Russia, RUSSIAN FEDERATION

The Cr or Fe doped ZnSe(S) crystals are the most promising materials for powerful tunable lasers in the 2-5 mm range. Dopant profile distribution in the active laser element strongly effects on the lasing characteristics. High concentration of the dopant on the surface increases probability of the laser breakdown at high power density. This problem can be solved by ensuring the maximum concentration of the dopant is in the sample volume and a zero one on the surface. We proposed a new approach for obtaining Fe^{2+}:ZnS and Fe^{2+}:ZnSe samples with undoped faces, combining the advantages of hot pressing and diffusion techniques. As a raw material we used CVD-ZnSe(S). Iron film (~1 mm) was deposited by electron-beam technique on one of the flat polished surfaces of CVD-ZnS (Se) discs Ø20×2 mm. The elements were touched in contact by iron surfaces, placed in a hot press die and heated under vacuum to 1000°C during 30 minutes with the application of 10 MPa uniaxial pressure. The iron film dissolved in ZnSe(S) matrix and elements welded together. The samples were subjected to hot isostatic pressing (HIP) during 28 hours at 100 MPa argon pressure and 1100-1300°C. After polishing we obtained three composite samples (Ø20×3.5 mm) with the following compositions: ZnSe/Fe^{2+}:ZnSe/ZnSe; ZnS/Fe^{2+}:ZnS/ZnS and ZnSe/Fe^{2+}:ZnSe/Fe^{2+}:ZnS/ZnS and required dopant distribution. The influence of sintering conditions and HIP processing on local morphology and properties of the interface of welded elements was studied by SEM and two-photon confocal microscopy. For all composite elements the lasing was obtained at a pumping by HF-laser at RT with relatively high efficiency. The proposed technique removes restrictions on the size of laser elements and appears to be very promising for the management of the distribution profile of the doping component. The work was supported by the Russian Science Foundation grant №15-13-10028.

GROWTH OF SCHEELITE-LIKE DISORDERED DOUBLE MOLYBDATE AND TUNGSTATE SINGLE CRYSTALS FROM STOICHIOMETRIC AND NON-STOICHIOMETRIC MELTS

Kirill A. Subbotin[1], Denis A. Lis[1], Valerii V. Voronov[1], Anatolii I. Titov[1], Valerii G. Senin[2], Viktoriia V. Sanina[1], Evgenii V. Zharikov[1]

[1]A.M.Prokhorov General Physics Institute Russian Academy of Sciences, RUSSIAN FEDERATION, [2]Vernadsky Institute of Geochemistry and Analytical Chemistry RAS, RUSSIAN FEDERATION

Scheelite-like disordered double molybdate and tungstate single crystals with general formula $NaLn(TO_4)_2$ ($Ln = La^{3+}$, Gd^{3+}, Y^{3+}, Bi^{3+}; $T = Mo^{6+}$, W^{6+}), doped with trivalent rare-earths ions (Nd^{3+}, Yb^{3+}, Tm^{3+}, Er^{3+}, etc.) are promising active media of tunable and femtosecond solid-state lasers. The optical absorption and photoluminescence bands of rare-earth dopants are rather strong and inhomogeneously broadened in these hosts. It is favorable for diode-pumped ultrashort laser pulses generation. Furthermore, these hosts doped by Yb^{3+} were recently shown to be promising quantum cutting materials, converting blue and UV quanta of Solar light to a double amount of 1 mm quanta. The latter ones are efficiently absorbed by photovoltaic cells made of crystalline silicon. Besides that, such crystals can be easily grown by Czochralski with high segregation coefficients of rare earths ions. However, properties of the crystals (including their durability and thermal conductivity) are substantially depend on even slight deviations of the crystal composition out from the stoichiometry. Meanwhile, the crystal and melt compositions of such compounds are quite unstable because of both segregation, and selective evaporation, but particular studies of this subject are practically absent. We have grown by Czochralski the series of $NaGd(WO_4)_2$ and $NaGd(MoO_4)_2$ crystals from melts with the compositions, shifted out from the stoichiometry for different directions. The actual compositions of the crystals were measured by microprobe analysis and compared with the melts compositions. The measurements in numerous points along the boule have not shown any sustainable compositions drift during the growth run. The measurements with small spot sizes and short steps allowed to reveal the scale of composition fluctuations at growth striations. Measurements of the crystals densities and the unit cells parameters allowed to calculate the molar mass of the crystals, as well as to refine their compositions, including the contents of vacancies. Besides that, the microhardness of all the grown crystals was measured. The obtained results are summarized and discussed in the presentation.

INFLUENCE OF RAW MATERIALS' PURITY ON GROWTH AND PROPERTIES OF β-BBO CRYSTALS

Andrey Sadovskiy[1], Marina Zykova[2], Elena Mozhevitina[2], Andrew Khomyakov[2], Alexander Ostrovskiy[3], Roman Avetisov[4], Alexander Yurkin[3], Igor Avetissov[2]

[1]IPG IRE-Polus, RUSSIAN FEDERATION, [2]Dmitry Mendeleev Univeristy of Chemical Technology of Russia, RUSSIAN FEDERATION, [3]Crystals of Sybiria Ltd., RUSSIAN FEDERATION, [4]ARMOLED Ltd., RUSSIAN FEDERATION

To date, nonlinear optical crystals of b-barium borate (b-BaB_2O_4 - BBO) are used in optoelectronics to convert the frequency of laser radiation by the mechanisms of second and higher harmonics generation [1,2], as well as the mechanisms of transformation with the use of stimulated Raman scattering [3]. BBO crystals are the best transducers for obtaining ultraviolet radiation at wavelengths less than 200 nm [4]. Because of the low thermal conductivity of the crystal along the optical axis (growth axis) of the crystal, there are a number of technological difficulties in obtaining crystals longer than 20 mm. An accumulation of impurities with a distribution coefficient of less than 1 occurs at the crystallization front. This leads to a breakdown in cellular growth. Therefore, in order to increase the mass of grown BBO crystals, it is necessary to improve the quality of the initial reagents. In the present research, we investigated the influence of purity of the raw materials on the growth process and quality of BBO crystals grown from a melt solution. The raw materials used were: $Na_2B_4O_7$´10 H_2O as a melt solvent, $BaCO_3$ as a source of barium, and H_3BO_3 or B_2O_3 as a source for BBO synthesis. The purity of the initial reagents ranged from 4N5 to 6N. Special attention was paid to water content. We prepared initial reagents ($Na_2B_4O_7$, B_2O_3) with water content no more than 500 ppm. The incorporation of impurities into the grown crystals has been studied as well as their distribution across and along the BBO crystals. It was found out that an increase in the purity of all reagents up to 6N made it possible to increase the length of grown crystals up to 2 times which followed by the improving of the structural characteristics of the BBO crystals. The research was financially supported by The Ministry of Education and Science of Russian Federation by grant RFMEFI57716X0218. 1. P. S. Banks, M. D. Feit, M. D. Perry *J. Opt. Soc. Am. B* **2002** 19 (1) 102-118 2. Qi Liu, Yan Wang, Xiaoyan Wang, Xue Qin, Lihua Bai, Huifang Zhang, Xiaona Yan *Optik - International Journal for Light and Electron Optics* **2015** 126(9-10) 985-989 3. Jun Liu, Jun Zhang, Takayoshi Kobayashi *Optics Letters* **2008** 33(13) 1494-1496 4. S. Galtier, F. Nez, L. Julien, F. Biraben *Optics Communications* **2014** 324(8) 34-37

GROWTH AND CHARACTERIZATION OF PHTHALIC ACID CRYSTALS IN PRESENCE OF HEXAMETHYLENETETRAMINE

Subbiah Meenakshisundaram, C Balakrishnan, S Sivaraman, R Markkandan, Rm Sockalingam

Annamalai university, INDIA

Single crystals of the complex of hexamethelenetetramine and phthalic acid are grown from water-ethanol (4:1, v/v) at room temperature by slow evaporation solution growth technique. It belongs to orthorohombic system and the cell parameters are, a = 6.4197(11) Å, b = 10.236(2) Å, c = 26.176(14) Å, V = 1720.0(9) Å^3. The cell parameters are quite different from that of the hexamethelenetetramine (a = b = c = 6.08 Å) and phthalic acid (a = 4.99 Å, b = 14.17 Å, c = 9.51 Å) indicating a new product. The powder X-ray diffraction pattern reveals the good crystallinity of the as-grown specimen. The functional groups are identified by FT-IR. Direct band gap energy is estimated as 4.09 eV by Kubelka–Munk algorithm. The scanning electron microscopy studies reveal the surface morphology. Second harmonic generation (SHG) efficiency of the specimen is estimated by Kurtz and Perry technique. NLO character is further analyzed by first-order molecular hyperpolarizability (β) values and the results are rationalized. Third-order nonlinear susceptibilites are to be probed, if the product crystallizes in a cetrosymmetric structure. Theoretical investigations using density functional theory method at B3LYP level with 6-31G (d,p) basis set are carried out and results are compared with experimental data.

GROWTH AND CHARACTERIZATION OF DIAQUATETRAKIS (1H-IMIDAZOLE-KN3)-MAGNESIUM DICHLORIDE SINGLE CRYSTAL

H Arul[1], Nagaradona Suneetha[2], D Rajan Babu[2], R Ezhil Vizhi[2]

[1]Department of Science and Humanities, Kumaraguru College of Technology (Autonomous),, INDIA, [2]Advanced Materials Research Centre, Department of Physics, School of Advanced Sciences, VIT University, INDIA

Semiorganic materials have been succeeded in achieving a great task in the field of nonlinear optics by overcoming the difficulties from the organic and inorganic materials. They possess the characteristics of both which is essential for nonlinear optical applications. In the present study Diaquatetrakis (1H-imidazole-**K**N3)-magnesium dichloride $[Mg\ (C_3H_3N_2)_4(H_2O)_2]Cl_2$ is a metal organic single crystal grown by slow evaporation at room temperature. Crystal structure was confirmed from single crystal XRD and lattice parameters are a = 12.48 A°, b = 11.14 A°, c = 14.63 A° and the crystal belongs to monoclinic with space group C2/c. The presence of functional groups was confirmed by FTIR spectrum. Optical properties like transmittance, energy band gap were estimated from UV-vis analysis. Refractive of the grown crystal was measured using Metricon prism coupler. The dielectric nature of the grown crystal was studied at different frequencies with respect to temperature. TG-DSC analysis revealed the stability and melting point up to which the material is stable. Nonlinear optical property was identified by Kurtz Perry powder technique.

CYCLOHEXYLAMMONIUM CINNAMATE SINGLE CRYSTAL FOR NONLINEAR OPTICAL APPLICATIONS

R Gomathi[1], S Madeswaran[1], D Rajan Babu[1], **H Arul**[2]

[1]Advanced Materials Research Centre, Department of Physics, School of Advanced Sciences, VIT University, INDIA, [2]Department of Science and Humanities, Kumaraguru College of Technology (Autonomous),, INDIA

Organic single crystal has much consideration in optical applications such as image processing and biomedical applications including sensing treatment and tissue engineering due to its high nonlinear optical susceptibility, high piezoelectric coefficient and bio compatibility [1,2]. Cyclohexylammonium cinnamate crystal (CYHC) was grown by slow evaporation technique. Single crystal XRD provides the crystalline characteristics of the compound and it belongs to monoclinic P21/n crystal system. The presence of various functional groups in the crystal was verified by FTIR analysis. Thermal analysis showed the melting point of crystal is 175 °C and decomposition point is 237.4 °C. Dielectric studies were carried out using Numetric Q impedance analyzer. Third order nonlinear optical studies were carried out using diode pumped CW Nd:YAG Laser (Coherent CompassTM215M-50 at 632.8 nm) and crystal's optical limiting behavior was tested (Fig. 1). The limiting threshold value and clamping output are found to be 18.62 mW and 1.72 mW respectively. Fig. 1 Optical limiting spectrum of CYHC crystal. **References:** [1] Yong Qian, Hong-Jia Zhang, Hao Zhang, Chen Xu, Jing Zhao and Hai-Liang Zhu, Bioorg. Med. Chem.,18 (2010), 4991-4996. [2] A.S. Nuraeva, D.S. Vasileva, S.G. Vasilev, P.S. Zelenovskiy, D.A. Gruzdev, V.P. Krasnov, V.A. Olshevskaya, V.N. Kalinin & V.Ya. Shur, Ferroelectrics, 496 (2016), 1-9.

PECULIARITIES OF BULK BAY$_2$F$_8$ SINGLE CRYSTALS GROWTH FOR OBTAINING LUMINESCENCE IN THE UV REGION.

Anastasiia Uvarova[1], Aleksandr Pushkar[2]

[1]National University of Science and Technology "MISIS", RUSSIAN FEDERATION, [2]Doctor Web, RUSSIAN FEDERATION

Single crystal BaY$_2$F$_8$, jointly activated Ce^{3+}, Pr^{3+} and Yb^{3+} is one of the prospects of active media for visible and UV spectral emitters. On this crystal, UV luminescence is demonstrated upon pumping by IR laser diodes [1]. Currently, the emitters for the UV range are cumbersome and inconvenient in operation compared to laser diodes, that are used for the IR range. For example, semiconductor lasers (laser diodes), which have the dimensions of several mm. can generate radiation of several hundred mW (they are structurally composed of a heterostructure at a quantum-size scale). In comparison with them, the dimensions of lasers for the ultraviolet (UV) spectral range of the same power are hundreds of cm. or meters. The use of laser diodes as pumping sources will significantly reduce the dimensions of UV emitters. The article considers the technological problems and ways for solution which are arising , when growing crystals of the BaY$_2$F$_8$ activated

by Yb^{3+}, Pr^{3+}, Ce^{3+}. 1. The problems for single crystal growth of host BaY$_2$F$_8$ are: - the formation of an opaque phase in the form of banded inclusions in the volume of a crystal; - the formation of an opaque phase in the form of a clearly expressed cap at the end of the crystal; - the absence of seeding and the formation of a completely opaque boule. 2. The problem at introduction of activators is: - low concentrations of Pr^{3+} and Ce^{3+} as a result of the non isomorphic entrance of these activators into the matrix crystal. In systems with trifluorides of rare-earth elements of the cerium subgroup, to which cerium and praseodymium ions relate, monoclinic compounds are not formed. Then this activators are non isomorphic and the limiting concentration of these ions in the crystal BaY$_2$F$_8$ does not exceed

0,67 at. %. In systems with trifluorides of rare-earth elements of the yttrium subgroup, monoclinic compounds, in particular BaYb$_2$F$_8$, are formed and form with the matrix BaY$_2$F$_8$ crystal a series of solid solutions up to a 100% Y^{3+} substitution by the Yb^{3+} ion. A technique for introducing these activators in a wide range of concentrations will be presented. [1] N. Kozlova[1], S. Kuznetsov[2], A. Pushkar[3], A. Uvarova[2], and T. Uvarova[3] * Up-conversion luminescence in the ultraviolet range excited by

IR-laser diodes in active medium BaY$_2$F$_8$:Yb^{3+}, Pr^{3+}, Ce^{3+} P hys. Status Solidi C 9, No. 12, 2362–2365 (2012) / DOI 10.1002/pssc. 201200492

SINGLE-CRYSTAL FIBER OF TETRAPHENYLPHOSPHONIUM BROMIDE FOR STIMULATED RAMAN SCATTERING

Yan Ren, Guang Qiang Wang, Xu Tang Tao

INSTITUTE OF CRYSTAL MATERIALS SHANDONG UNIVERSITY, CHINA

Stimulated Raman scattering (SRS) is an important frequency-conversion technique that can substantially extend the spectral coverage of solid lasers [1]. The rich spectral lines provided by this technique are the results of strong stimulated Raman scattering in inorganic or organic compounds. Among active Raman media of different physical configurations, optical fiber has much distinct advantages of reduced pump threshold, low attenuation, excellent heat dissipation, and flexibility for device applications. In particular, optical fibers made of single-crystal Raman media have the unique advantage because of their high concentration of active Raman centers [2]. However, few single-crystal fibers studies for SRS generation have so far been reported primarily because of the challenge of crystal growth. Here, we report a high quality one-dimensional organic single-crystal fiber of tetraphenylphosphonium bromide (TPPB) grown by a fast nucleation and growth in solution. The TPPB single-crystal fibers obtained possess high optical quality with large length-to-diameter ratios typically over 10^6:1 and diameters ranging from less one micron to tens of micron. TPPB single-crystal fibers exhibit excellent optical wave-guiding properties and efficient multiple wavelength SRS generation at 562 nm, 580 nm and 636 nm simultaneously under a continuous-wave pump at 532 nm. The SRS generation threshold of TPPB single-crystal fiber was found to be less than 0.7 mW using a CCD assembly that images the unpolished exit facet, which is far less than that of bulk crystal in a cavity under continuous laser excitations. The fast crystal growth method demonstrated here is simple and effective for growth of high optical quality one-dimensional single-crystals in solution. The crystal growth dynamics under such non-equilibrium conditions is an important field of study and also of vital technological importance in order to achieve high-quality high-yield single crystal fibers with uniform diameters. The TPPB single-crystal fiber developed here may find practical use in miniature optical frequency devices such as Raman lasers. References [1] H. M. Pask, “The design and operation of solid-state Raman lasers,” Prog. Quant. Electron **27**, 3-56 (2003). [2] Y. Urata, S. Wada, H. Tashiro, “Fiber-like lanthanum tungstate crystal for efficient stimulated Raman scattering,”App. Phys. Lett. 75, 636-638 (1999).

MULTIFRACTAL SPECTRUM INVARIANCE OF SPATIAL NANOFORMS ON THE SURFACE OF ZNXCD1-XTE-SI HETEROSTRUCTURES SYNTHESIZED BY VARIOUS TECHNOLOGIES.

Vladimir Kuznetsov[1], Pavel Moskvin[2], Vlad Rudnitskiy[2]

[1]Saint-Petersburg State Electrotechnical University, RUSSIAN FEDERATION, [2]Zhytomyr state technology University, UKRAINE

$Zn_XCd_{1-X}Te$ solid solutions layers were obtained by VD method with evaporable anode [3]. Single-crystal silicon was used as a substrate. Growth time, deposition rate and substrate temperature were variable parameters for the process of material obtaining from gas phase. The thickness of the films was measured using a mechanical ALPHA STEP 100 profilometer. The morphology of the structures was studied by atomic force microscopy (AFM) in a mode of periodic contact. Obtained AFM images of surface layers were processed by numerical methods in accordance with the MF analysis [1,2,4,5]. Rényi numberand parameter of fractal order were used as comparison parameters for the surface state. MF spectra for surfaces and volumes of spatial nanoform, which formed the surface relief are calculated and analyzed. The obtained experimental and calculated information has allowed to obtain dependences of specified parameters of MF spectra on substrate temperature at synthesis of layers with approximately identical speed of solid phase formation. Comparison of dependences of parameters MF of spectra from various geometric parameters of the nanoforms for layers synthesized by VD method and a hot wall method has been made. MF spectra for surfaces and bulks of spatial nanoform, which formed the surface relief are calculated and analyzed. The obtained experimental and calculated information has allowed to obtain dependences of specified parameters of MF spectra from substrate temperature at synthesis of layers with approximately identical velocity of solid phase formation. The comparison results show that Rényi number and disorder parameters for values and surfaces of nanoform which are formed on the surface of the heterostructures synthesized by above-mentioned methods are similar in magnitude, and their changes are symbate to substrate temperature changes. The latter indicates the possibility of obtaining layers with practicallythe same MF spectrum parameters (the same surface morphology) by different technological methods, while providing identical thermodynamic conditions of heterostructure synthesis. In addition, appearing invariance by the application of theory of power functions to the description of space of semiconductor heterostructure surface irregularity in nanoscale makes it possible to suggestthe possibility of using fractal concepts to describe the symmetric surface states formed during the synthesis process. [1] Moskvin P., Kryzhanivskyy V., Rashkovetskyi L., et.al. J.Cryst. Growth 2014, 404, p.204. [2] Moskvin P.P, Kryzhanivskyy V*., Rashkovetskyi* L., Lytvyn P.J. Crystal Growth, 2016, 450, p.28. [3] Moskvin P.P., Rudnitskiy V.A.Visnyk [4] Feder J. Fractals. New-York: Plenum Press, 1988. [5] Vstovsky G.V. Found. Phys. 1997, v.27, 1413.

OPTIMIZATION OF THE INTERFACIAL MISFIT ARRAY GROWTH MODE OF GASB EPILAYERS ON GAAS SUBSTRATE

Djalal Benyahia[1], Łukasz P. Kubiszyn[2], Krystian Michalczewski[1], Artur Kębłowski[2], Piotr Martyniuk[1], Józef Piotrowski[2], Antoni Rogalski[1]

[1]Military University of technology, POLAND, [2]Vigo System S.A., POLAND

The growth of high-quality epilayers on suitable substrates is a vital aspect for many technologies. Generally, a mismatch between the epilayer and the substrate exists, and produces strain at the interface. Thus, this strain should be controlled to obtain high-quality layers. GaSb layers grown on GaAs substrates are a typical model for investigating this issue, due to the large lattice mismatch (7.8%) between GaSb and GaAs. In the present work, we report on the growth of undoped GaSb layers on GaAs (001) substrate with 2° offcut towards <110> by a solid-source molecular beam epitaxy system. In order to control the strain and reduce the large lattice mismatch between GaAs substrate and GaSb layer, the interfacial misfit array mode was used. This mode is very beneficial to have a buffer-free layer, and to impede the propagation of the threading dislocations through the layer. The strain energy is relieved via the formation of a periodic array of misfit dislocation at the interface GaAs/GaSb. Moreover, we investigate three approaches of this technique. The difference between these approaches consists on the chronological events after the growth of GaAs buffer layer. In the first approach, the substrate temperature is decreased to the GaSb growth temperature under arsenic overpressure, while in the second one, the cooling was done without any group V flux. Furthermore, the temperature decreasing in the third approach was performed under antimony overpressure. High resolution X-ray diffraction analysis was used to investigate the presence of a periodic array of misfit dislocations, the strain, and the dislocations density in the grown layers. The surface morphology was assessed by Nomarski Microscopy, and high-resolution optical profilometry. Whilst the electrical parameters were determined by Hall Effect measurement. The third approach was found to acquire the best structural and electrical properties. In addition, X-ray analysis demonstrates the formation of a periodic array of 90° misfit dislocations in the layers grown using the third approach. The relaxation between GaSb layer and GaAs substrate was determined to be 99.8%. Acknowledgments:

We acknowledge the support by The Polish Science Centre – grant no.2015/19/B/ST7/02200.

EX-SITU PROFILING OF TiO_2 FILM GROWTH USING SYNCHROTRON RADIATION

Kyle A. Kulinski[1], Daniel Steckhahn[1], Brandon Gunn[1], Chris Tassone[2], Andrew S. Ichimura[3]

[1]San Francisco State University, CA, UNITED STATES OF AMERICA, [2]Stanford Synchrotron Radiation Lightsource, CA, UNITED STATES OF AMERICA, [3]San Francisco State University, UNITED STATES OF AMERICA

Control over crystallite orientation in thin-films is important for improving charge carrier transport in heterojunction devices such as solar cells. We have synthesized anatase TiO_2 films with strong <001> texture on gold substrate that may improve the efficiency since charge transport and electron injection were found to have reduced barriers along the [001] direction. Anatase thin films were synthesized by a hydrothermal method using titanium (IV) fluoride as the titanium source and evaporated gold on silicon wafers as the substrate. An additional fluoride source, HF_{aq} or NH4F, was also used to modify the composition of the starting solution. The films were characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), and atomic force microscopy (AFM). The <001> texture of the anatase films was determined at the Stanford Synchrotron Radication Lightsource (SSRL) beamline 11-3, employing a MarCCD area detector. The 2D patterns reveal fiber texture with the <001> axis normal to the substrate. SEM images reveal that the grains are small near the substrate and expand into a wedge shape at the exterior surface of the film. To elucidate film nucleation and growth, the films were polished such that one end of the film had a thickness of 10 nm and the other end, a distance 12 mm away, had a thickness of ~400 nm. Electron micrographs were acquired at select thicknesses between 10 – 400 nm and the film was characterized at each point by synchrotron X-ray diffraction employing the area detector. To quantify the <001> texture, pole figures of the (004) anatase reflection were constructed from rocking curves and grazing incidence patterns after correction for background, polarization, and absorption effects. The TiO_2 films exhibit <001> texture that is strong at the surface of the film and weaker close to the substrate. However, analysis of the {101} reflection shows that three orientations exist ($\chi = \pm 68^{o}, \pm 38^{o}, \pm 18^{o}$) at a film thickness of 10 nm. Films grown with additional fluoride (HF or NH_4F) have only two initial orientations. This unexpected finding suggests that nucleation is not random and may be influenced by the substrate and solution composition. As the films grow, the dominant orientation prevails at thickness greater than 200 nm such that the (001) plane is parallel to the substrate. An understanding of crystal nucleation and growth under hydrothermal conditions will allow control over the film texture, thickness, and faceting, thus improving charge transport properties in opto-electric applications.

ELECTRICAL CHARACTERIZATION OF ALD DEPOSITED PBTIO3 THIN FILMS

Nick Sbrockey[1], Gary Tompa[1], Aaron Welsh[2], Jung I. Yang[2], Susan Trolier-Mckinstry[2], Ronald Polcawich[3], Daniel Potrepka[3]

[1]Structured Materials Industries, NJ, UNITED STATES OF AMERICA, [2]Penn State University, UNITED STATES OF AMERICA, [3]U.S. Army Research Laboratory, UNITED STATES OF AMERICA

Piezoelectric and ferroelectric thin films are needed for applications such as micro-electro mechanical systems (MEMS) and ferroelectric memory (FRAM) devices. Deposition of these films onto complex device geometries will require atomic layer deposition (ALD) processes. Piezoelectric films deposited on to vertical sidewalls will enable 3-D actuation in MEMS. Ferroelectric films deposited in to high aspect ratio trenches will enable high density memory devices. This work is developing ALD process technology for lead-titanate ($PbTiO_3$) films. The precursors used were tetraethyl lead and tetrakis dimethylamino titanium (TDMAT). The substrates were platinum coated silicon wafer sections. Substrate temperature was 250 C. The reactant for both the Pb and Ti precursors was approximately 1% ozone in oxygen, produced using a commercial ozone generator. The Pb/Ti content of the film could be controlled by the relative number of Pb and Ti precursor doses during the ALD process. The as-deposited films were amorphous, as evidenced by x-ray diffraction. The films were crystallized by subsequent rapid thermal annealing in oxygen. Formation of the Perovskite phase was found to depend strongly on the film composition and the annealing conditions. Films with stoichiometric to Pb rich compositions crystallized to the Perovskite phase. Pb deficient films did not show Perovskite phase formation by x-ray diffraction. Films with composition close to stoichiometric $PbTiO_3$ showed the highest ferroelectric properties, as evidenced by hysteresis in the polarization versus applied field behavior and a non-zero irreversible Rayleigh constant.

ANALYSIS OF THE FLOATING SILICON METHOD (FSM) FOR THE HORIZONTAL GROWTH OF CRYSTALLINE SILICON RIBBONS

Kerry Wang, Jeffrey J. Derby

University of Minnesota, MN, UNITED STATES OF AMERICA

The Floating Silicon Method (FSM), under development by Dr. Peter Kellerman and his team at Varian Semiconductor Equipment Division, Applied Materials, is an extremely promising process for the growth of single-crystal ribbons of silicon [1]. This approach is classified as a horizontal ribbon growth (HRG) method and promises higher-quality, crystalline silicon at growth rates that are orders of magnitude greater than attained by vertical ribbon growth technologies. If successful, this process would enable the production of single-crystal silicon substrate at a fraction of the cost of current production techniques. This fascinating process was first conceived by Shockley in late 1950’s for silicon growth and was practiced by Bleil on the late 1960’s for germanium growth. Large-scale efforts were subsequently carried out by Kudo in Japan in the late 1970’s and by the Energy Materials Corporation in the US in the early 1980’s; however, neither process was commercialized. We present a thermal-capillary model based on finite-element methods to study the coupled phenomena of heat transfer, melt flow, segregation, and interfacial phenomena during the growth of crystalline silicon via the FSM process. This approach was successfully employed to model a similar horizontal ribbon growth process by Bleil [2,3]. These analyses employed steady-state, bifurcation theory coupled with transient computations to reveal process limitations and failure modes that were consistent with prior experimental observations. In this presentation, we describe our progress toward understanding the behavior of the FSM system, which employs a significantly different geometry and heat transfer conditions than the system of Bleil. We also attempt, via our thermal-capillary model, to address melt undercooling near the solidifying edge of the ribbon. A more complete understanding the heat transfer in this system may point a way to achieving substantially higher growth rates. [1] P. Kellerman, “Floating Silicon Method for Single Crystal Kerfless Wafering: Observation and Theory,” Presentation at e-MRS 2014, Lille, France (2014). [2] P. Daggolu, A. Yeckel, C.E. Bleil, and J.J. Derby, “Thermal-capillary analysis of the horizontal ribbon growth of silicon crystals,” J. Crystal Growth 355, 129–139 (2012). [3] P. Daggolu, A. Yeckel, C.E. Bleil, and J.J. Derby, “Stability limits for the horizontal ribbon growth of silicon crystals,” J. Crystal Growth 363, 132–140 (2013). --------------- This research was supported by the National Science Foundation, CBET-1336164; no official endorsement should be inferred.

GROWTH OF VERY THIN AL2O3 LAYER BY ATOMIC LAYER DEPOSITION AND ITS MODULATION OF ELECTRICAL PROPERTIES IN METAL/INP CONTACTS

Hogyoung Kim, Byung Joon Choi

Seoul National University of Science and Technology, KOREA, REPUBLIC OF

InP and related materials can be applied to optoelectronic devices such as laser diodes (LDs), solar cells and high speed metal insulator semiconductor field effect transistors (MISFITs) due to their direct band gap and high electron saturation velocity. In such devices, ohmic contact with low contact resistance and Schottky contact with high barrier height are highly required. Recently, insertion of very thin interfacial layer grown by atomic layer deposition (ALD) has been researched intensively. To modulate the electrical properties of metal/InP contacts, we deposited Al_2O_3 layer on n-InP with different thicknesses. Transmission electron microscope (TEM) data showed that the native oxide on InP was removed during the H_2O prepulse treatment. In addition, the diffusion of Au atoms into InP layer was blocked effectively by Al_2O_3 layer. The barrier heights increased from 0.47 to 0.62 eV with 1.3 nm thick Al_2O_3 layer. Then the barrier heights remained almost constant with increasing the thickness. Series resistance did not increase monotonically with increasing the thickness. At each thickness, the dominant current transport was found to be different. The detailed analyses and results based on the data will be presented later.

III-V NANO-RIDGE GROWTH ON (001) SI FOR OPTOELECTRONICS

Bernardette Kunert[1], Yves Mols[1], Yuting Shi[2], Dries Van Thourhout[2], Marianna Pantouvaki[1], Joris Van Campenhout[1], Robert Langer[2]

[1]Imec, BELGIUM, [2]INTEC Department Ghent University, BELGIUM

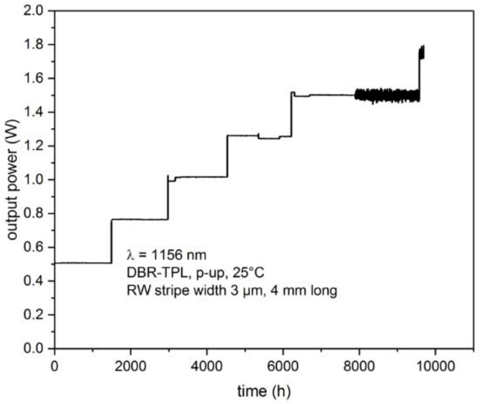
The monolithic growth of III-V compound materials on (001) Si substrate offers a huge potential for new device functionalities combining the mature Si technology with the excellent optoelectronic properties of III-Vs. The selective area growth (SAG) of III-V nano-ridges on trench-patterned Si substrate is a new integration approach combining two aspects: The growth of mismatched III-V material in very narrow oxide trenches ensures an efficient defect reduction by high aspect ratio trapping whereas the continuous growth out of the trench leads to an increased III-V volume for novel optoelectronic devices on Si such as laser diodes, modulators, detectors, etc. In this paper, we first discuss the monolithic growth of GaAs based nano-ridges on trench-patterned 300 mm (001) Si substrates by MOVPE. The nano-ridge shape on top of the trenches can be manipulated by the applied growth conditions in order to achieve a box-, diamond- or triangle-shaped nano-ridge. Besides GaAs the SAG of different materials such as InGaAs, InGaP and InP was also investigated to control the ridge shape formation. Especially the growth of ternary compound materials reveals a sensitive dependence of the In-incorporation efficiency on the different crystal facets of a nano-ridge. The box-shaped GaAs nano-ridges allow for a new laser integration concept, the so-called nano-ridge laser. An InGaAs/GaAs multi-quantum well structure on top of the (001) facet acts as the optical gain medium whereas the nano-ridge itself functions as the waveguide. Although the successful demonstration of first optically pumped laser operation emphasizes the high crystal quality, achieving an overall low defect density is the only path towards a long device life-time. Therefore, different methods beyond transmission electron microcopy (TEM) such as cathodoluminescence measurements or defect etching are discussed to determine the current defect density of the III-V nano-ridge material. The threading dislocation density clearly decreases with rising aspect ratio of the patterned trenches whereas the presence of stacking faults and twins is rather related to the pre-treatment of the Si wafers before deposition. The presented results enable a critical review on the current development status and the future prospective of III-V nano-ridges on Si substrate for new device applications.

DEGRADATION BEHAVIOR OF LASER DIODES WITH HIGHLY STRAINED INGAAS QWS WITH EMISSION WAVELENGTH BETWEEN 1120 NM AND 1180 NM

Frank Bugge, Gunnar Blume, David Feise, Nils Werner, Katrin Paschke, Markus Weyers

Ferdinand-Braun-Institut, GERMANY

Laser diodes emitting in the yellow-green range are key components for many applications, e.g. laser cooling of sodium atoms and time resolved fluorescence spectroscopy. Unfortunately, this yellow-green spectral region is currently not accessible directly with laser diodes. One solution for such sources is based on high-brilliance laser diodes with a highly strained InGaAs quantum well (QW) emitting between 1120 nm and 1180 nm and non-linear frequency conversion. Several groups reported about laser diodes in this spectral range but without giving reliability data [1-3]. In this work we investigate the growth of different epitaxial structures for this wavelength range. The challenges are defect free growth of such QWs with respect to a high reliability and the integration of a grating for manufacturing high brilliance laser diodes. With the aim of a satisfying reliability we processed structures with different active regions having different QW composition, different number of QWs, different strain compensation and different QW thicknesses. These variations have rather low effect on the electro-optical properties of broad area laser diodes. All laser structures were designed for the integration of a distributed Bragg reflector (DBR) into the rear part of a ridge waveguide (RW) and a taper section to obtain a high output power at a nearly diffraction-limited beam on a single frequency. Such diodes are well suited for a frequency conversion to 560 nm - 590 nm. The effect of these different structures on reliability was investigated in step-stress tests or at constant output powers, as for DBR ridge waveguide lasers with 4 µm stripe width, DBR tapered or 50 µm wide broad area laser diodes. In dependence on the active region, the emission wavelength and the device structure lifetimes between 400 h and 20000 h were obtained. Devices with laser diodes emitting at 1120 nm, 1156 nm and 1180 nm and periodically poled $MgO:LiNbO_3$ for frequency conversion emit more than 75 mW at 561 nm and 589 nm (DBR-RW laser) and more than 1 W at 578 nm (DBR tapered laser).



Step-stress test for a DBR tapered laser diode with a 3 µm ridge waveguide. The test still runs.

EXTREMELY RAPID GAAS GROWTH BY MOVPE FOR LOW-COST PV APPLICATIONS

Akinori Ubukata[1], Hassanet Sodabanlu[2], Kentaroh Watanabe[2], Syuichi Koseki[1], Yoshiki Yano[1], Toshiya Tabuchi[1], Takeyoshi Sugaya[3], Koh Matsumoto[1], Yoshiaki Nakano[2], Masakazu Sugiyama[2]

[1]Taiyo Nippon Sanso, JAPAN, [2]The university of Tokyo, JAPAN, [3]National Institute of advanced industrial science and technology, JAPAN

III-V multiple junction solar cells (MJSCs) have been attractive for their high conversion efficiency, such as the record of 46% achieved by 4-junction structure under a concentration light of 508 sun. Generally, there are two approaches to improve cost effectiveness: increasing performance and reducing cost. For the first approach, the conversion efficiency of MJSCs can be improved by utilizing more p-n junctions to lower the thermalization loss and by balancing the photo-current generated in each subcell. Meanwhile, considerable effort has recently been devoted to reduce the production cost of MJSCs, including the use of epitaxial lift-off, wafer reuse, and high- speed crystal growth by metalorganic vapor phase epitaxy (MOVPE). Epitaxial growth of GaAs was investigated in a horizontal MOVPE reactor with a same concept as III-nitride reactor in order to realize extremely high growth rate. In this study, GaAs growth rateexhibited almost linear relationship with the amount of trimethylgallium (TMGa) supply up to 90 μm/h; the maximum value was limited by the full scale of the mass-flow controller. Without susceptor rotation, the distribution of growth rate was observed over a 2 inch wafer along the flow direction, and the normalized profile of the distribution was independent of growth rate from 20 to 90 μm/h. These tendencies indicate that the parasitic pre-reactions in gas-phase to generate clusters was not significant in this range of growth rate. Carrier concentration of both n- and p-type doped GaAs could be directly controlled by adjusting the supply ratio of a dopant precursor to TMGa regardless of growth rate. GaAs p-n solar cells were successfully fabricated at growth rates of 20, 60, and 90 μm/h. The conversion efficiency of the cell grown at 90 μm/h was comparable with that of the 20 μm/h cell, indicating the good quality and properties of GaAs. Though the surface roughness of GaAs increased with the increasing growth rate, it did not influence the PV performance. The epitaxial growth exhibited good uniformity, as evidenced by the uniformity of the cell performance across a wafer, from the center to the edge of a wafer. The result indicates the potential of high-throughput MOVPE for low cost production, not only for PV devices, but also for other semiconductor applications.

SETUP FOR IN-SITU ELECTRON MICROSCOPIC STUDIES OF SEMICONDUCTOR GROWTH

Kerstin Volz

Philipps-University Marburg, GERMANY

The MOVPE (metal organic vapour phase epitaxy) growth of III/V semiconductors has reached a great maturity. However, our understanding, how semiconductor heterostructures grow at an atomic scale, is still incomplete. Nevertheless, this knowledge could lead to optimized structures. This study presents in-situ growth investigations in a transmission electron microscope. The Protochips Inc. *in-situ* TEM setup has been extended by a gas mixing system for the safe usage of toxic and pyrophoric III/V semiconductor precursors. The samples were prepared for the in-situ STEM investigation using a focused ion beam system, which guarantees that the specimens can be observed in zone axis orientation and high resolution can be achieved. A double Cs-corrected JEOL JEM-2200 FS operating at 200 kV was used for the STEM observations. With the example of TBP (tertiary butyl phosphine)-stabilized annealing of Ga(NAsP)/(BGa)(AsP) structures on Silicon substrates the functionality of the system is demonstrated. Atomically-resolved high angle annular dark field (HAADF) images in scanning TEM mode were achieved at high temperatures up to 700 °C and at high TBP partial pressures of 140 hPa. We monitor the incongruent evaporation of phosphorous from the TEM specimen by measuring its thickness as a function of temperature for different TBP partial pressures. This study allows us to determine the activation energy for P-evaporation, but also shows that the setup is completely functional and that the TBP is decomposed in the holder. In a further step, the quantum well homogeneity as well as Arsenic and Nitrogen interdiffusion into the barrier are studied as a function of temperature. In summary, this presentation will introduce the in-situ setup as well as the necessary TEM specimen preparation and depict some examples to prove the functionality of the system.

PHOTOLUMINESCENCE EXCITATION SPECTROSCOPY OF ANTIMONY DONORS IN ZINC OXIDE

Simon Watkins[1], Faezeh Mohammadbeigi[2], Senthil Kumar[1], Katrina Stirling[1]

[1]Department of Physics, Simon Fraser University, BC, CANADA, [2]Department of Physics, SimonFraser University, BC, CANADA

Antimony has been investigated intensively as a potential p-type dopant in ZnO, however several studies have shown that the defect incorporation mechanism is not as simple as first anticipated. Channelling studies indicate that Sb resides on the Zn lattice, which has led to a proposal that the Sb acceptor consists of a triple donor compensated by two neighboring Zn vacancies. We have shown that controlled doping of ZnO with very low trimethylantimony concentrations results in the observation of a new low temperature photoluminescence peak at 3.3643 eV which we attributed to a donor bound exciton. In this work we have succeeded in producing samples in which the Sb-related emission is the dominant near gap PL peak. This was achieved by introducing a small amount of hydrogen during growth which appears to reduce the incorporation of carbon impurities. Using a tunable uv excitation source we have further strengthened the assignment of this line as donor-related. By resonantly excited the principal donor bound exciton emission we successfully resolved the two electron satellite giving a donor binding energy of 42.4 meV, the shallowest known donor in ZnO. We further explored the excited state spectra of this donor by monitoring the ground state PL while tuning through the excited states with the UV source. The excited states are similar to those of other shallow donors, however with some notable differences which may reflect the extended nature of the defect complex. An excited state associated with the B valence band is observed at an energy of 5.0 meV, which is measurably higher than the value observed in other shallow donors (4.5meV). In addition the electronic and vibrational exited states do not closely follow the trends previously observed for simpler substitutional group III donors. We propose that the antimony donor defect consists of single Sb atom paired with a single Zn vacancy giving a single donor impurity. An understanding of the structure of this defect is important in order to understand the more challenging Sb acceptor complex.

SPATIO-TIME-RESOLVED CATHODOLUMINESCENCE STUDY OF THICK III-POLAR AND N-POLAR INGAN

Zakaria Y. Al Balushi, Joan M. Redwing

Dept. Materials Science and Engineering, The Pennsylvania State University, PA, UNITED STATES OF AMERICA

InGaN quantum wells (QWs) has been well established as active layers in LEDs and laser diodes. Recently, there has been interest in the growth of thick InGaN to serve as strain-reducing layers for deep-green and red emitters. The growth of thick layers is, however, challenging. The miscibility gap between InN and GaN leads to InGaN phase separation and indium clustering. In addition, low indium incorporation at high growth temperatures and a high density of V-pits are observed in InGaN films grown in the III-polar direction. Alternatively, the growth of films in the N-polar direction offers advantages that are attractive for the growth of thick InGaN. N-polar growth enables higher indium incorporation and V-pits are less favorable to form. Despite these advantages, limited studies on thick N-polar InGaN films have been reported. This is because N-polar InGaN grown by MOCVD typically suffer from high densities of hexagonal hillocks that originate from low quality N-polar GaN templates. Therefore, in order to assess the quality of thick N-polar InGaN films, it is necessary to probe the local structure and optical properties of high quality grown films. In this study, we compare the structural and optical properties of thick III-polar and N-polar InGaN. Both III-polar and N-polar InGaN growth was carried out by MOCVD under identical conditions (130 nm, 780°C, 300 Torr, V/III=2450) on high quality GaN base layers. The N-polar InGaN films were free of hexagonal hillocks and exhibited a reduced RMS roughness of 0.66 nm in comparison to the RMS roughness of 2.30 nm for III-polar InGaN. High resolution XRD, SIMS and EDX measurements revealed higher indium incorporation in the N-polar films (13%) when compared to III-polar InGaN (7.5%). From PL measurements, two distinct peak emissions located at different depths of the film were observed for both film polarities. One peak originating from a pseudomorphically strained region and the other from a partially relaxed region. To further investigate the optical properties of InGaN films, we preformed both steady state and time-resolved cathodoluminescence (TRCL) mapping of the III-polar and N-polar films at room and liquid helium temperatures. From CL measurements, distinct emission from indium clusters and threading dislocation around V-pits were observed in III-polar InGaN films. In the case of N-polar InGaN, CL emission was homogenous across the film surface. With the combination of spectroscopic techniques, this study elucidates the differences in the luminescence in thick InGaN as a function of film polarity.

RECENT DEVELOPMENTS AND UNDERSTANDING OF HIGH-PERFORMANCE PIEZO-/FERROELECTRIC SINGLE CRYSTALS OF COMPLEX PEROVSKITE

Zuo-Guang Ye

Simon Fraser University, BC, CANADA

Single crystals of relaxor-based complex perovskite solid solutions, $Pb(Mg_{1/3}Nb_{2/3})O_3$–$PbTiO_3$ [PMN-PT] and $Pb(Zn_{1/3}Nb_{2/3})O_3$–$PbTiO_3$ [PZN-PT], exhibit extraordinary piezoelectric performance - with extremely high piezoelectric coefficients, very large electromechanical coupling factors and exceptionally high strain levels, making them the materials of choice for the next generation of high-end electromechanical transducers for a wide range of applications, including (i) high-power underwater projectors and medical therapy, (ii) medical diagnostic imaging and nondestructive evaluation, (iii) sensors and receivers, such as hearing aid devices and pyroelectric applications. However, to further improve the binary materials' properties, new generations of piezocrystals have been developed, including ternary relaxor-PT solid solutions (Generation II), doped relaxor-PT solid solutions (Generation III), and other crystal systems with higher Curie temperature (T_C) and high-performance. On the other hand, understanding the relationship between the complex domain structures and macroscopic properties is a key to this development. In this talk we present an overview on the recent developments in high-performance piezo-/ferroelectric single crystals, and the fundamental understanding of their complex domain structures, phase transitions and structure - property relations. The design, crystal growth, phase symmetry, domain structure, and dielectric, piezoelectric and ferroelectric properties of several crystal systems will be discussed, including (i) ternary solid solution $Pb(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ [PIN-PMN-PT]-based Generation II piezocrystals with a complex morphotropic phase boundary region where the rhombohedral $R3m$ à monoclinic M_A (Cm) phase transition preserves the piezoelectric performance of the rhombohedral phase up to T_C, overcoming the depoling effect and extending the operating temperature range of the piezocrystals; (ii) $Bi(Zn_{0.5}Ti_{0.5})O_3$ [BZT]-based binary and ternary crystals that exhibit a high-T_C; (iii) $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbSnO_3$-$PbTiO_3$ [PMN-PSn-PT] ternary system which shows high piezoelectricity with a piezoelectric memory effect attributed to a self-polarization mechanism based on the defect-dipoles due to the presence of mixed valence states of $Sn^{2+/4+}$; and (iv) $Pb(Zr_{1-x}Ti_x)O_3$ [PZT] single crystals that form a class of high-T_C and high-performance piezo-/ferroelectric materials potentially useful for high-power electromechanical transducers that can operate in a wide temperature range and at high fields. In addition, the development of the Standard for Piezoelectric Single Crystals will be presented. This document covers the physical and electromechanical requirements for relaxor-based piezoelectric single crystals of PMN-PT and PZN-PT solid solutions. *This work is supported by the U. S. Office of Naval Research (Grants No. N00014-12-1-1045 and N00014-16-1-6301) and the Natural Science and Engineering Research Council of Canada.*

CRYSTAL GROWTH AND DOMAIN MEMORY EFFECT OF PMN-PT NEAR MPB

Qiang Li, Chao Xu

Department of Chemistry, Tsinghua University, CHINA

Relaxor-based (1-x)Pb($Mg_{1/3}Nb_{2/3}$)O_3-xPbTiO_3(PMN-PT) single crystals have attracted extensive attentions for more than three decades due to their ultrahigh electromechanical coupling and piezoelectric coefficients. Bulk single crystals of PMN-PT near Morphotropic Phase Boundary (MPB) have been be grown successfully using a modified Bridgman-Stockbarger method. However the phase structure of PMN-PT system is polytropic and susceptible to composition, temperature and biased electric field. Close to the MPB region, the microstructure remains controversial, viewing from the initial rhombohedral (R) and tetragonal (T) phases coexistence theory to the discovery of the monoclinic phase. In order to understand the phase structure in the as-grown PMN-PT single crystal, polarized light microscope(PLM) was applied to study its temperature-induced domain behavior. The temperature dependent domain structure was investigated in the [100]-oriented PMN-0.30PT single crystals. The domains of the rhombohedral phase were bounded in the domain framework of the parent tetragonal phase during the cooling process and a domain memory effect was observed when reheating to the tetragonal phase. A dense square network of crossing domains is observed in the tetragonal phase, in which the domain boundaries are nearly immobile upon phase transition. When phase transforming and transforming back, the result domains are bounded in the domain framework of the parent phase and the original domain structures can be memorized. This domain memory effect may be associated with the weak phase transformation behavior mediated by the domain boundaries.

GROWTH, SIMULATION AND PROPERTIES CHARACTERIZATION OF LARGE SIZE $PB(IN_{1/2}NB_{1/2})O_3$-$PB(MG_{1/3}NB_{2/3})O_3$-$PBTIO_3$SINGLE CRYSTAL BY MODIFIED BRIDGEMAN METHOD

Kexin Song[1], Zhuo Xu[1], Zhenrong Li[1], Fei Li[2], Shiji Fan[1], Sanhong Wang[1], Haisheng Guo[1], Ming Ma[1], Yao Liu[1]

[1]Xian Jiaotong university, CHINA, [2]Material Research Lab, Pennsylvania State University, UNITED STATES OF AMERICA

Relaxor based ferroelectric single crystals $Pb(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$(PIN-PMN-PT) with composition near morphotropic phase boundary exhibit extraordinary piezoelectric properties. Large bulk single crystal with 108mm in diameter and 170mm in length was successfully grown by modified Bridgeman method. Dielectric, piezoelectric and ferroelectric properties of the [001] samples along single crystal growth direction were systematically measured. The excellent properties (d_{33}-2774pC/N, k_{33}-0.94, E_C-4kV/cm, T_C-180°C, T_{RT}-100°C) were found near morphotropic phase boundary. However, due to composition segregation, morphotropic phase boundary is narrow region in the as-grown crystal boule. It is found that the uniform composition with relatively high properties was appeared in the rhombohedral phase near MPB which occupied 70% length of crystal boule. In this region, piezoelectric constant d_{33}, T_{RT} and Curie temperature are about 1500-1800pC/N, 110°C and 160-180°C, respectively. In the same range of boule, PIN, PMN and PT content are around 24mol%, 44mol% and 32mol%. In order to make large crystal growth more efficient, the characteristics of heat and mass transport in the growth process of PIN-PMN-PT single crystal were also simulated by changing macro parameters, such as furnace structure, temperature distribution, and interface shape. It is found that the suitable conditions would reduce the production costs, save time and improve crystal quality.

HIGH CURIE-TEMPERATURE (TC) PIEZO-/FERROELECTRIC SINGLE CRYSTALS WITH BISMUTH-BASED COMPLEX PEROVSKITES: GROWTH, STRUCTURES AND PROPERTIES

Zuo-Guang Ye, Zenghui Liu, Hua Wu, Alisa Paterson

Simon Fraser University, BC, CANADA

Complex perovskite solid solutions based on Bi(B'B'')O_3-$PbTiO_3$ are potentially interesting ferroelectric and piezoelectric materials with high Curie temperature (T_C). In this work, large-size (1-x)Bi($Zn_{1/2}Ti_{1/2}$)O_3-$x$$PbTiO_3$ (BZT-PT), and (1-x)Bi($Zn_{2/3}Nb_{1/3}$)O_3-$x$$PbTiO_3$ (BZN-PT) single crystals have been successfully grown by the high-temperature solution growth method and the top-cooled solution growth method. A comparative study of the (001)-oriented BZT-PT and BZN-PT crystals is carried out and significant differences are found in their crystal structures and physical properties. The crystal structures and electric properties of these crystals are investigated by various techniques. The crystal structure is refined to be of tetragonal symmetry by means of powder X-ray diffraction, but their local crystal structures shows remarkable differences in terms of cationic displacements. The T_C is determined to be around 570 ºC and 420 ºC for the BZT-PT and BZN-PT single crystals, respectively. The optical crystallography and domain structures studied by polarized light microscopy reveal different types of domain structures in the BZT-PT and BZN-PT crystals and their effects on ferroelectricity are investigated. The high T_C and large coercive electric field, as well as the high remanent polarization of the BZT-PT and BZN-PT single crystals make them promising candidates for applications in high-power electromechanical transducers that can operate in a wide temperature range. *This work is supported by the U. S. Office of Naval Research (Grants No. N00014-12-1-1045 and N00014-16-1-6301) and the Natural Science and Engineering Research Council of Canada.*

LEAD-FREE CRYSTAL GROWTH: FROM KTN TO KNN

Hao Tian, Peng Tan

Harbin Institute of Technology, CHINA

Lead-free crystals, as a classic example of environmentally-friendly materials, have received the extensive concern and key development recently at the forefront of high-technology advanced materials. Among these lead-free candidates, $KTa_{1-x}Nb_xO_3$ (KTN) and $K_{1-y}Na_yNbO_3$ (KNN) are the most potential systems due to their giant electro-optic and piezoelectric properties. However, large-size and high quality KTN and KNN crystals are difficult to grow, which limits their development and application. In this work, we successfully grew a series of large-size and high-quality KTN and KNN crystals by the top-seeded solution growth method. The as-grown KTN and KNN crystals exhibit good crystallinities and have large quadratic electro-optic coefficients ($s_{11} = 1.04 \times 10^{-14}$ m^2V^{-2}) and large piezoelectric coefficients ($d_{33} =$ 161 pC/N) respectively, indicating their quality and suitability for device application. We investigate the segregation of as-grown crystals which enables precise control of the individual components of crystals during growth, and propose effective energy models to explain the crystal morphology and guide the size uniformity crystal growth which ensures the quality of as-grown crystals. Further, the variable gradient functional materials engineering is proposed. Niobium composition gradient KTN crystals were designed and successfully grown to achieve the controllable gradient of quadratic electro-optic coefficients by controlling growth conditions. Based on this variable gradient refractive index KTN, a 2.2 MHz high-speed electro-deflector was produced. The controllable growth of high-quality KTN and KNN crystals will be valuable for the lead-free crystal performance improvement and photonic and electronic device development, and provides a basis for exploring the origin of giant electro-optic and piezoelectric effects.

COMPOSITION DESIGN AND PIEZOELECTRIC PROPERTY OF PURE KXNA1-XNBO3 SINGLE CRYSTAL FABRICATED BY SEED-FREE SOLID-STATE CRYSTAL GROWTH

Minhong Jiang, Chongyan Hao, Zhengfei Gu

Guilin University of Electronic Technology, CHINA

Recently, we developed and reported the using of traditional ceramic technology (that is a seed-free solid-state crystal growth(SFSSCG) method) to prepare the $K_xNa_{1-x}NbO_3$(KNN)-based single crystal of the size of the centimeter level or above. The addition of Bi and Li species gives rise to an increasing of mobile ionic defects and space charge which then leads to high dielectric loss in the KNN-based single crystal. Therefore, exploring a pure KNN single crystal with low defect density and high quality is very attractive for factual applications, and also useful for further clearing the mechanism of ceramic→single crystal transformation in the system. In the present work, we designed a pure KNN single crystal without any other additions by adjusting the ratio of K and Na in $K_xNa_{1-x}NbO_3$. Pure $K_{0.52}Na_{0.48}NbO_3$ lead-free piezoelectric single crystal with an orthorhombic structure and a maximum dimension of $4 \times 4 \times 2$ mm^3 was successfully prepared by SFSSCG method. At the same time, we also report the microstructure, piezoelectric, dielectric and ferroelectric properties of the pure KNN single crystals. Reference [1] M.H. Jiang, C.A. Randall, H.Z. Guo, G.H. Rao, R. Tu, Z.F. Gu, G. Cheng, X.Y. Liu, J.W. Zhang, and Y.X. Li, *J. Am. Ceram. Soc.* 2015, 98, 2988.

THE SYNERGY OF MODELING AND NOVEL EXPERIMENTS FOR MELT CRYSTAL GROWTH RESEARCH

Jeffrey J. Derby

University of Minnesota, MN, UNITED STATES OF AMERICA

We present recent examples of how computational modeling and novel experiments together have enabled the identification of fundamental mechanisms important during the growth of bulk crystals from the melt. We first discuss how microgravity experiments, carried out via sounding rockets, motivated a reexamination of classical theories for foreign particle engulfment during crystal growth. Via the development and application of rigorous numerical models, we were able, for the first time in over a decade of research on this system, to quantitatively describe data on the engulfment of SiC (silicon carbide) particles during the growth of crystalline silicon. Moreover, the model results allowed for the unambiguous identification of previously unascertained interactions responsible for the behavior of this system and, via this insight, the analytical derivation of a new scaling law for the dependence of critical engulfment velocity on particle size. We finish with an overview of exciting, new research that employs neutron imaging experiments that are allowing us to directly “see” growth of a crystal, *in operando*, during a gradient freeze experiment. We argue that the synergies of “seeing” via these tools will dramatically improve our fundamental understanding and provide for a closed-loop approach of optimizing of the growth of large, single crystals from the melt. --------------- This research was supported in part by NASA NNX10AR70G, DOE/NNSA DE-NA0002514, DOE/NNSA/DNN R&D (LBNL subcontract AC0205CH11231); no official endorsement should be inferred.

STRUCTURE OF SOLID-LIQUID GROWTH INTERFACES: GAN-GA AND SI/GE-IN

Elias Vlieg[1], Aryan De Jong[1], Vedran Vonk[2]

[1]Radboud University, Institute for Molecules and Materials, NETHERLANDS, [2]DESY, GERMANY

In crystal growth from solution, it is well known that the solution can have a large effect on the crystal morphology or polymorph. In order to fundamentally understand this role the atomic-scale structure of the crystal-solution interface needs to be determined. We use in situ X-ray diffraction to achieve this and will present two examples involving semiconductors to illustrate the information that can be obtained. GaN is the most used semiconductor material after Si and is for example used in LED lighting, blue lasers and high-temperature and high-power applications. High quality material can be grown from the liquid phase, using Ga as the solvent. Due to the inert nature of N_2, such solution growth typically requires very high temperatures and pressures. It was recently found that the addition of Na to the solution can significantly reduce these pressures and temperatures, leading to a possible route for high-quality GaN growth at reduced cost [1]. We have developed a set-up that allows in situ observation of the growth interface using high-energy X-ray diffraction up to a temperature of 1100 K and a pressure of 50 bar [2]. Using this set-up and high-quality GaN substrates, it is possible to prepare atomically-smooth interfaces between GaN and Ga. This enabled us to acquire large X-ray diffraction data sets, providing a unique, atomic-scale view of the interface. Epitaxial layers of Ge can be grown on Si using liquid-phase epitaxy (LPE). We have studied the early stages of this process and find that already in an undersaturated solution, a thin precursor film of Ge is formed at the interface. This near-equilibrium layer will act as the template for subsequent growth at supersaturation. [1] F. Kawamura et al., J. Cryst Gr. 310 (2008) 3946. [2] A.E.F. de Jong et al., J. Cryst Gr. 420 (2015) 84. [3] V. Vonk et al., Langmuir 33 (2017) 814.

GROWTH OF MOLECULAR SYSTEMS

Frank Schreiber

Tuebingen University, GERMANY

We discuss the peculiarities of structure formation in molecular systems, with particular emphasis on the differences to the growth of elemental (atomic), simple crystals or thin films. We focus on two qualitative differences between atoms and molecular systems. The first is the existence of internal degrees of freedom, i.e. in particular the orientational degrees of freedom, which can introduce new equilibrium phases (as is obvious in liquid crystals) and also additional complexities in non-equilibrium structure formation, such as orientational transitions during growth and possibly different scaling laws [1,2]. The second concerns the typically different distance dependence (i.e., range) of the interaction potentials, which also impact of course the equilibrium phase diagram (with the appearance / disappearance of the liquid phase depending on interaction range as a famous example). We show that the interaction range has profound impact on the diffusion behavior of adsorbates and thus on the structure formation [3]. Finally, we comment on consequences for structure formation of mixtures of molecular systems [4-6]. Contributions by A. Hinderhofer and A. Gerlach as well as numerous external collaborators are gratefully acknowledged. [1] Dürr et al., PRL 90 (2003) 016104 [2] Kowarik et al, PRL 96 (2006) 125504

[3] Kleppmann et al., PRE 95 (2017) 020801(R)

[4] R. Banerjee et al., PRL 110 (2013) 185506

[5] A. Aufderheide et al., PRL 109 (2012) 156102

[6] C. Lorch et al., APL 107 (2015) 201903

DISLOCATION AIDED ORIENTATION ALIGNMENT DURING INITIAL STAGES OF CRYSTAL GROWTH

Amit Samanta, Andrew Lange, Tammy Olson, Selim Elhadj

Lawrence Livermore National Laboratory, CA, UNITED STATES OF AMERICA

The oriented attachment of molecular clusters and nanoparticles is a commonly reported mechanism of crystal growth in many materials, yet the microscopic mechanisms associated with the alignment of nanoparticles during coalescence has not been established. We studied the coalescence of prototypical gold and copper nanoparticles using *in situ* electron microscopy coupled to atomic level simulations. At variance with the oriented attachment hypothesis, alignment of nanoparticles post-contact irrespective of their initial misorientation is driven by extensive dislocation activity that is followed by twinning or surface diffusion aided neck growth and subsequent surface diffusion aided shape evolution. We found that in contrast to macro-crystalline particles, in nanoparticles the energy barriers associated with the stability of grain boundaries formed during coalescence are very low. Consequently, with small thermal fluctuations the grain boundaries readily disintegrate or migrate to the surface. Our atomistic simulations suggest that the dislocation-aided alignment of nanoparticles in vacuum happens much faster than diffusion aided processes such as neck growth, or shape. The fact that many nanoparticles with different orientation coalesce to form single crystal aggregates suggests a revision of the scope of oriented attachment during crystal growth by nanoparticle aggregation. Our findings also reveal that the temperature sensitivity and the multi-scale nature of coalescence of nanoparticles are distinctly different from the classical picture of diffusion aided sintering of macro-scale particles. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

TWINNING DURING CZOCHRALSKI GROWTH OF HEAVILY-DOPED, DISLOCATION-FREE SINGLE CRYSTAL SILICON

Joel K. Kearns

NASA John H. Glenn Research Center, OH, UNITED STATES OF AMERICA

Lower voltage power electronics are needed to enable low power consumption computers, routers, telecommunications and automotive devices. Low voltage power MOSFETs are made from dislocation free silicon heavily doped with arsenic, phosphorous or antimony to provide low electrical resistivity. As crystal resistivity is lowered by increased dopant concentration, twinning of the crystal has unexpectedly occurred during growth. Twinning renders that part of crystal unusable for devices. The only mechanism previously proposed to explain growth twinning in diamond cubic semiconductors such as silicon does not predict twinning under these conditions. It is possible that the high electronic impurity content or impurity concentration gradients in the crystal or melt provide a different mechanism to generate twins during growth. The source of the twins must be identified so that crystal growth process conditions can be designed to eliminate this defect mechanism, allowing lower resistivity crystals to be grown reliably. Several potential models are reviewed which may explain the growth twinning. Crystals that twinned during attempted growth are characterized for electrical, chemical and structural defects related to the proposed twin mechanisms. The presence of defects during growth, which encourage twin nucleation, are examined by electrical resistivity measurements, transmission and scanning electron microscopy, energy dispersive X-ray spectroscopy, secondary ion mass spectrometry, photoluminescence and x-ray diffraction. Initial results of optical microscopy, SEM, EDS and diffraction by Laue back-reflection will be discussed.

HIGH MOBILITY BASNO3 FILMS GROWN BY MOLECULAR BEAM EPITAXY AND FIELD EFFECT TRANSISTOR

Jisung Park[1], Hanjong Paik[1], Debdeep Jena[2], Darrell Schlom[3]

[1]Department of Material Science and Engineering, Cornell University, NY, UNITED STATES OF AMERICA, [2]School of Electrical and Computer Engineering, Cornell University,, NY, UNITED STATES OF AMERICA, [3]Kavli Institute at Cornell for Nanoscale Science, NY, UNITED STATES OF AMERICA

$BaSnO_3$ is a promising wide band gap perovskite semiconductor with high mobility at room temperature and excellent oxygen stability. The reported mobility is 320 $cm^2/V·s$ in single crystals at room temperature and 70 $cm^2/V·s$ in thin films grown by pulsed-laser deposition. Our epitaxial $BaSnO_3$ thin films grown by molecular beam epitaxy have mobilities of about 150 $cm^2/V·s$ on a variety of substrates including $SrTiO_3$ and MgO for carrier densities in the mid 10^{19} cm^{-3} range. The dependence of the mobility on the carrier density shows that the mobility is limited by defects such as threading dislocations. Nonetheless, a La-doped $BaSnO_3$ film with a mobility of 36 $cm^2/V·s$ and a carrier concentration of $1×10^{18}$ cm^{-3}, which is the highest mobility yet reported at low carrier concentration, was achieved. This is promising for field effect transistor devices. The fabrication and measurement of field effect transistors with $BaSnO_3$ channel layers will be discussed.

ADSORPTION-CONTROLLED GROWTH OF LA-DOPED BASNO$_3$BY MOLECULAR-BEAM EPITAXY

Hanjong Paik[1], Zhen Chen[2], Edward Lochocki[3], Ariel Seidner[1], Amit K. Verma[4], Nicholas Tanen[1], Jisung Park[1], Masaki Uchida[5], Shunli Shang[6], Bi-Cheng Zhou[6], Zi-Kui Liu[6], Debdeep Jena[1], Kyle Shen[3], David A. Muller[2], Darrell G. Schlom[1]

[1]Department of Material Science and Engineering, Cornell University, UNITED STATES OF AMERICA, [2]Applied and Engineering Physics, Cornell University, UNITED STATES OF AMERICA, [3]Department of Physics, Cornell University, UNITED STATES OF AMERICA, [4]School of Electrical and Computer Engineering, Cornell University, UNITED STATES OF AMERICA, [5]Department of Applied Physics and Quantum-Phase Electronics Center (QPEC), University of Tokyo, JAPAN, [6]Department of Materials Science and Engineering, The Pennsylvania State University, UNITED STATES OF AMERICA

Epitaxial La-doped BaSnO$_3$ thin films have been grown in an adsorption-controlled regime by molecular-beam epitaxy, where the excess volatile tin oxides desorb from the film surface. Fully relaxed films grown on (001) DyScO$_3$ substrates exhibit mobilities as high as 183 cm^2/V·sec at room temperature and 400 cm^2/V·sec at 10 K at carrier concentration of 1.2×10^{20} cm^{-3} despite the high concentration of threading dislocations (1.2×10^{11} cm^{-2}). The mobility remains over 120 cm^2/V·s even at carrier concentrations as low as 4.0×10^{18} cm^{-3}. In comparison to other reports, we observe a much lower concentration of (BaO)$_2$Ruddlesden-Popper crystallographic shear faults. This suggests that in addition to threading dislocations, (BaO)$_2$ crystallographic shear defects can significantly reduce electron mobility and their reduction is key to reducing the electron scattering in La-doped BaSnO$_3$ thin films grown on highly mismatched substrates.

NOVEL RADICAL-BASED MOLECULAR BEAM EPITAXY APPROACH FOR METAL OXIDE FILMS CONTAINING ELEMENTS OF LOW OXIDATION POTENTIAL

Bharat Jalan

University of Minnesota, MN, UNITED STATES OF AMERICA

Metals possessing high oxidation potential are readily oxidized, whereas those with lower potential require stronger reaction conditions. For ternary oxides such as perovskite oxides (ABO_3, where A and B are elemental metals), a difference in oxidation potentials of metal A and B can make synthesis more demanding as compared to their binary oxide counterparts. For instance, if metal B has a lower oxidation potential than that of metal A, a more severe oxidation condition may be required to achieve full oxidation of B in the presence of A. Modern MBE approaches overcome these challenges to a certain extent by using high oxygen pressure, reactive gases such as ozone or by employing oxygen containing metal-organic precursors. The first two approaches often accompany undesirable consequences in MBE such as metal flux instability due to the surface oxidation, or filament oxidation, or even damage to the vacuum pumps due to high oxygen pressure. The latter approach although works for titanates and vanadates, it is not always possible to find an oxygen-containing metal precursor that is compatible with the MBE system, i.e. those with the high vapor pressure, and thermal stability. [1] We will present our recent development of the radical MBE approach, which utilizes the highly reactive metal radicals to not only overcome the oxidation challenges in oxide MBE but to also provides potential routes to grow metal oxides of elements possessing low oxidation potentials (such as V, Sn, Ni, Ir, W, etc) or in other words, elements, which are hard to oxidize under standard MBE growth conditions. Using a model materials system, a detailed study of MBE growth of $BaSnO_3$ and $SrSnO_3$ doping and electronic transport properties and their relationships with structural defects/disorder will be presented. [2] [1] A. Prakash, J. Dewey, H. Yun, J.S. Jeong, K.A. Mkhoyan, and B. Jalan, “Hybrid molecular beam epitaxy for the growth of stoichiometric $BaSnO_3$”, J. Vac. Sci. Technol. A **33**, 060608 (2015) [2] A. Prakash, P. Xu, A. Faghaninia, S. Shukla, J. W. Ager III, C. S. Lo, and B. Jalan, “Wide Bandgap $BaSnO_3$ Films with Room Temperature Conductivity Exceeding 10^4 Scm^{-1}” Nat. Comm. (2017) (in press)

SYNTHESIS STRATEGIES FOR CONTROLLING THE IN-PHASE OCTAHEDRAL ROTATION AXIS IN *PBNM*-TYPE PEROVSKITES

Steven May

Drexel University, PA, UNITED STATES OF AMERICA

The last few years have seen considerable interest in engineering BO_6 octahedral rotations to gain new control over the properties of ABO_3 perovskite heterostructures. One example is the prediction of hybrid improper ferroelectricity in short-period superlattices consisting of centrosymmetric constituent layers that in bulk form exhibit the *Pbnm* space group (orthorhombic, $a^-a^-c^+$ structures).[1,2] To realize this prediction, the in-phase rotation axis of the perovskite layers must be oriented parallel to the growth direction of the superlattice. I will discuss strategies for growing superlattices in which the in-phase axis can be deterministically controlled and the implications of these strategies on synthesis efforts to realize polar superlattices. I will show how rotational imprinting from *Pbnm* substrates offers a straightforward approach for engineering the orientation of the rotational pattern, while epitaxial strain typically yields multiple domains of varying crystallographic orientations.[3] Additional considerations such as the role of growth temperature will be discussed. Finally, I'll describe how the measurement and analysis of half-order diffraction peaks can be used to quantify octahedral rotations and *A*-site displacements in *Pbnm*-type heterostructures.[4] This work is supported by the NSF (DMR- 1151649). [1] J. M. Rondinelli and C. J. Fennie, *Adv. Mater*. **24**, 1961 (2012). [2] A. T. Mulder, N. A. Benedek, J. M. Rondinelli, and C. J. Fennie, *Adv. Funct. Mater*. **23**, 4810 (2013). [3] A. K. Choquette, C. R. Smith, R. J. Sichel-Tissot, E. J. Moon, M. D. Scafetta, E. Di Gennaro, F. Miletto Granozio, E. Karapetrova, and S. J. May, *Phys. Rev. B* **94**, 024105 (2016). [4] M. Brahlek, A. K. Choquette, C. R. Smith, R. Engel-Herbert, and S. J. May, *J. Appl. Phys.* **121**, 045303 (2017).

PUSHING THE ENVELOPE ON UNDERSTANDING AND SUPPRESSING ATOM AND ION DIFFUSION ACROSS COMPLEX OXIDE INTERFACES

Scott A. Chambers, Steven R. Spurgeon, Yingge Du, Peter V. Sushko

Pacific Northwest National Laboratory, WA, UNITED STATES OF AMERICA

In our quest to synthesize atomically precise heterostructures and superlattices, the ability to make interfaces with a high degree of perfection is critical and highly sought after. Yet, the same thermal energy that gives incoming atoms sufficient mobility to nucleate an epitaxial layer can also drive cation and anion diffusion across the interface, particularly when the two oxides have some degree of mutual miscibility and/or vacancies are present in the substrate. In addition, when making polar/nonpolar interfaces, the energy gain associated with eliminating the interface dipole can also promote cation mixing. While oxygen vacancies have attracted much attention, anti-site defects resulting from cation mixing are often neglected in experimental and theoretical studies. The true structure of the interfaces is often approximated using a “chemically sharp” model that is subsequently used to interpret electronic and magnetic data. However, the accuracy of this approximation is limited and this approach cannot result in substantive and sustainable growth of the field as a whole. Meaningful progress requires adequate understanding and characterization of the intermixing process, as well as strategies to kinetically limit the extents of diffusion for specific elements. In this talk, we present our recent work on perovskite/perovskite and perovskite/Group IV semiconductor interfaces. In both cases we model the interface as a quasi-two-dimensional defect structure and aim to resolve its properties in the most definitive way possible. On the experimental side, we combine atomic-scale structural and chemical imaging (STEM-HAADF, EELS, and EDS) with volume-averaged techniques such as x-ray photoelectron spectroscopy and associated modeling to explain materials properties and device performance. We show that STEM-EDS chemical maps are prone to significant errors that obscure the true interface structure due to strong interaction between the probe electron beam and specimen. After accounting for these errors, we accurately map the spatial distributions of each cation species. On the theoretical side, we apply electrostatic considerations to generate plausible interface structures and refine them with the help of classical *ab initio* simulations. These models are then validated against the experimental data to determine the most likely atom configurations for a given extent of intermixing. Taken together, our results illustrate the powerful insight into real interfaces generated by combining a correlative analysis approach with refined theory calculations based on experiments. Strategies for suppressing interdiffusion center around deposition at temperatures close to ambient and subsequent recrystallization at elevated temperature. Results from these experiments will also be presented.

GROWTH, STABILITY, AND APPLICATIONS OF GAAS1-XBIX MATERIALS THROUGH THE LENS OF MICROSTRUCTURAL DEVELOPMENT

Susan E. Babcock[1], Thomas F. Kuech[2], Luke J. Mawst[1], Dane Morgan[1], Weixin Chen[3], Kamran Forghani[1], Yingxin Guan[2], Honghyuk Kim[1], Guangfu Luo[1], Adam Wood[1]

[1]University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA, [2]University of Wisconsin Madison, UNITED STATES OF AMERICA, [3]Department of Materials Science and Engineering, University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA

Motivated by the high sensitivity of the band structure of $GaAs_{1-x}Bi_x$ to the Bi concentration, our team has explored $GaAs_{1-x}Bi_x$ solid solutions as model materials for the synthesis, stability, and application of the broad range of promising ternary and quaternary compound semiconductor alloys that have extensive miscibility gaps in their phase diagrams. $GaAs_{1-x}Bi_x$ is an exemplar for the epitaxial OMVPE deposition and stability of such materials because of the very low solubility of Bi in GaAs. The near-atomic-scale, three-dimensional element mapping capability of atom probe tomography (APT) and high-angle annular dark field (HAADF) scanning transmission electron microscopy (STEM) have been applied to study the Bi distribution in as-OMVPE-deposited and annealed materials as a means to elucidate growth and Bi dissolution mechanisms. The low solubility of Bi demands films be grown at temperatures (~400^{o}C) more than two hundred degrees Celsius below those typically used to deposit high-quality GaAs epitaxial films (~650^{o}C). The observed Bi distributions in as-grown materials support models that describe Bi as accumulating on the surface of the growing film prior to incorporation when certain growth chemistries are employed, behavior that can result in composition profiles in the growth direction of superlattices that deviate substantially from square wave form. They also suggest that Bi incorporates uniformly across the growth front even when it does not in the growth direction. Studies of annealed materials provide insight into mechanisms by which Bi might phase separate from the solid solution film during post-growth processing and use. Combined APT and HAADF-STEM have revealed both the preservation of the composition profile, indicating minimal solid-state diffusion, and the formation of nanometer-scale precipitates. These precipitates are bifurcated into Bi and Ga rich zones with compositions that are consistent with the Bi-Ga binary phase diagram. Substantially-extended Bi-denuded “tails” frequently are associated these precipitates, suggesting that phase separation can occur by the formation of nano-scale liquid droplets that accelerate Bi dissolution from the $GaAs_{1-x}Bi_x$ solid solution by moving through it. Observed gradients in precipitate number density with distance from the sample surface support simulations implicating Ga vacancies in precipitate nucleation processes (Punkkinen *et al.* (2014) *Semicond. Sci. Tech* **29** 115007). These results suggest that Bi dissolution might be mitigated by inhibiting Ga vacancy formation. Experiments designed to test this hypothesis are underway. This research primarily is supported by NSF through the University of Wisconsin Materials Research Science and Engineering Center (DMR-1121288).

EPITAXIAL GROWTH OF III-V QUANTUM DOT LASERS ON SILICON SUBSTRATES FOR SILICON PHOTONICS

Huiyun Liu

University College London, UNITED KINGDOM

As a future driving force technology, Si photonics can improve the low-cost and high speed inter-chip communication by using optical transmission instead of electrical connection. However, Si based light-emitting sources have been considered as “holy grail” for silicon photonics due to Si has in-direct bandgap. By using InAs/GaAs quantum dots (QDs) as active region in laser structure, III-V laser monolithically grown on silicon is a promising solution to be the role of active region on Si platform, which has been proved on GaAs substrate. The challenge of monolithic growth is that high density of threading dislocations (TDs) will propagate into laser active region due to the lattice mismatch between GaAs and Si. To stop the TD propagation, defect filter layers (DFLs) formed by InGaAs/GaAs strained-layer superlattices (SLSs) have been applied, which significantly reduce the density of TDs from $\sim 10^{10}/cm^2$ at the interface between III-V and Si to $<10^6/cm^2$ in III-V active region. As a zero-dimensional material, QD has three-dimensional quantum confinements, which create delta-function like density of states. QD lasers thus have low threshold currents, temperature insensitive operation, and less sensitivity to threading dislocations. Therefore QD is the ideal candidate to form active region in III-V lasers grown on group IV substrates. High performance QD lasers grown on GaAs substrates have been well-established, which proves its potential of growing on group IV platforms . In this presentation, we will review our development of InAs/GaAs QD lasers monolithically grown on Ge, Se/Si, and Si substrates in last few years. Low threshold current density of 62.5 A/cm^2, which corresponds to 12.5 A/cm^2 for each of the five QD layers, has been demonstrated under cw operation at room temperature. The lasing wavelength is at 1315 nm. The output power is as high as 105 mW at an injection current density of 650 A/cm^2, with no evidence of power saturation up to this current density. The ageing test was performed at a fixed temperature of 26 ^{o}C, with the output power monitored for a constant cw drive current of 210 mA. An extrapolated mean time to failure (MTTF) of over 100,158 hours was demonstrated here.

INTERFACE ANALYSIS FOR STRAINED LAYER SUPERLATTICES BY ATOM PROBE TOMOGRAPHY

Ayushi Rajeev[1], Weixin Chen[2], Jeremy D. Kirch[1], Susan E. Babcock[2], Luke J. Mawst[1], Thomas F. Kuech[3], Tom Earles[4]

[1]Department of Electrical and Computer Engineering, University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA, [2]Department of Materials Science and Engineering, University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA, [3]Department of Chemical and Biological Engineering, University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA, [4]Intraband LLC, WI, UNITED STATES OF AMERICA

Quantum Cascade Laser (QCL) devices have active regions constituting of ~30-40 repetitions of a superlattice (SL) structure with quantum wells and barriers of various thicknesses (typically 1-5nm each). Growing the quantum wells and barriers with high precision in thickness and sharp compositional interfaces is critical for obtaining the desired emission wavelength of QCLs. Moreover, for strained layer SLs, minor thickness variations can lead to imbalance in the overall strain thickness product, which may result in strain relaxation of the thick active region. Analysis of high-resolution x-ray diffraction (HRXRD) data provides details about the compositions and periodicity in the SL layers. Transmission electron microscopy techniques offer atomic resolution structural and chemical analysis in a 2-D projection of the 3-D structure, but revelation of 3D detail is generally of poorer chemical sensitivity. Here we report the three dimensional characterization of the interfaces using atom probe tomography (APT) in III-V strained layer SL structures grown by Organometallic Vapor Phase Epitaxy (OMVPE). Such measurements have proven valuable in explaining the red-shifted emission wavelength for QCLs consisting of SL layers lattice matched to InP [1]. Strained-layer SL samples composed of: a.) 5 periods of $In_{0.365}Al_{0.635}As$(20.1nm) / $In_{0.673}Ga_{0.327}As$(23.35nm) and b.) 124 periods of $In_{0.44}Al_{0.56}As$(1.86nm) / $In_{0.6}Ga_{0.4}As$(2.23nm) were grown on InP substrates at 605°C and 100 torr reactor pressure, with a 5sec interruption between the layer growth. Pusled-laser APT was used to investigate the three-dimensional compositional structure of these superlattices. The superlattice period and compositions deduced from the HRXRD scans were used to validate the reconstruction of the specimen atom positions from the atom probe data. Concentration profiles across the interface for each of the component elements were deduced from this reconstruction. Interface widths were quantified by fitting lines to the linear portions of the concentration gradients at the interfaces in these concentration profiles and measuring the distance between the intersection points of these lines with the uniform concentrations measured in the abutting layers. The compositional thicknesses of the interfaces determined in this way were less than 1nm in all cases investigated. With this information, the effects of OMVPE growth parameters (such as interruption times) on these interface widths can be quantified and used to improve strained layer QCL designs.
Acknowledgement: This work is supported by The National Science Foundation (PFI) 1317292, Navy STTR N68335-11-C-0432, and Air Force Research Laboratory FA8650-13-2-1616 [1] C.A. Wang et al., Journal of Crystal Growth, http://dx.doi.org/10.1016/j.jcrysgro.2016.11.029

SUBSTRATE EVALUATION FOR HIGH QUALITY BORON PHOSPHIDE GROWTH

Yu Yang[1], Xuejing Wang[2], Jianqiu Guo[1], Balaji Raghothamachar[1], Michael Dudley[1], Balabalaji Padavala[3], Clint Frye[3], James H. Edgar[3]

[1]Stony Brook University, UNITED STATES OF AMERICA, [2]Purdue University, UNITED STATES OF AMERICA, [3]Kansas State University, UNITED STATES OF AMERICA

Due to its numerous outstanding properties, boron phosphide (BP) has emerged as a promising candidate for solid state neutron detectors which are compact, sensitive and economic. However, the scale up of the crystalline BP by bulk growth is challenging since it incongruently decomposes into its constituents at temperatures below its melting point. Therefore, heteroepitaxial growth using chemical vapor deposition (CVD) method is a more viable synthesis technique. In our study, extensive growth processes and characterizations were conducted on two types of substrate systems: BP||SiC and BP||AlN. In synthesis part, BP was deposited on a variety of polytype crystals of SiC (3C-, 4H-, 6H) and on the AlN-buffered sapphires films with different intentional misorientations (both in tilt angles and tilt directions). In order to compare the crystalline quality of these BP epitaxies, Synchrotron White Beam X-ray Topography (SWBXT) technique was utilized for investigating the existence of defects, hetereostructures ($B_{12}P_2$) and rotational twins. The surface morphologies of different BP films were characterized with Scanning Electron Microscope (SEM). The imperfections and strain in different BP epitaxies were also analyzed with High Resolution X-ray Diffraction (HRXRD). Defect structures and the relaxation conditions at interfaces between BP and the different substrates were thoroughly studied in atomic scale using High Resolution Transmission Electron Microscope (HRTEM). The topography shows that the BP grown on 3C-SiC eliminates the rotation twin completely as the result of it being isostructural with respect to the substrate crystal. The BP||AlN substrate system produced better quality films, since the AlN has high thermal stability, lower lattice constant mismatch and is composed of elements isoelectronic with BP. In general, the good substrate crystalline quality rather than the off-cut angle plays a significant role in influencing the BP film property. Ongoing investigations of the surface structures of off-axis substrates and their influence on the quality of the epitaxial growth of BP will be correlated with the X-ray data and the results discussed.

GROWTH, TRANSFER, AND CHARACTERIZATION OF GE AND SIGE NANOMEMBRANES ON III-V SUBSTRATES

Abhishek Bhat[1], Xiaorui Cui[1], Yingxin Guan[2], Shelley Scott[1], Thomas F. Kuech[3], Max G. Lagally[1]

[1]Department of Material Science and Engineering, University of Wisconsin-Madison, UNITED STATES OF AMERICA, [2]Department of Material Science and Engineering, University of Wisconsin Madison, WI, UNITED STATES OF AMERICA, [3]University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA

It has been proposed that heterostructures comprising high-Ge-content Si(1-x)Ge(x) alloys (x>0.65) can exhibit large quantum confinement in the electronic L valleys. These structures can further be engineered and exploited for the development of L valley quantum cascade lasers[1], [2]. Simultaneously, tunable light emitters in the wavelength range 2.1-2.5 μm have applications in chemical and biological sensing as well as communication. The introduction of biaxial tensile strain into the Ge lattice makes the band structure go from indirect to direct, introducing the ability to have a strain controlled wavelength tunable light emitting diode[3]. A major hindrance in the development of such hetereostructures and strain tunable devices has been the lack of availability of high-quality germanium-on-insulator (GOI) material. Growing SiGe and Ge on III-V materials not only has the potential to provide us with the desired high-quality material, but also presents opportunities to explore new nanomembrane (NM) based architectures. The near perfect lattice match between Ge and GaAs as well as the availability of lattice matched release layers such as AlAs and InGaP allows for the fabrication of high-quality and freestanding crystalline compounds. Critical thickness constraints not being a major concern in such growth systems also makes it possible to obtain a range of thicknesses with strain introduced deliberately only after transfer to a flexible host. We present here initial results of MOCVD and MBE growth of Ge and high-Ge-content SiGe films on GaAs. Results on the characterization of these membranes are also presented, along with details of release and transfer of wafer-scale NMs without etch holes. Results from Raman measurements of externally induced strain, x-ray diffraction structure determinations, and AFM images of surface roughness of successfully grown and released membranes are presented in comparison to commercially obtained GOI. We believe these NMs present a crucial first step towards generating hybrid III-V/IV NM materials. References: [1] K. Driscoll and R. Paiella, “Design of n-type silicon-based quantum cascade lasers for terahertz light emission,” *J. Appl. Phys.*, vol. 102, no. 9, p. 93103, Nov. 2007. [2] K. Driscoll and R. Paiella, “Silicon-based injection lasers using electronic intersubband transitions in the L valleys,” *Appl. Phys. Lett.*, vol. 89, no. 19, p. 191110, Nov. 2006. [3] J. R. Sanchez-Perez *et al.*, “Direct-bandgap light-emitting germanium in tensilely strained nanomembranes,” *Proc. Natl. Acad. Sci.*, vol. 108, no. 47, pp. 18893–18898, Nov. 2011.

IN SITU DIAGNOSTICS OF SCINTILLATOR CRYSTAL GROWTH PROVIDED BY ENERGY-RESOLVED NEUTRON IMAGING

Anton S. Tremsin[1], Didier Perrodin[2], Adrian Losko[3], Sven C. Vogel[3], Mark Bourke[3], Jeffrey H. Peterson[4], Jeffrey J. Derby[4], Takenao Shinohara[5], Gregory A. Bizarri[2], Edith D. Bourret[2]

[1]University of California at Berkeley, CA, UNITED STATES OF AMERICA, [2]Lawrence Berkeley National Laboratory, CA, UNITED STATES OF AMERICA, [3]Los Alamos National Laboratory, NM, UNITED STATES OF AMERICA, [4]University of Minnesota, MN, UNITED STATES OF AMERICA, [5]Japan Atomic Energy Agency, JAPAN

High resolution energy resolved neutron imaging at pulsed neutron sources enables various non-destructive and in-situ studies where other conventional techniques fail due to the opacity of the sample and the processing equipment. In-situ diagnostics of several parameters important for the optimization of crystal growth procedure becomes possible now due to recent developments of neutron imaging techniques, enabled by the advances at bright pulsed neutron beam facilities and the development of high resolution neutron counting detectors suitable for time-of-flight applications. The experiments presented here demonstrate the unique possibility to obtain real-time characteristics of crystal growth process, such as location and shape of the liquid/solid interface, the elemental composition, distribution of temperatures and others. Neutrons are unique probes for crystal growth processes due to their high penetration capability through the growth equipment and the ability to differentiate the liquid/solid phases by coherent neutron scattering and their sensitivity to elemental composition and temperature through resonance absorption. We demonstrate the possibility of in-situ imaging during vertical gradient-freeze growth of several gamma scintillator materials. The neutron imaging experiments conducted at the LANSCE and J-PARC pulsed neutron sources reveal the dynamics of the liquid/solid interface and segregation of particular elements during the growth of BaBrCl:Eu, $Cs_2LiLaBr_6$:Ce and NaI:Eu crystals sealed in quarts ampules. The spatial distribution of several elements was measured with sub-mm spatial resolution, demonstrating the possibility to quantify the segregation of these elements (Eu, Li and Cs in particular) within the solid and liquid phases. Coherent neutron scattering by the solid phase and the change of elemental concentration across the liquid/solid interface is used for the visualization of that interface in real time. Our results demonstrate that energy resolved neutron imaging can provide unique information for the optimization of crystal growth through feedback control, in conjunction with detailed process simulation. *This work is supported by the Department of Energy/NNSA/DNN R&D and carried out at Lawrence Berkeley National Laboratory under contract #AC02-05CH11231.*

FINITE-ELEMENT MODELING OF SCINTILLATOR CRYSTAL GROWTH WITHIN A BRIDGMAN FURNACE IMAGED VIA NEUTRON SCATTERING

Chang Zhang[1], Jeffrey H. Peterson[1], Jan Seebeck[1], Anton S. Tremsin[2], Didier Perrodin[3], Gregory A. Bizarri[3], Edith D. Bourret[3], Sven C. Vogel[4], Jeffrey J. Derby[1]

[1]University of Minnesota, MN, UNITED STATES OF AMERICA, [2]University of California, CA, UNITED STATES OF AMERICA, [3]Lawrence Berkeley National Laboratory, CA, UNITED STATES OF AMERICA, [4]Los Alamos National Laboratory, NM, UNITED STATES OF AMERICA

Since the pioneering work of Bridgman in 1925, there have been no direct methods to observe what transpires within refractory crucibles that are moved through high-temperature furnaces during vertical Bridgman crystal growth. Indeed, we have only been able to infer the conditions of phase change and crystal growth indirectly, by measurement of discrete temperatures during a growth run, by observation of quenched interfaces after aborted runs, or via determination compositional profiles in the grown crystal. In companion research presented at this conference, Tremsin et al. discuss groundbreaking experiments that employ spallation neutrons to visualize, in situ, the compositional field that is developed during the growth of a mixed halide scintillator crystal via the Bridgman method. These measurements provide, for the very first time, a direct observation of melt crystal growth within a system large enough to display the complex interplay of heat transfer, fluid flow, segregation, and phase change characteristic of an industrially relevant process. In this presentation, we apply finite element models to predict the macroscopic transport of heat, mass, and momentum along with phase-change phenomena in the crystal growth system employed in these neutron imaging experiments. Not only do the experimental observations serve to validate the modeling results, but, more importantly, the model provides a rigorous framework in which to understand the mechanisms that are responsible for the complicated evolution of interface shape and dopant distribution observed in the growth experiment. We discuss how ongoing synergies between modeling and experiment will allow for unambiguous interpretation of growth experiments. This is particularly significant, since there is a lack of fundamental understanding of how microstructural defects arise during growth. If we can directly observe these phenomena via imaging and real-time measurements and correlate their behavior with growth conditions provided by the model, we have a path by which we can begin to understand and quantify the responsible mechanisms. Ultimately, the understanding obtained by model and experiment will truly allow the closing of the loop between materials quality, growth conditions, and process development, an undertaking that in the past has relied on empiricism and experience to typically achieve only incremental advances. --------------- This work has been supported by DOE/NNSA DE-NA0002514 and DOE/NNSA/DNN R&D (LBNL subcontract AC0205CH11231); no official endorsement should be inferred.

PREPARATION AND CHARACTERIZATION OF TERNARY CESIUM HAFNIUM CHLORIDE SINGLE CRYSTALS

Robert Kral[1], Petra Zemenova[1], Ales Bystricky[1], Vitezslav Jary[1], Vladimir Babin[1], Antonin Cihlar[1], Karel Nitsch[1], Pavel Veverka[1], Martina Kohoutkova[2], Shohei Kodama[3], Shunsuke Kurosawa[4], Yuui Yokota[5], Akira Yoshikawa[3], Martin Nikl[1]

[1]Institute of Physics, Czech Academy of Sciences, CZECH REPUBLIC, [2]University of Chemistry and Technology Prague, CZECH REPUBLIC, [3]Institute for Materials Research, Tohoku University, JAPAN, [4]Faculty of Science, Yamagata University, JAPAN, [5]New Industry Creation Hatchery Center, Tohoku University, JAPAN

Recently, ternary cesium hafnium chloride (Cs_2HfCl_6) has been identified as promising scintillating material [1],[2]. Furthermore, Kang and Biswas [3] presented first principle calculations of Cs_2HfCl_6 electronic and optical properties which, among others, indicate the self-trapping of holes and electrons in the form of V_K and polaron centers, respectively. The Cs_2HfCl_6 belongs into group of halide materials with general formula A_2MX_6, where A is alkali metal (Li, Na, K, Rb, Cs), M is metal in 4+ valence state (e.g. Ti, Zr, Hf, Sn, Se, Te), and X is halide (F, Cl, Br, and I). Due to its high atomic number Z = 58, high light yield around 54 000 ph/MeV, energy resolution of 3.3% at 662 keV, moderate density 3.86 g/cm^3, and low hygroscopicity, it is suitable candidate for application in radiation detectors as scintillator. The Cs_2HfCl_6 is formed by CsCl and $HfCl_4$ mixed together in stoichiometric ratio 2:1 and melts congruently at 826 °C. The crystallographic structure of Cs_2HfCl_6 is cubic with lattice parameters a = 10.42 ± 0.01 Å and space group of Fm-3m, which is isostructional to K_2PtCl_6 and analogous to anti-fluorite CaF_2 structure [4]. This work deals with the direct synthesis of undoped Cs_2HfCl_6 from starting CsCl and $HfCl_4$ mixed in required ratio in quartz ampoules and reacted in molten state under ambient pressure. However, the direct synthesis of Cs_2HfCl_6 is complicated by the fact that $HfCl_4$ sublimates and is highly hygroscopic. The Cs_2HfCl_6 single crystals were grown by unseeded vertical Bridgman method. Prepared Cs_2HfCl_6 material as well as grown crystals were characterized using X-ray fluorescence, X-ray diffraction, and thermal analyses to determine the purity, phase content, and thermal properties. Moreover, the absorption, radioluminesnce, and photoluminescence spectra as well as decay measurements on prepared optical specimens from grown crystals will be discussed. **Acknowledgement** The bilateral ASCR-JSPS project and projects of Frontier Research Institute for Interdisciplinary Sciences, Tohoku University and International Collaboration Center Institute for Materials Research (ICC-IMR), Tohoku University are gratefully acknowledged. The authors thank to Mrs. A. Beitlerova and Mrs. S. Randakova for radioluminescence and XRF measurements of the grown crystal, respectively. **References** [1] A. Burger et al., Appl. Phys. Lett. 107 (2015) 143505. doi:10.1063/1.4932570. [2] K. Saeki et al., Appl. Phys. Express. 9 (2016) 042602. doi:10.7567/APEX.9.042602. [3] B. Kang, K. Biswas, J. Phys. Chem. C. 120 (2016) 12187–12195. doi:10.1021/acs.jpcc.6b02496. [4] S. Maniv, J. Appl. Crystallogr. 9 (1976) 245–245. doi:10.1107/S0021889876011114.

SOLUTION GROWTH OF BULK ORGANIC CRYSTALS

Natalia Zaitseva[1], Leslie Carman[2], Andrew Glenn[2], Andrew Mabe[2], Stephen Payne[2]

[1]Lawrence Livermore National Laboratory, UNITED STATES OF AMERICA, [2]Lawrence Livermore National Laboratory, CA, UNITED STATES OF AMERICA

Low-temperature solution growth has been traditionally used for crystal growth from aqueous solutions. Due to the high polarity of water, the method has been successfully applied to inorganic ionic crystals like dihydrogenphosphate (KDP) grown to a super-large size for laser applications. Recent demand for advanced solid-state materials for radiation detection, led to the development of a new direction in solution crystal growth now applied to the production of molecular organic crystals which, due to the lack of solubility in water, can be grown only from pure organic solvents. Application of the rapid growth technique like that used previously for the KDP-type of crystals, enabled the growth of large-scale (~10cm) crystals of aromatic hydrocarbons (e.g. trans-stilbene, bibenzyl, 2-5-diphenylanthracene) that have high content of hydrogen and fluorescence properties for deployment as efficient scintillators in high-energy neutron detectors. The method also contributed to a better understanding of the similarities and differences introduced into the growth mechanisms by the molecular and crystallographic structures. In-situ observations of growth step sources revealed that the combination of traditional dislocation growth accompanied by step generation from the crystal edges (described previously for KDP-type crystals) may be typical only for some crystal facets. A surprising finding was that the 2-dimensional (2D) growth often becomes dominant on the other facets of the same growing crystal, leading to formation of severe defects specific for most organic crystals. Additional contributions into growth rates and defect formation can be attributed to the attachment of 3D clusters to the growing surfaces exposed to high supersaturation. Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S.Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.This work has been supported by the U.S. Department of Energy NA-22, and by the US Department of Homeland Security, DNDO, under competitively awarded IAA HSHQDC-09-X-00743. This support does not constitute an express or implied endorsement on the part of the Government.

THE GROWTH AND DECOMPOSITION OF METASTABLE SEMICONDUCTING ALLOYS

Thomas F. Kuech[1], Yingxin Guan[2], Susan E. Babcock[3], Luke J. Mawst[4], Dane Morgan[5], Guangfu Luo[5]

[1]University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA, [2]Department of Material Science and Engineering, University of Wisconsin Madison, WI, UNITED STATES OF AMERICA, [3]Department of Materials Science and Engineering, University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA, [4]Department of Electrical and Computer Engineering, University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA, [5]Department of Material Science and Engineering, WI, UNITED STATES OF AMERICA

New semiconductor device concepts often demand incorporation of semiconducting materials with highly tuned electronic properties, specifically band gap, and lattice parameter, a requirement for epitaxial growth. The electronic properties, optical properties, and lattice parameter of a semiconducting ternary or quaternary alloy of almost any composition can be predicted with relative ease, offering tantalizing solutions to this demand. However, many of these promising alloy compositions lie within miscibility gaps in their respective equilibrium phase diagrams, severely limiting the range of materials that currently are deployed to those few that are thermodynamically stable and lattice matched to available substrates. Development of strategies to form homogeneous alloys with independently tune band gap and lattice parameter from within these miscibility gaps should greatly expand the range of materials that could be incorporated in new device designs, thereby greatly enhancing device capability. The formation of such metastable semiconducting alloys generally requires growth conditions which are far from thermodynamic equilibrium. These conditions favor phase separation, which must, however, occur at the growth surface where the atomic mobility and mass motion is sufficiently high to allow local compositional variations to form under typical growth conditions. The formation of homogeneous metastable alloys therefore requires a high degree of control over mass transport at the growth front. This control can be achieved through low growth temperatures, which reduce the diffusion coefficients, and control over the surface chemistry, which alters surface structure and site occupancy, as well as modifying local mass transport. The talk will present recent results on the formation of complex multinary alloys with compositions that are deep within the miscibility gap of the alloy compositional field. The use of growth chemistry to control alloy composition at low growth temperatures will be discussed.

THERMODYNAMICS OF DEPOSITION-FLUX DEPENDENT INTRINSIC FILM STRESS

Marcel J. Rost[1], Amirmehdi Saedi[2]

[1]Huygens-Kamerlingh Onnes Laboratory, NETHERLANDS, [2]Leiden Institute of Chemistry, NETHERLANDS

Vapour deposition on polycrystalline films can lead to extremely high levels of compressive stress, exceeding even the yield strength of the films. A significant part of this stress has a reversible nature: it disappears when the deposition is stopped and re-emerges on resumption. Chason [1] even showed the corresponding inverse behavior during electrochemical etching.

Although the debate on the underlying mechanism still continues, insertion of atoms into grain boundaries seems to be the most likely one. However, the required driving force has not been identified. To address the problem we analyzed the entire film system using thermodynamic arguments.

Surprisingly, we find that the observed, tremendous stress levels can indeed be explained by the flux-induced entropic effects in the extremely dilute adatom gas on the surface. Our analysis justifies any adatom incorporation model, as it delivers the underlying thermodynamic driving force. Counterintuitively, we also show that the stress levels decrease, if the barrier(s) for adatoms to reach the grain boundaries are decreased.

[1] Shin and Chason, Phys. Rev. Lett. **103**, 056102 (2009)

STRESS-DIRECTED COMPOSITIONAL PATTERNING OF COMPOUND SEMICONDUCTORS AND STRESS MAPPING BY 2D MICRO-RAMAN IMAGING

Brian Rummel, Michael Rimada, **Sang M. Han**

University of New Mexico, NM, UNITED STATES OF AMERICA

We have recently shown that a patterned elastic stress field can be used to change the near-surface atomic composition in an epitaxial compound semiconductor film.[1] This compositional patterning laterally manipulates quantum barriers within the film in a press-and-print manner. For the initial proof of concept, an array of Si pillars is pressed against a relaxed $Si_{0.8}Ge_{0.2}$ substrate in a mechanical press, and the entire assembly is heated to high temperatures. This serves to promote Ge diffusion away from the compressed regions, leaving 100% Si-enriched areas. Careful design of nanopillar array and press assembly allow patterning of Si- or Ge-enriched regions, which can ultimately produce thermo-mechanically triggered quantum dot circuits. In expectation of building an addressable circuit, we demonstrate that 2D micro-Raman imaging can be used to map the post-pattern stress field and therefore surface compositions. We are currently extending this work to InGaAs/GaAs systems. [1]S. Ghosh, D. Kaiser, J. Bonilla, T. Sinno, and S. M. Han, "Stress-Directed Compositional Patterning of SiGe Substrates for Lateral Quantum Barrier Manipulation," *Appl. Phys. Lett.* **107,** 072106-1:5 (2015).

OPTOELECTRONIC PROPERTIES OF EPITAXIALLY STRAINED COMPLEX OXIDES FROM FIRST PRINCIPLES

Sebastian E. Reyes-Lillo, Jeffrey B. Neaton

Molecular Foundry, LBNL, CA, UNITED STATES OF AMERICA

Bismuth vanadate ($BiVO_4$) and strontium titanate ($SrTiO_3$) have long been explored for solar energy water splitting applications due to their robust photo-catalysis, stability against degradation in water, and technological properties (e.g. ferroelasticity and ferroelectricity). However, the photo-electrochemical performance of these materials is severely limited by relatively large band gaps and low electron mobilities. Previous theoretical work has focused on the role of extrinsic and intrinsic defects to control and tune the optical properties of complex oxides; however, the effect of anisotropic strain remains largely unexplored. Recently, (001)-$BiVO_4$ and (111)-$SrTiO_3$ thin films have been grown using molecular beam epitaxy, opening new possibilities to design oxide-based renewable solar-energy devices. In this work, using $BiVO_4$ and $SrTiO_3$ as model materials, we use density functional theory and many-body perturbation theory calculations to investigate the interplay of optoelectronic properties and epitaxial strain in complex oxides. Our results show that in both cases, compressive epitaxial strain leads to a moderate decrease of band gap at room temperature due to structural symmetry mechanisms. For $BiVO_4$, compressive (001) strain enhances the hole effective mass and majority carrier small polaron formation energy. For $SrTiO_3$, (111) strain induces novel ferroelectric phases that are not present in bulk or (001) strained perovskites. This work is supported by DOE; computational resources are provided by NERSC.

ELASTIC STRAIN ENGINEERING OF PBTIO3 THIN FILMS GROWN BY REACTIVE MOLECULAR-BEAM EPITAXY

Eric Langenberg[1], Eva H. Smith[1], Hari P. Nair[1], Neus Domingo[2], Gustau Catalan[2], Darrell G. Schlom[3]

[1]Department of Material Science and Engineering, Cornell University, UNITED STATES OF AMERICA, [2]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC, Barcelona Institute of Science and Technology, Campus Universitat Autònoma de Barcelona, SPAIN, [3]Kavli Institute at Cornell for Nanoscale Science, UNITED STATES OF AMERICA

Epitaxial strain of complex oxide thin films imposed by the underlying substrate has been widely used to gain access to novel phases, absent in bulk specimens, with new or enhanced functional properties. In ferroelectric oxides, strain engineering may be used to tune ferroelectric-ferroelastic domain configurations. In archetype ferroelectric-ferroelastic $PbTiO_3$, sufficiently large compressive strain is predicted to produce only c-domains (i.e. domains with the polarization along the out-of-plane direction, P_3), whereas on applying sufficiently large tensile strain, a1/a2 domains are favored (i.e. domains with the polarization pointing along the in-plane crystallographic directions: P_1 and P_2). However, at intermediate strains, a wide variety of domains and domains configurations are predicted such as a/c domain configurations (mixture of a- and c-domains) or more complex monoclinic r-domains ($P_1 = P_2 \neq 0$, $P_3 \neq 0$) or ca*-domains ($P_1 \neq 0$, $P_2 = 0$, $P_3 \neq 0$). To provide experimental evidence of the strain-ferroelectric domain phase diagram in $PbTiO_3$, we report the growth of $PbTiO_3$ films on several single crystal perovskite substrates, namely, $SrTiO_3$, $DyScO_3$, $GdScO_3$, $SmScO_3$, $PrScO_3$, and $LaLuO_3$ by reactive Molecular-Beam Epitaxy (MBE). All the substrates have pseudocubic (001) orientation with an average pseudocubic lattice parameter ranging from 3.905 Å to 4.184 Å, thus approximately spanning from the *a* to the *c* lattice parameters of bulk $PbTiO_3$ tetragonal structure (3.904 Å and 4.152 Å, respectively). Single phase $PbTiO_3$ thin films are achieved through continuous codeposition of Pb, Ti, and distilled ozone in an adsorption-controlled growth regime. In-situ reflection high-energy electron diffraction (RHEED) patterns, continuously monitored during growth, confirm the layer-by-layer growth fashion of $PbTiO_3$ thin films, which gives rise to very flat surfaces (typically RMS < 0.5 nm) as verified by atomic force microscopy. Thus, the high crystal quality and atomically flat surfaces achieved by adsorption-controlled 2D growth of $PbTiO_3$ on $SrTiO_3$ by reactive MBE can be extended to a large variety of different lattice-parameter perovskite substrates. Both X-ray diffraction and piezoresponse force microscopy are used to probe the evolution of the ferroelectric-ferroelastic domains in $PbTiO_3$ as functions of both epitaxial strain and film thickness. In agreement with theoretical predictions, our results show that for moderate compressive strain pure c-domain $PbTiO_3$ thin films are obtained, whereas at large tensile strain a1/a2 domain configuration is observed. Interestingly, at intermediate strains a thickness-dependent competing scenario of different domain configurations is found.

STRAIN CONTROL OF CATIONIC DISTRIBUTION IN $BI_4TI_3O_{12}$-$BIFEO_3$ COMPOSITE FILMS

Changhee Sohn, Dongkyu Lee, Xiang Gao, Ho Nyung Lee

Oak Ridge National Laboratory, TN, UNITED STATES OF AMERICA

Strain engineering has been a powerful way to improve or to develop novel functionalities of materials by modulating the bond angle/length between atoms as well as inducing defects. Beyond these well-known mechanism, a recent theoretic calculation predicted that strain engineering can even control the cation distribution of ions in the well-known Aurivillius multiferroic system, $Bi_4Ti_3O_{12}$-$BiFeO_3$ composite [A. Y. Birenbaum and C. Ederer, Appl. Phys. Lett. **108**, 082903 (2016)]; while Ti and Fe ions are randomly distributed in bulk, Fe ions can preferentially locate at the inner or outer octahedral layers in the Aurivillius structure depending on the type of strain. To attest the prediction, we have fabricated $Bi_4Ti_3O_{12}$-$BiFeO_3$ epitaxial films on $SrTiO_3$, LSAT, and $LaAlO_3$ substrate by using pulsed laser epitaxy to control the sign and degree of strain. Scanning transmission electron microscopy with electron energy loss spectroscopy revealed that Fe ions have site-preference when compressively strained, whereas no preferential positioning was observed in the tensile strained films. This experimental result supports well the theoretical prediction particularly for the case of compression, while further theoretical and experimental attempts are required for the tensile case. Effects of the site preference on magnetic and ferroelectric properties were investigated by using SQUID and second harmonic generation and will be discussed. This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

SHARPENED VO2 PHASE TRANSITION VIA CONTROLLED RELEASE OF EPITAXIAL STRAIN

Chang-Beom Eom

University of Wisconsin-Madison, UNITED STATES OF AMERICA

Phase transitions in correlated materials can be manipulated at the nanoscale to yield emergent functional properties, promising new paradigms for nanoelectronics and nanophotonics. Vanadium dioxide (VO_2), an archetypal correlated material, exhibits a metal–insulator transition (MIT) above room temperature. At the thicknesses required for heterostructure applications, such as an optical modulator discussed here, the strain state of VO_2 largely determines the MIT transition dynamics critical to the device performance. We develop an approach to control the MIT dynamics in epitaxial VO_2 films by employing a large lattice mismatch SnO_2 intermediate template layer over the TiO_2 substrate to relieve the interfacial lattice constraints, contrary to conventional thin film epitaxy which favors lattice match between the substrate and the growing film. A combination of phase-field simulation and *in situ* real-time nanoscale imaging reveals continuous MIT dynamics at structurally discontinuous domain boundaries and significantly sharpened MIT in SnO_2-templated VO_2 films. Utilizing the sharp MIT, we demonstrate a fast, electrically switchable optical waveguide. This study offers unconventional design principles for heteroepitaxial correlated materials, as well as novel insight into their nanoscale phase transitions. This work has been done in collaboration with D. Lee, J. Lee, K. Song, F. Xue, S.Y. Choi, Y. Ma, J. Podkaminer, D. Liu·, S.C. Liu, B.W. Chung, W. Fan, W. Zhou, J.C. Lee, L.Q. Chen, S. H. Oh, Z. Ma and C.B. Eom

HIGH-INDEX-CONTRAST PHOTONIC CRYSTAL (HC-PC) QUANTUM CASCADE LASERS FABRICATED BY OMVPE

Luke J. Mawst[1], Chris Sigler[1], Colin Boyle[1], Jeremy D. Kirch[1], Don Lindberg Iii[2], Tom Earles[2], Dan Botez[1]

[1]Department of Electrical and Computer Engineering, University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA, [2]Intraband LLC, WI, UNITED STATES OF AMERICA

Phase-locked arrays of antiguided lasers have proven to be a viable approach to coherently scale the output power of semiconductor lasers. In the near-IR, watt-range peak pulsed and CW near-diffraction-limited powers were demonstrated more than 15 years ago for devices designed to exhibit resonant leaky-wave coupling. Such devices represented high-index-contrast (Δn = 0.08-0.10) photonic crystals (PC) structures that allow global coupling between the array elements. Such device structures often require multi-step etching and OMVPE regrowth to form the antiguides within the array. We have developed a two-step OMVPE process to realize near-resonant leaky-wave coupled QCLs emitting at 4.7 mm, which operate to 6 W peak pulsed power with a narrow beamwidth *(<3.7xD.L. at Pmax)*. Such devices exhibit curved layer formation within the interelement regions of the array that must be accurately controlled to achieve resonantly coupled emitters within the array. OMVPE-regrowth studies indicate that regrowth of the interelement regions at relatively high temperature 675^{o}C results in improved surface morphology and controllable thickness for the layers within the interelement regions. The interelement regions of the array have InGaAs layers and lowered Au regions that create a higher effective refractive index than in the element regions. As a result an array of antiguides of large index step ($\Delta n > 0.05$) is formed. Resonant leaky-wave coupling occurs when the interelement regions' width S_t is basically equal to half the projected wavelength λ_1 in the lateral direction. A 35-stage core region with 0.5 μm-thick InP spacer layer was grown by OMVPE using a strain-balanced InGaAs/AlInAs core-region structure designed for emission at 4.6-4.7 μm. Low-doped (2×10^{16}cm^{-3}) 2 μm-thick cladding layers were grown around the core region. An additional 2 μm of higher-doped InP is grown to complete the upper cladding layer. Wet and dry (ECR) chemical etching were used to make deep trenches that stopped at the InP-spacer layer. Fe:InP and InGaAs layers were preferentially regrown by OMVPE in the trenches by using the SiN mask employed for trench etching. After regrowth of the interelement regions, a SiN mask was placed, for current confinement, 5 μm away from the array edges. Then, Ti and Au films were evaporated for metal contact. The measured modal properties of such devices are then correlated with optical models using the actual measured array geometry obtained from SEM imaging. This work was supported in part by the Air Force Research Laboratory under Grant FA8650-13-2-1616 and Navy STTR N68335-15-C-0073

TUNING PHASE-SEPARATION AND ATOMIC-ORDERING IN ALGAINP FOR METAMORPHIC DEVICES

Kunal Mukherjee[1], Eugene A. Fitzgerald[2]

[1]University of California Santa Barbara, CA, UNITED STATES OF AMERICA, [2]Massachusetts Institute of Technology, MA, UNITED STATES OF AMERICA

Vapor phase growth of III-V alloys often results in significant deviations from random solid-solutions [1]. These deviations, in the form of phase-separation and atomic ordering, have an impact on the optoelectronic properties of the semiconductor. With increasing success in the heterogeneous integration of III-V materials and lattice-mismatched substrates, we revisited non-random alloys to determine if they offer additional barriers against carrier recombination at dislocations. In the first part of this study, we systematically varied non-randomness in the alloy microstructure using growth temperature modulation of lattice-mismatched AlGaInP heterostructures. The recombination process around dislocations was then quantified using cathodoluminescence spectroscopy at room-temperature. Our results suggest a somewhat reduced impact of dislocations in the non-random samples. In the second part of the study, lattice-hardening due to non-randomness was investigated using room-temperature nanoindentation. Lattice-hardness could be an important proxy for the long-term reliability of devices against recombination-enhanced defect reactions [2]. Through an analysis of dislocation pop-in events, we noted a small improvement in the mechanical properties of non-random AlGaInP layers as well. In conclusion, microstructural engineering at present offers marginal improvements, but as we develop an understanding of the mechanisms involved, avenues for enhancing these effects can be studied. [1] S. Mahajan, Two-dimensional phase separation and surface-reconstruction driven atomic ordering in mixed III–V layers, Mater. Sci. Eng. B. 30 (1995) 187–196. doi:10.1016/0921-5107(94)09013-0. [2] S. Mahajan, V.G. Keramidas, J.H. Wernick, InP and InGaAsP Semiconducting Materials for Optical Communications, JOM. 36 (1984) 37–41. doi:10.1007/BF03338527.

DOMAIN EPITAXY IN ANATASE TiO_2-SAPPHIRE THIN FILM HETEROSTRUCTURE: A NOVEL EPITAXIAL MATCH DERIVED FROM SOLUTION PHASE SYNTHESIS

Marissa S. Martinez[1], **Andrew S. Ichimura**[2], Christopher J. Tassone[3]

[1]University of Colorado, CO, UNITED STATES OF AMERICA, [2]San Francisco State University, UNITED STATES OF AMERICA, [3]Stanford Synchrotron Radiation Lightsource, CA, UNITED STATES OF AMERICA

In this report, we describe the growth, structure, and photophysical properties of anatase films that have a heteroepitaxial match to C-plane sapphire substrate, $(001)_{anatase}||(001)_{sapphire}$. This is the first report of this out-of-plane orientation for these two phases. Anatase films were grown on single crystal sapphire by a hydrothermal route using titanium (IV) fluoride as the titanium source. The structure and morphology of the thin films were characterized by X-ray diffraction (XRD) and field emission scanning electron microscopy (FESEM), respectively. The in-plane and out of plane orientations of anatase on sapphire were determined by phi (ϕ) and θ-2θ scans at the Stanford Synchrotron Radiation Lightsource (SSRL) on beamlines 7-2 and 2-1 operating at 12.7 keV (0.9744 Å), and with a Bruker D8 diffractometer ($Cu(K_\alpha=1.54$ Å$)$). The out-of-plane heteroepitaxial relationship was found to be $(001)_{anatase}||(001)_{sapphire}$. The in-plane orientation relationship was determined by phi-scans that focused on the (101) anatase and (102) sapphire reflections. It was found that anatase [101] occurs 15° from the sapphire [102] direction. Due to the three-fold rotational symmetry of the substrate, the anatase film consists of three domains offset from each other by 120°. A domain matching epitaxy model is proposed to account for the growth of anatase on sapphire in which the four-fold symmetric tetragonal base of the anatase lattice is bound to the hexagonal oxygen sublattice of c-plane sapphire. FESEM images show square {101} facets of anatase ~400 nm in size at the external surface. Film cross-sections reveal a structure with small grains near the substrate that develop into well-formed columns after ~100 nm of growth. The total film thickness is ~700 nm. Depth profiling of the film by sequential polishing to different film thickness shows that the <001> anatase texture begins at or near the substrate surface. Anatase films with strong <001> texture and {001} facets at the external surface grown on insulating and transparent substrates are excellent photocatalysts. In addition, they are ideal for fundamental studies to reveal orientation-dependent photophysical properties such as photoconductivity and EPR spectroscopy of electron and hole states, and facet dependent photooxidation chemistry. The results of fundamental photophysical studies will be reviewed.

IN-SITU SURFACE X-RAY SCATTERING INVESTIGATION INTO HYBRID OXIDE MOLECULAR BEAM EPITAXY GROWTH MECHANISMS FOR PEROVSKITE MATERIALS

Tassie Andersen[1], Say Young Cook[1], Hawoong Hong[2], Laurence Marks[1], Dillon Fong[2]

[1]Northwestern University, IL, UNITED STATES OF AMERICA, [2]Argonne National Laboratory, IL, UNITED STATES OF AMERICA

Perovskite oxide materials are a playground for the crystal growth community due to the wide range of complex heterostructures that can be created through controlled growth strategies. Transition metal oxides offer tunable magnetic, electronic, and catalytic properties, and hybrid molecular beam epitaxy (MBE) growth methods combining metal-organic sources with effusion cells offer additional freedom in film fabrication. These methods increase film growth speed, improve cation stoichiometric control for oxides such as the titanates and vanadates, and promote full oxidation of B-site cations by providing already-oxidized precursors. To fully exploit the capabilities of hybrid growth systems, understanding of the growth mechanisms and first stages of film growth are necessary. This work focuses on the construction and utilization of a hybrid oxide MBE integrated into an in-situ surface x-ray scattering diffraction system at Sector 33-ID of the Advanced Photon Source at Argonne National Laboratory. With this instrument, we aim to understand oxide growth behavior and allow comparison between existing reflection high energy electron diffraction and x-ray datasets by providing real-time information about film growth and structure. As a starting point, growth of $SrTiO_3$ perovskite and Sr_2TiO_4 Ruddlesden-Popper structures were considered. Thin films, ~10nm thick, were grown on strontium titanate, $SrTiO_3$ (001), and lanthanum strontium aluminum tantalum oxide, LSAT (001), substrates via hybrid oxide MBE. Titanium was supplied via titanium tetraisopropoxide (TTIP) precursor while strontium was supplied via effusion cell. Growth was conducted in a background pressure of 1E-6 Torr $O_{2(g)}$ and substrate temperatures ranged from 750-800°C. Scattering along the in-plane direction was measured at 15 keV to assess film structure and in-situ scattering was monitored during growth at the 0 0 ½ position to maximize sensitivity to changes in the film's surface. Growth of the Sr_2TiO_4 Ruddlesden-Popper endmember has been achieved. Films show good quality based on the presence of thickness fringes. In-situ surface scattering data give insight into the initial growth modes of these films. While a smooth transition (or appropriate combination of phases) from one $Sr_{n+1}Ti_nO_{3n+1}$ member to the next is expected with decreasing Sr:Ti ratio until the perovskite endmember, $SrTiO_3$, is achieved, this system displays unusual phase separation under certain growth conditions. The Sr_2TiO_4 phase persists and decreases as the Sr:Ti ratio is reduced while the presence of epitaxial anatase TiO_2 increases. Further investigation of this system and its endmembers' growth will provide insight into synthesis of other common perovskite and Ruddlesden-Popper oxide materials via hybrid oxide MBE.

TRACKING FERROELECTRIC DOMAIN GROWTH USING LASER SCATTERING TOMOGRAPHY

Robert S. Feigelson, Howard Lee, Robert Demattei

Stanford University, CA, UNITED STATES OF AMERICA

The movement and growth of ferroelectric domains in a crystal under an electric field (poling voltage) has been studied using laser scattering tomography, a technique heretofore used mainly for studying defects in crystals. This technique involves scanning successive planes in a crystal with a micron size laser beam and collecting the scattered light in a computer. The data collected can then be arranged to display 2- or 3-dimensional images and can be viewed along any axis in the crystal. Using this technique we were able to generate images of domain wall nucleation and growth as a function of electric field strength and time. It also allowed for the observation of domain wall movement along any crystallographic direction including down the poling axis which is covered with opaque metallic electrodes. Details of the technique and its use during the poling of a strontium barium niobate crystal is discussed.

MANUFACTURING AND UNIFORMITY OF GRAIN TEXTURED PIEZOELECTRIC CERAMICS

Mark Fanton[1], Richard J. Meyer[2], Elizabeth R. Kupp[2], Beecher H. Watson[2], Yunfei Chang[2], Gary L. Messing[2]

[1]Penn State University, UNITED STATES OF AMERICA, [2]Penn State University, PA, UNITED STATES OF AMERICA

For many decades metals and polymers benefitted from the ability to enhance electrical and mechanical performance by creating highly directional microstructures via rolling, drawing, directional cooling, or other similar processing techniques. Directional tailoring of performance for oxide materials has been largely limited to taking advantage of anisotropies in single crystal materials. Meanwhile traditional technical ceramics remain unimproved with respect to commercialized products. This presentation outlines the process technology and scale up considerations for tailoring asymmetric, directionally oriented ceramic microstructures, with a focus on achieving near single crystal performance from highly oriented ceramic piezoelectric materials. The key principle exploited is the ability of highly anisotropic grains to be added to and then aligned inside a ceramic green body such that they seed pronounced asymmetric grain growth. Critical processes including template synthesis, template alignment via tape casting, part fabrication, process controls, and process characterization will be discussed. The engineering challenges associated with scaling each step will be outlined. Process and performance variabilities across large individual parts and part quantities will be discussed in terms of sensitivity to process variables and other factors critical to economically feasible manufacturing.

PROCESSING-ELECTROMECHANICAL PROPERTY RELATIONSHIPS IN TEXTURED PMNT

Richard J. Meyer[1], Mark Fanton[2], Gary Messing[1], Elizabeth Kupp[1], Yunfei Change[1], Beecher Watson[1]

[1]Penn State University, PA, UNITED STATES OF AMERICA, [2]Penn State University, UNITED STATES OF AMERICA

Textured PMN-PT ceramics are produced by the templated grain growth (TGG) method, whereby platelet-shaped seed crystals of a perovskite phase are used to control grain growth in the PMN-PT ceramic during thermal processing. These seed crystals are aligned by shear forces during tape casting of a slurry containing the seed crystals and a fine PMN-PT powder. At the Pennsylvania State University (PSU) textured materials have been produced in plate, ring, and monolithic cylinder geometries. In <001> textured (1-x)Pb(Mg1/3Nb2/3)O3-xPbTiO3 (PMN-PT), strong preferred grain alignment results in more single-crystal-like piezoelectric response. Current PMN-PT based textured ceramics show d33 = 900-1200 pC/N – about 70-75% of the PMN-PT single crystal value, and a greater than 3-fold improvement over conventional ceramics. These materials also show substantial increases in electromechanical coupling (k33 ≥ 0.83) and dielectric constant (εT33 ≥ 3800) compared to PZT ceramics. To facilitate further adoption of this technology, PSU has been engaged in a two-prong development effort that is looking at scaling the current processing techniques for manufacturing and also at improving the performance of textured PMNT through composition and processing enhancements. This presentation will provide an overview of that effort highlighting key process-electromechanical property relationships.

SHEAR PIEZOELECTRIC PROPERTIES OF RELAXOR-PBTIO3 SINGLE CRYSTALS

Ming Ma, Fei Li, Kexin Song, Yangbin Liu, Zhenrong Li, Shiji Fan, Sanhong Wang, Zhuo Xu

Electronic Materials Research Laboratory, Key Laboratory of the Ministry of Education and International Center for Dielectric Research,Xi'an Jiaotong University, CHINA

Relaxor-$PbTiO_3$ single crystals with ultrahigh shear piezoelectric properties are promising candidates for accelerator and hydrophone applications. In this work, shear piezoelectric and dielectric properties of [111]-poled $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ and [111]-poled $Pb(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$- $PbTiO_3$ single crystals are investigated along the [011] growth direction. Crystals with compositions around morphotropic phase boundary possess optimum properties, in which the shear piezoelectric coefficient d_{15} is found to be higher than 5000 pC/N, electromechanical coupling factor k_{15} is higher than 0.90 and dielectric permittivity $\varepsilon_{11}^T/\varepsilon_0 >$ 10000. These properties are much better than the state-of-the art PZT ceramics (P5H, d_{15}

~800 pC/N, k_{15}~0.75, $\varepsilon_{11}^T/\varepsilon_0 \sim 4000$).

Fig.1. (a) $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ and (b) $Pb(In_{1/2}Nb_{1/2})O_3$- $Pb(Mg_{1/3}Nb_{2/3})O_3$- $PbTiO_3$ single crystal. (c) Crystal samples.

ELECTRO-OPTIC AND NONLINEAR-OPTICAL PROPERTIES OF PB($MG_{1/3}NB_{2/3}$)O_3-PBTIO$_3$SINGLE CRYSTAL

Zhuo Xu, Xin Liu, Xiaotian Fu, Ye Zhao, Weigang Zhao, Yongyong Zhuang, Xiaoyong Wei, Peng Luan

Xian Jiaotong University, CHINA

Pb($Mg_{1/3}Nb_{2/3}$)O_3-PbTiO_3（PMNPT）has long been known as a relaxor ferroelectric with ultrahigh piezoelectricity. In this work, we prepared the single domain PMNPT crystal chip and systematically investigated its electro-optic and nonlinear-optical characterization. A refractive index of 2.5~2.6 is achieved among visible and near infrared range, as well as a 70% transmission between 500nm to 2500nm. Furtherly, we obtained much higher electro-optic coefficient and 2nd order nonlinear coefficient of PMNPT compared to the current nonlinear optical crystals. Herein, we fabricated periodic poled PMNPT aimed at quasi-phase matching for high-efficiency optical-frequency conversion. Additionally, we presented the dielectric permitivity in terahertz (THz) and gigahertz (GHz) frequency of PMNPT. The excellent electro-optic and nonlinear-optic performance of PMNPT shows a promising prospect in optical application.

ON ALLEVIATING MORPHOLOGICAL INSTABILITIES IN THE TRAVELING HEATER METHOD (THM) VIA THE ACCELERATED CRUCIBLE ROTATION TECHNIQUE (ACRT)

Jeffrey H. Peterson, Jeffrey J. Derby

University of Minnesota, MN, UNITED STATES OF AMERICA

The traveling heater method (THM) has seen wide use for the growth of detector-quality bulk crystals of cadmium zinc telluride (CZT). However, the traveling heater method suffers from growth rates that are an order of magnitude slower than other directional solidification processes such as the Bridgman method. Our recent work has shown that these slow growth rates may be caused by morphological instability of the growth interface brought on by constitutional supercooling [1]. Specifically, we observe constitutional supercooling at growth rates well below the expected limit due to lateral mass transport caused by the formation of lee waves in the melt flow. In this presentation, we discuss strategies for eliminating the lee wave and enhancing mass transport through the use of the accelerated crucible rotation technique (ACRT). We will examine the sensitivity of the system ACRT cycles of various lengths, acceleration rates, and maximum rotation rates. Conventional wisdom would predict that the forced convection in the melt would virtually eliminate the supercooling through a reduction in the composition gradient at the growth interface. However, our results show that the supercooling is only periodically alleviated at the growth interface. Further, we use the analysis by Mullins and Sekerka [2] to predict whether the interface will become morphologically unstable. We show that the interface undergoes cyclical stages of stability and instability throughout the ACRT cycle. Surprisingly, we also see that certain ACRT cycles with persistent undercooling do not lead to conditions of morphological instability. And conversely, other ACRT cycles that appear to relieve undercooling tend to destabilize the interface more than they stabilize it. Finally, we will provide insight on how to design appropriate ACRT cycles for the THM system. [1] Jeffrey H. Peterson, Michael Fiederle, and Jeffrey J. Derby, “Analysis of the traveling heater method for the growth of cadmium telluride", *Journal of Crystal Growth* **454**, pp. 45-58 (2016). [2] W. W. Mullins and R. F. Sekerka, “Stability of a planar interface during solidification of a dilute binary alloy”, *Journal of Applied Physics* **35**(2), pp. 444–451 (1964). -------------- This work has been supported in part by the National Science Foundation, under DMR-1007885, and no official endorsement should be inferred.

GROWTH TEMPERATURE OPTIMIZATION OF GAAS-BASED $IN_{0.83}GA_{0.17}AS$ PHOTODETECTOR STRUCTURES ON $IN_{X}AL_{1-X}AS$ BUFFERS

Xingyou Chen, Yi Gu, Yonggang Zhang, Yingjie Ma, Suping Xi, Ben Du, Jian Zhang, Yanhui Shi, Wanyan Ji, Yi Zhu

Shanghai Institute of Microsystem and Information Technology (SIMIT), Chinese Academy of Sciences (CAS), CHINA

$In_xGa_{1-x}As$ (0.53<x<1) photodetectors (PDs) and arrays have been extensively investigated on InP over the past decades due to their important applications in space remote sensing, environmental monitoring, etc[1]. Nowadays the $In_{0.53}Ga_{0.47}As$ PDs lattice-matched to InP with cutoff wavelength of 1.7 µm are mature commercially. Wavelength extended InGaAs PDs and linear arrays with response to the longer wavelength range are also available though large format focal plane arrays (FPAs) are still rare. To ameliorate this situation, the adoption of larger size, lower cost GaAs substrate instead of InP is preferred. However, a larger lattice mismatch had to be faced on GaAs. To acquire device-level high indium InGaAs on GaAs, more efforts should be considered including the optimization of the growth temperature and improvement of the metamorphic buffer structure. In this work, a series of $In_{0.83}Ga_{0.17}As$ with lattice mismatch up to 5.9% were grown on GaAs-based temperature-modulated $In_xAl_{1-x}As$ metamorphic buffer layers by gas source molecular beam epitaxy. Each structure was grown as follows: 0.2 µm GaAs, 0.1 µm $In_{0.1}Al_{0.9}As$, 2.5 µm $In_xAl_{1-x}As$ continuously graded buffer, 1 µm $In_{0.83}Al_{0.17}As$ template and 1 µm lightly Si-doped $In_{0.83}Ga_{0.17}As$ ($n=3\times10^{16}$ cm^{-3}). The X-ray diffraction reciprocal space mapping (XRD-RSM) results showed that the structure with low temperature (LT) grown InAlAs metamorphic buffer layers showed full relaxation with a little larger tilting angle along the growth direction and a much broader peak width along the Q_x direction in the (004) reflection of the $In_{0.83}Ga_{0.17}As$ layer comparing to that with high temperature (HT) grown buffer layers, as shown in Fig. 1(a) and 1(b). But the features of surface morphology and luminescence of $In_{0.83}Ga_{0.17}As$ were improved remarkably due to the superior interfacial effect of the LT buffer. Particularly when it comes to the structure on the LT InAlAs buffer coupled with the $In_{0.83}Al_{0.17}As$ template grown at 540 ºC, the room temperature (RT) photoluminescence (PL) intensity of $In_{0.83}Ga_{0.17}As$ was increased by several times, as shown in Fig. 1(c). These results were demonstrated further by the decrease of RT dark current for GaAs-based $In_{0.83}Ga_{0.17}As$ PDs grown on LT InAlAs buffers with respect to that on HT InAlAs buffers. These are encouraging for the implementation of large format InGaAs FPAs on GaAs substrate in future. Further results and detailed analysis will be contained in the presentation. [1] Y. G. Zhang, Y. Gu, Chapter 17, InTech, 2011. ISBN: 978-953-307-163-3.

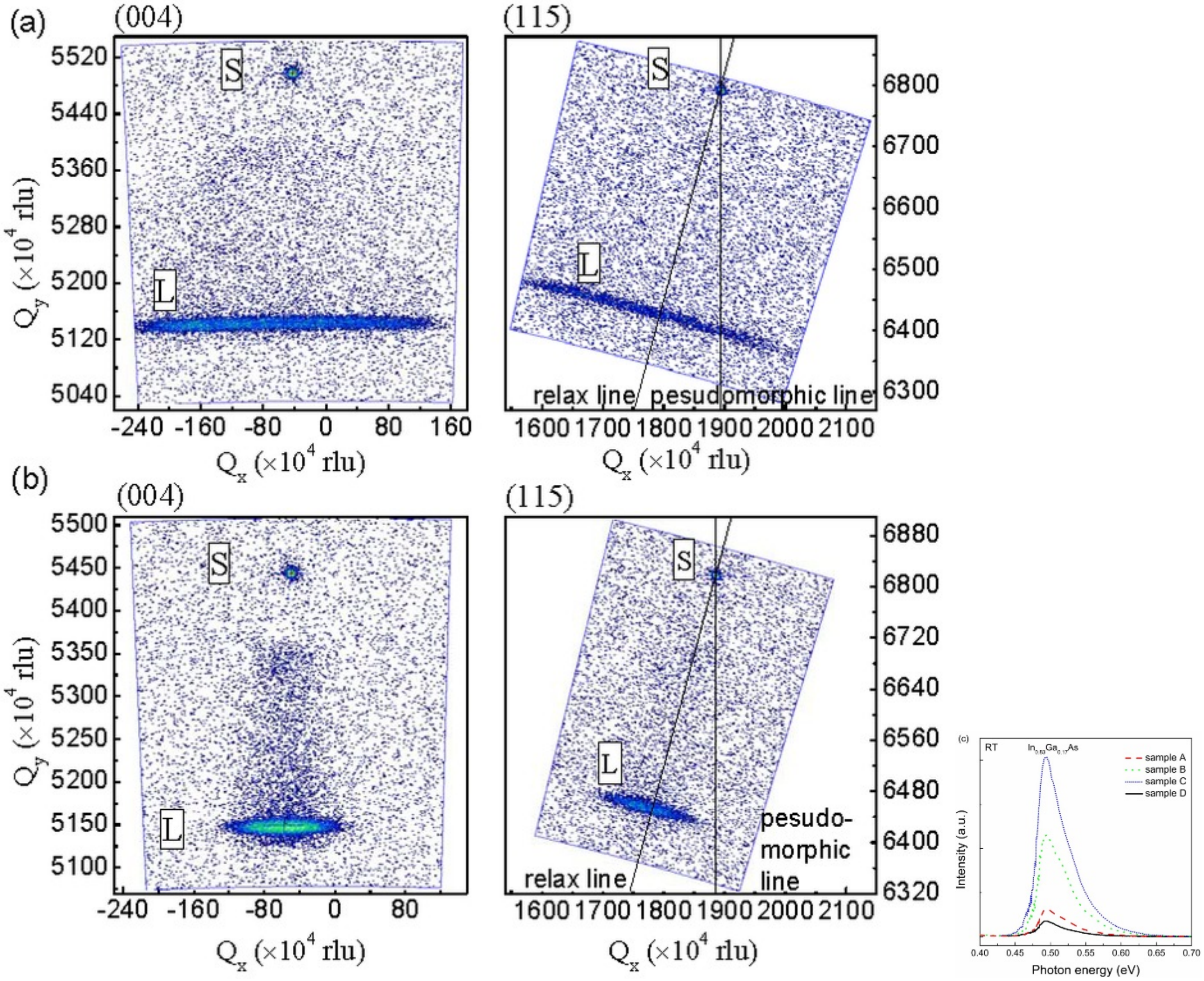


Figure 1. XRD-RSMs of (a) sample B and (b) sample D; (c) RT PL spectra of all samples.

INFLUENCE OF OXYGEN DIFFUSION ON DISLOCATION DENSITY IN SI SINGLE CRYSTAL

Satoshi Nakano[1], Wataru Fukushima[2], Hirofumi Harada[1], Yoshiji Miyamura[1], Koichi Kakimoto[1]

[1]Research Institute for Applied Mechanics, Kyushu University, JAPAN, [2]Kyushu University, JAPAN

Dislocation density is one of the major problem to reduce the quality for the Si single crystal. Oxygen atoms about 10^{18} atoms/cm^3 are in the Si single crystal grown by Czochralski growth method. It has been reported that dislocation could be immobilized by anchoring effect of oxygen atoms in the Si single crystal. Therefore, dislocation multiplication in the Si single crystal is suppressed during high-temperature processing. In this study, we investigated the relationship between the dislocation density and oxygen atoms in the Si single crystal by using numerical analysis. We developed a three-dimensional Haasen-Alexander-Sumino model to analyze the influence of oxygen atoms in the Si single crystal on dislocation multiplication during annealing process. We took into account unlocking stress which could release the fixing of oxygen atoms on dislocation core. Unlocking stress is a function of oxygen concentration at dislocation core. Therefore, we also took into account the diffusion equation for oxygen atoms around the dislocation core to obtain oxygen concentration at dislocation core. The results show that dislocation density is small in case of high oxygen concentration in the Si single crystal because of immobilization of dislocation by the effect of oxygen atoms. We also studied the relationship between dislocation multiplication and temperature in the Si single crystal. We found that dislocation density rapidly increased in the temperature range of 1200-1300K during heating-up process.

GA(NASSB) CLOSE TO 1 EV GROWN WITH DTBAA

Eduard Sterzer[1], Nattermann Lukas[1], Oliver Maßmeyer[1], Benjamin Ringler[1], Carsten Von Hänisch[2], Wolfgang Stolz[1], Kerstin Volz[1]

[1]Philipps-Universität Marburg, Material Sciences Center and Faculty of Physics, GERMANY,
[2]Philipps-Universität Marburg, Faculty of Chemistry, GERMANY

Nitrogen containing III/V materials are discussed for solar cell as well as laser applications. In particular the (GaIn)(NAs) material is well known and can be grown in metalorganic vapor phase epitaxy (MOVPE). The Ga(NAsSb) 1 eV material however, has been very challenging in terms of MOVPE growth so far. A strong N incorporation reduction in dependency of Sb supply makes the growth of Ga(NAsSb) material extremely difficult with the conventionally used N precursor 1,1-dimethyl hydrazine (UDMHy). The novel N/As precursor di-tertiary-butyl-arsano-amine (DTBAA), synthesized and purified in our lab, has an extremely efficient N incorporation in GaAs as well as in (GaIn)As. Based on these results, Ga(NAsSb) experiments with DTBAA were performed. In this study we will present N and Sb incorporation characteristics grown with tri-ethyl-gallium (TEGa), tri-ethyl-stebanum (TESb) and DTBAA. For the N and Sb content determination high resolution X-ray diffraction (HR-XRD) and Photoluminescence (PL)-measurements were used complementary. The surface quality was investigated with an atomic force microscope (AFM). Figure 1 shows the HR-XRD (left) as well as PL measurements (right) of Ga(NAs) and Ga(NAsSb) multi quantum wells (5x) grown on exact semi insulating GaAs (001) substrates.

Fig. 1: HR-XRD profile of Ga(NAs)/Ga(NAsSb) samples (left) as well as PL spectra of the same samples (color coded)

REVISITING THE TWINNING MECHANISM IN DIRECTIONAL SOLIDIFICATION OF MULTI-CRYSTALLINE SILICON SHEET

Chung-Wen Lan, H.K. Lin

Dept. of Chem. Eng., National Taiwan University, TAIWAN

The formation of the twin nucleus is an important phenomenon during the solidification of multi-crystalline silicon. However, the available model by Duffar and Nadri [Scripta Mater. 62(12) (2010) 955] was unable to predict a critical undercooling for twinning that was comparable with the experiments. Through the detailed analysis of the grain structures in the multi-crystalline silicon sheets grown by directional solidification, we find that the grain boundary plays a crucial role. By taking this into account, we revise the previous model. The free energy change (per unit length) when one or two facets anchor to the groove tri-junction and the critical undercooling for twinning are derived and compared with experiments. The predicted undercooling and the probability of forming a twinned nucleus at the groove based on the revised model are consistent with the experimental observations.

THICK HVPE GAN FILMS WITH DRAMATICALLY IMPROVED PROPERTIES

Jaime A. Freitas[1], James C. Culbertson[1], Nadeemullah A. Mahadik[1], Shuang Wu[2], Balaji Raghothamachar[3], Michael Dudley[2], Tomasz Socacki[4], Michal Bockowski[4]

[1]Naval Research Laboratory, DC, UNITED STATES OF AMERICA, [2]Dept. of Mat. Sc., Stony Brook University, NY, UNITED STATES OF AMERICA, [3]Dept. of Mat. Sc/., Stony Brook University, NY, UNITED STATES OF AMERICA, [4]UNIPRESS, Institute of High Pressure, POLAND

The fabrication of high performance GaN-based devices with high yields requires high crystalline quality substrates with controlled electronic transport properties. Recently, it was demonstrated that thick freestanding Hydride Vapor Phase Epitaxy films grown on ammonothermal substrates reproduce the high crystalline quality of those substrates, and conveniently have free carrier concentrations that are several orders of magnitude lower [1]. In this work we have verified that such thick HVPE GaN films can be used as substrates for further homoepitaxial growth. Thick HVPE film deposited on an epi-ready Ammono (0001) substrate was removed from the reactor and its surface was CMP polished . This template was placed back in the HVPE reactor and an additional ~800 mm was deposited. The final crystal consisted of two sequentially grown HVPE-GaN layers on the Ammono substrate. The top HVPE layer was sliced off and the surface of three samples were CMP finished. The lattice parameters were very close to the bulk lattice constants. The rocking curves for these samples had full widths at half maximum of ~16 arcsecs, indicating high crystalline quality. Raman scattering measurements were carried out on the front and back surfaces of two samples. The E_2^2 phonon frequency was mapped on both faces of two samples; the distribution of Raman shifts was 567.45±0.05 cm^{-1}, indicating stress free GaN. The A_1(LO) phonon frequencies and the linewidths measured on the Ga-polar face were larger than those measured on the N-polar face; this is consistent with a larger incorporation of donor impurities as the growth proceeds. Low temperature, photoluminescence measurements carried out on the Ga- and N-polar faces of these samples were also consistent with more doping as the growth proceeds [2]. SIMS depth profile measurements also confirm this observation. Defect configurations were investigated by synchrotron X-ray topography. Threading dislocations and basal plane dislocations are observed. The threading screw dislocation density was measured to be about 880 cm^{-2} while the threading edge dislocation density was about an order higher. The distribution of BPDs, which are formed due to deformation, was found to highly non-uniform with most regions of the wafer nearly BPD-free with high densities concentrated near one edge. Also, besides the surface features, arrays of threading dislocations can be seen from the transmission and grazing incidence topographs, which likely originate from scratches on the surface of the ammonothermal substrate. [1] T. Sochacki, et al., JCG (2014) [2] J.A. Freitas, Jr., et al., CG&D (2015)

SINGLE-CRYSTAL-LIKE III-NITRIDE THIN FILMS DIRECTLY GROWN ON METAL TAPE

Jae-Hyun Ryou[1], Shahab Shervin[2], Kamrul Alam[2], Kaveh Shervin[2], Seung-Hwan Kim[2], Tae Hoon Chung[3], Jie Chen[2], Wiejie Wang[2], Sara Pouladi[2], Rebecca Forrest[2], Jiming Bao[2]

[1]University of Houston, TX, UNITED STATES OF AMERICA, [2]University of Houston, UNITED STATES OF AMERICA, [3]KOPTI, KOREA, REPUBLIC OF

Recent developments of flexible display and electronics have demonstrated flexible visible LEDs. When the semiconductor structure becomes flexible on a flexible template/substrate, it can be used in many applications of wearable and implantable electronics. Most flexible device demonstrations relied on transfer techniques, including epitaxial lift-off, transfer printing, or 2-D material transfer. In this work, we developed a transfer-free direct deposition method of III-N films on a flexible metal substrate. We demonstrate high-crystalline-quality aluminum nitride (AlN) and gallium nitride (GaN) on a flexible metal substrate using graphene as an intermediate seed layer. There were a few reports on the growth of GaN on graphene in which the graphene layer was transferred from Cu or Ni foil to a target substrate. This method is transfer-free for easily-scalable and continuous roll-to-roll deposition-compatible process. We use a flexible Cu foil as the flexible substrate for the direct growth of III-N film as well as a nucleation layer for graphene. Graphene is grown on the Cu foil by well-established chemical vapor deposition procedure. Raman data confirm that monolayer graphene is obtained. Scanning-electron microscopy images show that graphene film is continuous and completely covers Cu grains. DC reactive magnetron sputtering is applied to deposit an AlN layer. Sputtering parameters, such as power, gas ratio, total pressure, temperature, and target-to-substrate distance, are optimized to achieve preferred growth of AlN in a *c*-axis orientation. GaN layers are grown by metalorganic chemical vapor deposition with optimized conditions to overcome technical issues, including thermal expansion coefficient mismatch between layers, thermal and mechanical stability of layers, etc. X-ray diffraction (XRD) shows that the *c*-plane of AlN film (from (0002) peak in 2θ-ω scan) is preferably grown. Atomic force microscopy characterization shows step-flow features of the AlN surface, confirming high crystalline quality of the layer. XRD results also show that GaN is grown epitaxially on the AlN buffer layer. Pole figure on GaN (10-12) plane also shows six-fold symmetry features which confirms the single-crystal-like wurtzite structure is formed during growth. The direct growth of GaN on the Cu foil/tape is expandable to other flexible substrates. A new focus is put on the direct growth of GaN and AlN on a foreign flexible substrate with Cu coating, leveraging the same deposition technique. This method is applicable to any inorganic substrate with either amorphous or polycrystalline structure; and offers potential for roll-to-roll fabrication of flexible electronic and photonic devices.

STRAIN RELAXATION PROPERTIES OF OMVPE-GROWN ALINN SEMICONDUCTORS

Wei Sun, Renbo Song, Jonathan J. Wierer, Jr., Nelson Tansu

Lehigh University, PA, UNITED STATES OF AMERICA

III-Nitride semiconductor has attracted tremendous attentions in recent decades for advantages in high efficiency solid-state lighting and power electronics applications. The InGaN has been well studied for the active region synthesis in the state-of-the-art light-emitting diodes. The AlGaN also draws much interests for deep-ultraviolet (UV) and power electronics applications attributed to its direct and wide bandgap. However, the valence bands crossover in AlGaN material with higher Al-content (>57%) results in the undesired dominant transverse-magnetic-polarized transition. Recently, the AlInN material has become an emerging candidate for UV applications. By adding small amount of Indium (<20%), the bandgap of AlInN fully covers the deep-UV regime, and the dominant transverse-electric-polarized transition can be achieved with In-content of higher than ~8%. Meanwhile, the nearly lattice-matched AlInN on GaN could be achieved when the In-content is ~17%, which could eliminate the strain effect and suppress the strain induced defect and polarization field. Furthermore, the AlInN also enables the potential of strain engineering in GaN based nanostructure by slightly changing the In-content than the nearly lattice-matched condition. In this work, we performed the organometallic vapor phase epitaxy (OMVPE) of the AlInN single crystal materials with In-content from ~3% up to ~20%. Afterwards, the strain analysis was conducted using the reciprocal space mapping (RSM) in an X-ray diffraction (XRD), PANalytical Empyrean. In our work, the AlInN was grown on top of the unintentionally-doped GaN template in the Veeco P-75 reactor. The trimethylaluminum and trimethylindium were used as the group-III precursors, while the ammonia was used as the nitrogenous precursor. The growth condition was firstly optimized for the nearly-lattice matched AlInN with ~17% In-content at growth temperature of ~780°C. Then different samples were grown by changing the growth temperature from ~740°C to ~860°C targeting In-content from ~20% to ~3%. Other growth parameters maintain constant. The RSM results show that the In-content of the AlInN material changed from ~3% to ~20% with growth temperature decreased from 860 °C to 740 °C. The strain relaxation of the AlInN epilayer ranges from ~80% to ~0% with the In-content from ~3% to ~17%. Furthermore, our study shows that the tensile strain in AlInN changed to compressive strain with strain relaxation within ~3% when the In-content changed from ~11% to ~20%. The switch of the type of strain in AlInN with large In-content variation and small strain relaxation shows the potential of applying the OMVPE-grown AlInN in quantum nanostructure for strain engineering.

THREADING DISLOCATION REDUCTION IN GAN ON SI(111) BY USING THREE DIMENSIONAL ISLAND GROWTH

Shane Chang

Material Science and Engineering, TAIWAN

3D GaN island growth was first introduced under the high growth pressure in metalorganic chemical vapor deposition, followed by 2D growth to form a smooth surface. X-ray diffraction shows a high-quality GaN film can be achieved Cross-sectional results in bending of the threading dislocations (TDs) and form dislocation loops thus producing a 1.2 mm-thick GaN with a low threading dislocation density of 2.5 $x10^8$ cm^{-2}. The mechanism and the role of maskless GaN islands were studied and discussed. The maskless GaN islands not only successfully reduce the TDs in the GaN film but also obtain smooth surface morphology.

IN SITU COHERENT X-RAY SCATTERING STUDIES DURING OMVPE OF GAN

Guangxu Ju[1], Dongwei Xu[1], Matt Highland[1], Andrew Ulvestad[1], Carol Thompson[2], Jeffrey Eastman[1], Peter Zapol[1], Angel Yanguas-Gil[1], Paul Fuoss[1], Gregory B. Stephenson[1]

[1]Materials Science Div., Argonne National Lab, IL, UNITED STATES OF AMERICA,
[2]Department Of Physics, Northern Illinois University, UNITED STATES OF AMERICA

High-energy x-rays provide a powerful tool for *in-situ* time-resolved studies of materials processes such as epitaxial film growth. Their penetrating nature allows observations inside growth chambers under actual process conditions, and their short wavelength provides sensitivity to atomic-scale structure. With the continued increase in coherent flux delivered by advanced synchrotron radiation facilities, coherent x-ray techniques promise to provide new insight into materials synthesis. The fluctuations observed by coherent x-ray methods can elucidate atomic dynamics in these systems more clearly than average quantities obtained from scattering with incoherent beams. These methods can reveal the atomic rearrangements underlying crystal growth mechanisms such as step motion, island nucleation, step-edge barriers, and surface transport. We have developed a new instrument [1] that exploits this ongoing revolution in synchrotron sources, optics, and detectors to enable *in situ* studies of OMVPE growth of III-nitride materials using coherent x-ray methods. The system includes: high-resolution positioning of the sample and detector; an x-ray transparent chamber wall for incident and diffracted beam access over a wide angular range; and a sample mount with minimal thermal motion, giving the sub-micron positional stability and reproducibility needed for coherent x-ray studies. To provide fundamental understanding of OMVPE processes, the instrument enables surface x-ray photon correlation spectroscopy, microbeam diffraction, and coherent diffraction imaging of atomic-scale surface and film structure and dynamics during growth. We present examples from our initial studies of surface coherent x-ray scattering during OMVPE of GaN. We will show simulations and initial measurements of speckle dynamics in coherent scattering from dynamic surfaces, both at equilibrium in the OMVPE environment at high temperature, and during non-equilibrium crystal growth. Initial exploration of surface coherent diffraction imaging will also be discussed. Work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Division of Materials Sciences and Engineering. [1] G. Ju et al., Review of Scientific Instruments, published online (2017), DOI: 10.1063/1.4978656

BROADBAND IN SITU OPTICAL MONITORING FOR OMVPE GROWTH

George Atanasoff, Christopher J. Metting

AccuStrata, Inc., MD, UNITED STATES OF AMERICA

In the typical OMVPE growth of LED structures the non-uniformity of the central wavelength over the individual wafers as well as run-to-run and reactor-to-reactor non-repeatability are primary contributors to delayed process tuning, reduced manufacturing yield and inflated product cost. On the epitaxial level, inferior device performance results from process variations leading to variations in the chemical composition and thickness of the individual compound layers and especially in the quantum well layers. Also, being extremely thin, from optical point of view, the individual quantum well layers remain beyond the resolution of the standard optical monitoring techniques. We have developed and made commercially available an in situ LED growth broadband spectroscopic monitoring and process control system for OMVPE application. The system monitors the LED thin films as they grow in real time on the individual rotating wafers, record the signal in a broad spectral range and process the information to retrieve the most important film parameters and their distribution over a single wafer, all the wafers in a batch and multiple batches. During the epitaxial growth of the thin quantum well films, the recorded 3D spectral signal from each wafer (reflectance as function of time and wavelength) is correlated to the process parameters such as substrate temperature and precursor gas composition. We deploy a novel algorithm for a real-time pattern search in the acquired broadband spectral data to display abnormalities and differences in the deposition of the individual wafers and specifically the differences in the quantum well layers. This information can be used by the OMVPE engineer to better tune the epitaxial process, and can be integrated into the OMVPE reactor to ensure better uniformity and repeatability. Presented are the experimental results from the broadband monitoring of multiple sapphire wafers during a single LED epitaxy run and during multiple epitaxy runs. Throughout the duration of the experiment the epitaxial process has been substantially improved by gradually tightening the parameter distribution functions and optimizing the process. The presented results illustrate how the epitaxial process has been tuned to achieve better uniformity and repeatability, speed up the process tuning time and improve manufacturing yield.

CHARACTERIZING AMPOULE PERFORMANCE FOR LOW VAPOR PRESSURE PRECURSOR DELIVERY

James Maslar[1], William Kimes[1], Brent Sperling[1], William Kimmerle[2], Kyle Kimmerle[2]

[1]NIST, UNITED STATES OF AMERICA, [2]NSI, UNITED STATES OF AMERICA

Low vapor pressure organometallic compounds are widely utilized as precursors for chemical vapor deposition and atomic layer deposition processes. Such precursors are often delivered using an inert carrier gas that is passed through either a bubbler (an ampoule with a dip tube) or a vapor draw ampoule (no dip tube: the gas in and gas out ports open directly into the ampoule headspace), depending on the precursor properties and process requirements. However, it can be difficult to predict how much precursor will be delivered for a given carrier gas flow rate, or even the relationship between precursor and carrier gas flow rate. A number of factors may contribute to this difficulty, including a pressure drop between the ampoule and the pressure control location, sublimative/evaporative cooling of the precursor (i.e., cooling reduces the precursor vapor pressure and hence the amount of material entrained in the carrier gas), incomplete saturation of the carrier gas (i.e., the precursor sublimation rate is too low to permit saturation of the carrier gas for a particular residence time in the ampoule), or slow mass transport processes in the ampoule. Furthermore, the relative importance of the factors depends on the precursor, ampoule design, and process conditions. The goal of this work is to characterize ampoule performance for delivering low vapor pressure precursors, including the development of analytical and numerical models to describe the relationship between precursor and carrier gas flow rate for both bubblers and vapor draw ampoule. A variety of low vapor pressure precursors, e.g., CCTBA and PDMAT, and precursor simulants, e.g., hexadecane, were employed in this investigation. The focus was on commercial 1.5 L ampoules (with a maximum fill of 1.2 L). All ampoule models were experimentally validated using data that was obtained with custom-designed non-dispersive infrared gas analyzers located downstream of the ampoule. For selected ampoules, resistance temperature detector arrays were employed in order to characterize the liquid temperature distribution in the ampoule and level sensors were employed to confirm liquid level in the ampoule. It is expected that the development of such models can facilitate both process optimization and development of improved ampoule designs.

HIGH TEMPERATURE OMVPE REACTOR WITH REDUCED PREMATURE REACTION AND IMPROVED HEATING EFFICIENCY

Kuang-Hui Li, Hamad S. Alotaibi, Xiaohang Li

King Abdullah University of Science and Technology (KAUST), SAUDI ARABIA

AlN is crucial for important applications including UV optoelectronics. However, high quality AlN thin films on commercially viable sapphire substrates by OMVPE have been difficult to realize. Higher temperatures have been shown more favorable for reduced defect density due to enhanced Al adatom mobility,[1] which is also essential for epitaxial lateral overgrowth.[2] The impurity incorporation can be suppressed at higher temperature as well.[1] However, most but a handful of III-nitride OMVPE reactor designs can reach wafer temperatures at or above 1500 °C. EpiQuest has created a horizontal reactor with a resistive heater which can reach wafer temperatures up to 1500 °C.[3] Yet, common resistive heaters could have reliability issue at this temperature range. In addition, a few institutions have utilized vertical quartz reactors encompassed by induction heaters to obtain temperatures over 1500 °C, which are low-cost and reliable.[4,5] However in this design, the gas inlets made of metals have to have large distance from the susceptor to avoid being heated by residual alternating magnetic field above the susceptor. Because of the long precursor flow path, the configuration would lead to considerable premature reactions between NH_3 and TMAl and thus particle formation, compromising the material quality and growth efficiency. In addition, the horizontal gap between the induction heater and susceptor reduces heating efficiency because of the unused magnetic flux. In this work, we proposed a novel design to circumvent these issues.[6] By introducing a specially-shaped metal susceptor and integrating the induction heater within a vertical quartz reactor (Figure 1), we can bring down strength of the magnetic field by eight times thanks to the susceptor's shielding (Figure 2). Consequently, the gas inlets in the form of a showerhead, can be brought as close as 5-20 mm away from the susceptor to minimize the premature reactions with a small carrier gas velocity. Additionally, most of the magnetic flux is utilized for susceptor heating, hence improving the heating efficiency considerably. Key parameters including heat transfer, induction heating, flow simulation, and chemical reactions have been modelled by SOLIDWORKS, COMSOL Multiphysics, and STR VR NE. More results will be discussed in the conference presentation. 1. M. Imura et al., J. Cryst. Growth (2008). 2. M. Imura, et al., Appl. Phys. Lett. (2006). 3. http://www.epiquest.co.jp/. 4. J. R. Creighton et al., J. Cryst. Growth (2016). 5. http://agnitron.com/. 6. US provisional application 62396669.

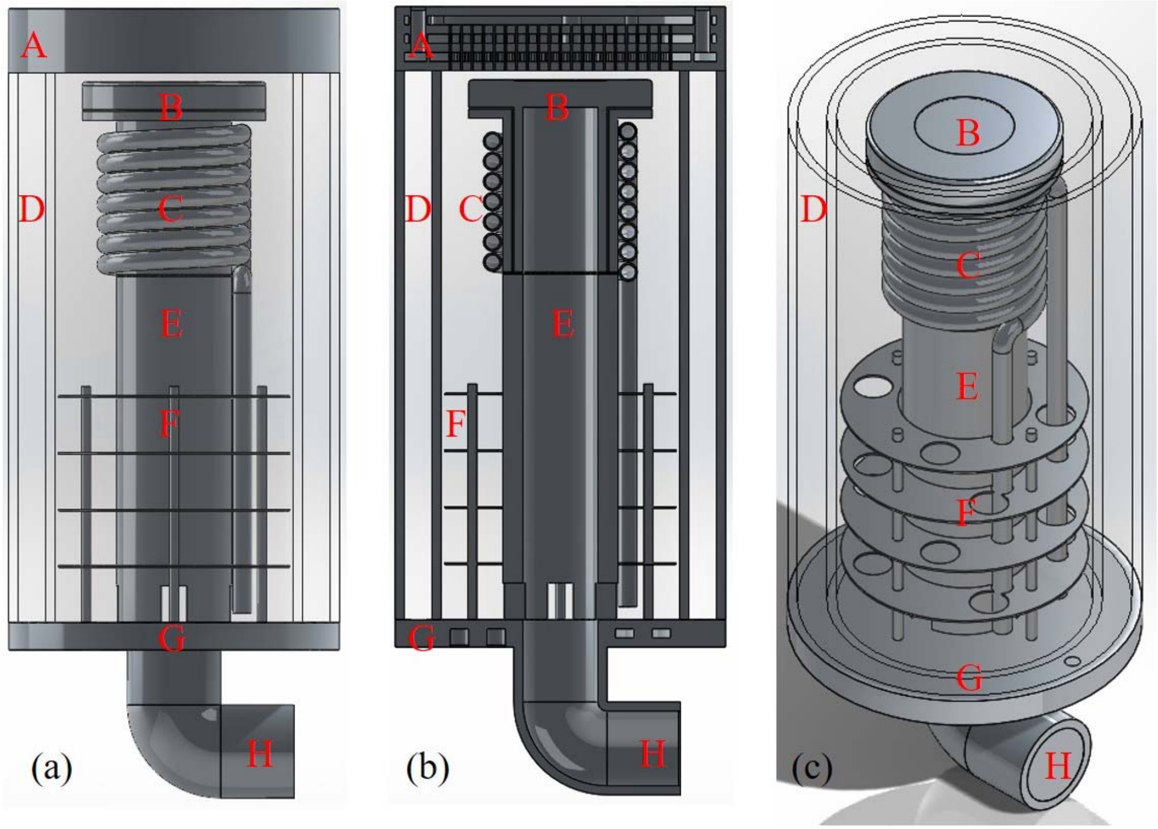


Figure 1. (a) Side view and (b) cross-sectional view of the reactor, and (c) isometric view of the reactor without the showerhead, where A, B, C, D, E, F, G, and H represent showerhead, susceptor, induction coil, double quartz wall, supporter, heat shield, bottom flange, and exhaust, respectively.

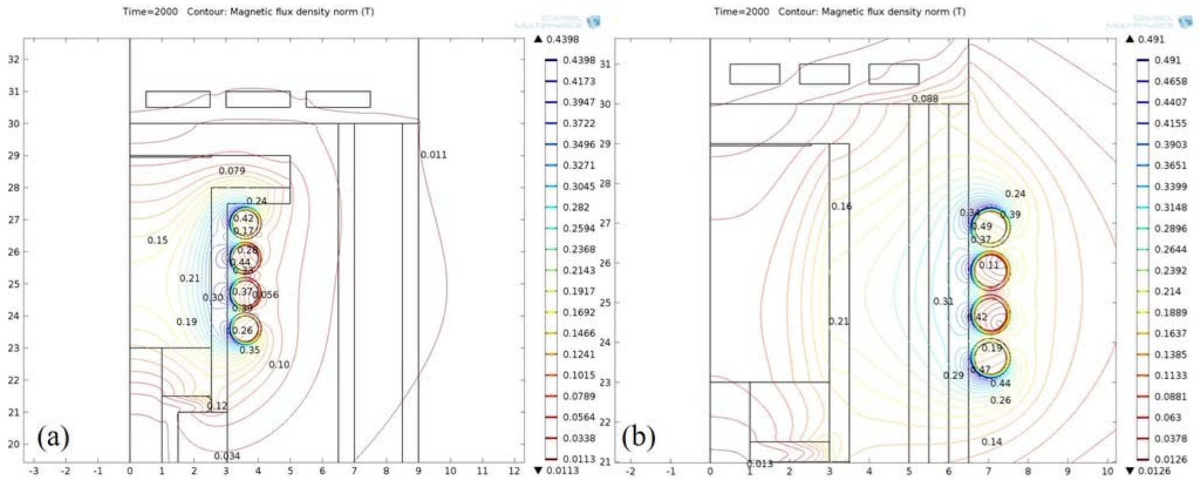


Figure 2. (a) Magnetic flux density distribution of the reactor with a 21 kW induction heater built inside the reactor, as shown in Figure 1. (b) Magnetic flux density distribution of a conventional reactor with a 35 kW induction heater built outside the reactor.

EPITAXIAL GROWTH OF GA_2O_3 BY MOCVD USING OXYGEN: EXPERIMENTAL STUDY AND MODEL VERIFICATION

Maxim Bogdanov[1], Anna Lobanova[1], Roman Talalaev[1], **Alex Galyukov**[2], Fikadu L. Alema[3], Brian Hertog[3], Andrei Osinsky[3]

[1]STR Group, Inc. – Soft-Impact, Ltd., RUSSIAN FEDERATION, [2]STR US, Inc., VA, UNITED STATES OF AMERICA, [3]Agnitron Technology, Inc., MN, UNITED STATES OF AMERICA

In recent years gallium oxide (Ga_2O_3) wide-bandgap semiconductor has attracted a lot of interest as a new material for electronic applications. Recently, Ga_2O_3 films grown by MOCVD with growth rate of up to 1 μm/hr in vertical rotating disk reactor were demonstrated. However, pronounced drop of growth rate with pressure pointed to significant effect of parasitic reactions [1]. It is mentioned that trimethylgallium (TMGa) precursor exhibits high reactivity with molecular oxygen (O_2) [2]. Model of Ga_2O_3 growth by MOCVD has been developed to get a better understanding of the physical phenomena underlying the growth. The model accounts for TMGa gas-phase decomposition, TMGa interaction with oxygen, formation of $DMGa\text{-}O\text{-}CH_3$ complex and $(DMGa\text{-}O\text{-}CH_3)_2$ dimer as well as surface chemical reactions leading to deposition. In the present work, we demonstrate growth of Ga_2O_3 epilayers from O_2 and TMGa using a custom designed low pressure close-coupled showerhead reactor. Argon is used as a carrier gas. The effect of the process conditions on the growth rate has been analyzed by variation of the growth pressure, temperature and TMGa precursor flow rate. The growth rate dependence on growth temperature (850-950°C) was found to be negligible. So, the decomposition of Ga_2O_3 in oxygen at given conditions is not pronounced. At the same time, the growth rate has been found to be highly sensitive to the growth pressure, rapidly decreasing with the increase of pressure from 40 to 90 Torr. This effect is attributed to the generation of $[DMGa\text{-}O\text{-}CH_3]_2$ dimers that are assumed not to contribute to the growth, which is accelerated with increasing the total pressure. Increase of the growth rate with TMGa flow rate was found to be slightly sublinear, which can also be attributed to increasing dimer generation. The growth rate as high as 10 μm/hr is obtained at T=900°C. References [1] Fikadu L. Alema, O. Ledyaev, R. Miller, B. Hertog, A. Osinsky, W. V. Schoenfeld, ICMOVPE XVIII, abstracts, 2016. [2] S. Yamashita, K. Watanuki, H. Ishii, Y. Shiba, M. Kitano, Y. Shirai, S. Sugawa, and T. Ohmi, Journal of The Electrochemical Society, 158, 2 (2011) H93.

PROGRESS IN CZOCHRALSKI CRYSTAL GROWTH OF DISLOCATION FREE SILICON, AND POTENTIAL OF CONTINUOUS CZOCHRALSKI FOR NEXT GENERATION SILICON

Joel K. Kearns

NASA John H. Glenn Research Center, OH, UNITED STATES OF AMERICA

Czochralski growth of dislocation free single crystal silicon continues to progress in different directions for different end wafer markets. Semiconductor silicon is focused on diameter scale up to 450mm (and potentially 675mm) diameter crystals, while maintaining micro-defect control and reducing costs. Solar “mono” silicon is focused on reducing cost while improving bulk properties for photovoltaic conversion efficiency. Crystals for optical and mechanical applications are also increasing in diameter even as silicon directionally solidified in a crucible offers an alternative. The Continuous Czochralski (CCz) method of crystal pulling has been developed by at least two manufacturers. The method can be used economically to produce crystals with either low or high resistivity values. There are several benefits of the CCz approach for single crystal silicon production, in particular as crystal diameters are increased. The oxygen concentration can be decoupled from crucible size and crystal diameter, and relatively low oxygen concentrations obtained over long crystal lengths without use of a magnet to change the melt flow conditions. The crystal length is determined by “height of building” (length of pull chamber) instead of crucible size. This allows longer crystals to be made in a run without increasing the size and cost of the consumables or the production equipment. The current status of silicon Czochralski crystal growth process development for these three major end wafer markets will be reviewed. Recent advances in CCz crystal growing will be described, as well as examples of crystal bulk property attributes produced by CCz process, drawn from the public domain literature. The benefits of applying CCz to crystal diameters over 300mm will be described.

TOWARDS GRAPHITE-FREE HOT ZONE FOR DIRECTIONAL SOLIDIFICATION OF SILICON

Natasha Dropka[1], Iryna Buchovska[1], Iris Herrmann-Geppert[1], Frank M. Kießling[1], Ulrich Degenhardt[2]

[1]Leibniz Institute for Crystal Growth (IKZ), GERMANY, [2]FCT Ingenieurkeramik GmbH, GERMANY

In the solar cells production, there is a compelling need for a cost-effective technology that can improve the ingot quality and increase the yield. For a progress towards these goals, it is important e.g. to control the level of carbon impurities in the ingot in order to prevent wire breakage during wafer slicing. In a typical industrial furnace, solar-grade polysilicon is loaded in a nitride-coated quartz crucible, which is placed inside a graphite susceptor, and then covered with a graphite plate. These parts are surrounded by graphite heaters and carbon-based insulation. All materials present in the hot-zone could be the source of ingot contamination. So far, the reduction of impurities was a subject of many scientific studies that proposed solutions for crucibles, coating and feedstock of various purity and price. Nevertheless, only a few studies were devoted to the search for an alternative material to graphite that will prevent the formation of SiC from the reaction between SiO, which evaporates from the melt or is coming from the silica crucible, and graphite parts. In the same time, this new material should sustain the high working temperatures in oxidative environment, has sufficient low concentration of metallic impurities (e.g. Fe), is free of health risks and has sufficient mechanical strength/durability. Up to now, the proposed layers of SiC, W, Mo and their alloys [1,2] on the graphite crucible cover only partly meet the heavy constrains. Therefore, there is still urgent need to find better solutions. The present study is focused on identifying carbon-free massive ceramic material for the crucible cover and support. For this purpose, we selected three advanced ceramics, adjusted a design of the crucible support and growth process to the ceramics material properties, and finally we compared crystals grown in them with ingots from the standard graphite design. Particularly, we studied directionally solidified n-doped Si ingots of G0 and G1 size. All Si ingots were compared with respect to O- and C-content, metal impurities and lifetime. In parallel, the composition, structure and mechanical properties of selected ceramic materials were determined. Furthermore, experimental studies were closely accompanied with numerical simulations. The first very encouraging results will be presented and the strengths and weaknesses of various ceramics in comparison to graphite will be discussed. References [1] http://www.schunk-carbontechnology.com [2] B. Gao et al., J. Cryst. Growth 318 (2011), 255-258. Fig.1 Graphite and ceramic crucible covers and supports: a) G1 size, b) G0 size.

NUMERICAL SIMULATION OF THE THERMAL AND FLOW FIELDS FOR A CZOCHRALSKI SILICON GROWTH WITH THE SYMMETRIC OR ASYMMETRIC CUSP-SHAPED MAGNETIC FIELD

Thi Hoai Thu Nguyen[1], Jyh Chen Chen[1], Chieh Hu[1], Chun Hung Chen[2]

[1]National Central University, TAIWAN, [2]Research and Development Division, GlobalWafers Co., Ltd., TAIWAN

In this study, the quasi-steady numerical simulations are used to investigate the effects of different magnetic ratios, which defined as the ratio of the lower coil current to the upper coil current, on the velocity, temperature, and oxygen concentration distribution in the silicon melt and the crystal-melt interface shape during the Czochralski growth of a 200 mm silicon crystal. The effects of an asymmetric cusp-shaped magnetic field on the Voronkov ratios based on analyzing the growth rate and temperature gradient are also presented. Moreover, it is well known that to avoid constitutional super-cooling the temperature gradient in the crystal (or the melt) must exceed the critical value. Using an asymmetric magnetic field may control the temperature gradient in the crystal (or the melt) and hence, this will affect the constitutional super-cooling during the growth process. This will be discussed with applying the different magnetic ratios.

INFLUENCE OF CONTAINMENT ON THE GROWTH OF GERMANIUM-SILICON IN MICROGRAVITY

Martin Volz[1], Konstantin Mazuruk[2], Arne Croell[2], Tina Sorgenfrei[3]

[1]NASA Marshall Space Flight Center, AL, UNITED STATES OF AMERICA, [2]University of Alabama in Huntsville, AL, UNITED STATES OF AMERICA, [3]University of Freiburg, GERMANY

A series of $Ge_{1-x}Si_x$ crystal growth experiments are planned to be conducted in the Low Gradient Furnace (LGF) onboard the International Space Station. The primary objective of the research is to determine the influence of containment on the processing-induced defects and impurity incorporation in germanium-silicon alloy crystals. A comparison will be made between crystals grown by the normal and “detached” Bridgman methods and the ground-based float zone technique. “Detached” or “dewetted” Bridgman growth is similar to regular Bridgman growth in that most of the melt is in contact with the crucible wall, but the crystal is separated from the wall by a small gap, typically of the order of 10-100 microns. A meniscus bridges this gap between the top of the crystal and the crucible wall. Theoretical models indicate that an important parameter governing detachment is the pressure differential across this meniscus. An experimental method has been developed to control this pressure differential in microgravity that does not require connection of the ampoule volume to external gases or changes in the temperature profile during growth. Experiments will be conducted with positive, negative or zero pressure differential across the meniscus. Characterization results of ground-based experiments, including etch pit density, synchrotron white beam X-ray topography and double axis X-ray diffraction will also be described.

DONOR IMPURITY INCORPORATION DURING LAYER GROWTH OF ZN II-VI SEMICONDUCTORS

Douglas Barlow

Santa Fe College, FL, UNITED STATES OF AMERICA

Maximum donor concentration in Zn II-VI semiconductors during layer growth is studied using a standard model from statistical mechanics. Here the driving force for incorporation is an increase in entropy upon mixing of the donor impurity into the available anion lattice sites in the host binary. A formation energy opposes this increase and thus equilibrium is attained at some maximum concentration. Considering the halogen donor impurities within the Zn II-VI binary semiconductors ZnO, ZnS, ZnSe and ZnTe, a heat of reaction obtained from reported diatomic bond strengths is shown to be directly proportional to the log of maximum donor concentration. The formation energy can then be estimated and an expression for maximum donor concentration derived. Values for the maximum donor concentration with each of the halogen impurities, within the Zn II-VI compounds, are computed. This model predicts that the halogens will serve as donors in these compounds in order of increasing effectiveness as: F, Br, I, Cl. Finally, this result is taken to be equivalent to an alternative model where donor concentration depends upon impurity diffusion and the conduction band energy shift due to a depletion region at the growing crystal's surface. From this we are able to estimate the diffusion activation energy for each of the impurities mentioned above. Comparisons are made with reported values and relevant conclusions presented.

AXIAL INFLECTION POINT TEMPERATURE PROFILES FOR THE ENGINEERING OF CONVEX CRYSTAL GROWTH INTERFACES IN BRIDGMAN SYSTEMS

Jeffrey H. Peterson, Jeffrey J. Derby

University of Minnesota, MN, UNITED STATES OF AMERICA

We present new insight on furnace designs that promote macroscopically convex interfaces in Bridgman crystal growth methods. Specifically, we posit that axial inflection points in the centerline thermal profile will produce radial heat flows consistent with conditions needed for convex interface shapes. We present a mathematical justification of this idea and demonstrate its efficacy through sample simulations. It has long been understood that a solid-liquid interface that is slightly convex with respect to the crystal is desirable for high-quality growth in directional solidification. However, such interface shapes do not occur for most materials grown in classical Bridgman systems. Recently, Zhang et al. [1] introduced a bell-curve thermal profile for an electrodynamic gradient freeze (EDG) furnace and showed, via computations, that it resulted in inwardly-directed radial heat fluxes near the growth interface that promoted convex interface shapes. We generalize these ideas in a mathematical framework that infers radial heat fluxes and interface shapes during growth from the axial thermal profile in the furnace. More specifically, we put forth an assertion the growth interface will tend to be convex when the temperature profile contains an axial inflection point (i.e., with d2T/dz2 = 0) that produces negative curvature (d2T/dz2 < 0) in the axial profile above the melting point, a generalization of conditions that were satisfied by our prior bell-curve profile. Additionally, we have used these principles in the design of a 4-zone Bridgman furnace for the growth of mixed halide scintillators, and we show through simulation results that the axial inflection point profile can lead to significant improvements in interface shape. [1] Nan Zhang, Andrew Yeckel, and Jeffrey J. Derby, "Maintaining convex interface shapes during electrodynamic gradient freeze growth of cadmium zinc telluride using a dynamic, bell-curve furnace profile", Journal of Crystal Growth 355(1), pp. 113 – 121 (2012). -------------- This work has been supported by the Department of Energy, NNSA, under DE-NA0002514, and no official endorsement should be inferred.

STRAIN TUNING OF ELECTRONIC GROUND STATE IN CA_2RUO_4 EPITAXIAL THIN FILMS

Hari P. Nair[1], Jacob P. Ruf[2], Yang Liu[3], Benjamin Grisafe[4], Nikhil Shukla[4], Celesta S. Chang[5], Qiang Han[6], Andrew Millis[6], David A. Muller[5], Suman Datta[4], Kyle Shen[2], Darrell G. Schlom[7]

[1]Department of Materials Science and Engineering, Cornell University, UNITED STATES OF AMERICA, [2]Department of Physics, Cornell University, UNITED STATES OF AMERICA, [3]Department of Physics, Zhejiang University, CHINA, [4]Department of Electrical Engineering, University of Notre Dame, UNITED STATES OF AMERICA, [5]Applied and Engineering Physics, Cornell University, UNITED STATES OF AMERICA, [6]Department of Physics, Columbia University, UNITED STATES OF AMERICA, [7]Kavli Institute at Cornell for Nanoscale Science, UNITED STATES OF AMERICA

Sizable strain tuning of a metal-insulator transition (MIT) has been a holy grail of condensed matter physics for decades. Bulk single crystal Ca_2RuO_4 undergoes an MIT at 357 K and becomes an antiferromagnet with a Neel temperature of 110 K. By leveraging a small tensile strain of 0.3 % in our molecular beam epitaxy grown Ca_2RuO_4 thin films, we have pushed this MIT to above 600 K compared to 357 K for bulk single crystals. Moreover, the MIT can be electrically triggered making Ca_2RuO_4 epitaxial thin films a very attractive candidate for Mott-based electronics, which require devices to operate above 400 K. On the other hand with a compressive strain of 1.6 % we have been able to suppress MIT to ~ 200 K. With increasing compressive strain, at 2.9 %, the insulating ground state is completely suppressed and the film remains metallic down to 4 K. Preliminary calculations confirm our experimental findings that the electronic ground state in Ca_2RuO_4 is extremely sensitive to epitaxial strain. Until now, such a dramatic effect of strain on the ground state electronic properties has not been observed in any other material system making Ca_2RuO_4 an excellent candidate for further explorations of strain-induced tuning of electronic and magnetic properties. To date there have been very few demonstrations of Ca_2RuO_4 epitaxial thin films. We will discuss how we determine the optimal growth conditions for Ca_2RuO_4 epitaxial films using the Ellingham diagrams calculated from bulk Ca_2RuO_4 thermodynamic data. The growth window for epitaxial films of Ca_2RuO_4 is narrow both in temperature and oxygen pressure, zeroing in on this narrow growth window is critical to achieve high quality epitaxial thin films of Ca_2RuO_4. We will also briefly touch upon some of the challenges involved in the growth of Ca_2RuO_4 on certain substrates, likely due to interface reactions and how we can surmount this with judicial use of appropriate buffer layers.

SUBSTRATE 'THERMINATION' AND THE ROLE OF SURFACE RECONSTRUCTION FOR THE EPITAXY OF PEROVSKITE OXIDES

Wolfgang Braun, Maren Jäger, Jochen Mannhart

Max Planck Institute for Solid State Research, GERMANY

Using direct, long-wavelength laser irradiation from the back side, we have developed a laser heating system to heat oxide substrates such as $SrTiO_3$ to temperatures well beyond 1350 °C. This procedure allows us to prepare substrates for epitaxy by high-temperature annealing directly before growth, rather than by using traditional ex-situ chemical termination. The resulting surfaces obtained by this *in-situ* process show the same terrace structure and surface reconstruction as found after chemical preparation. Also, the RHEED oscillations measured during homoepitaxial growth on these substrates are indistinguishable from those obtained from growth on chemically etched substrates. The substrates may be cooled with initial rates as high as 80 K/s by turning off the laser beam, allowing us to take snapshots of annealing and growing surfaces at different times during the procedure. Unstable homoepitaxy we find on mixed surface reconstructions involving areas of different surface structures on the same terraces. Stable homoepitaxy we achieve on single, uniform surface reconstructions.

MAGNETISM AT INTERFACES IN COMPLEX OXIDES GROWN USING MOLECULAR BEAM EPITAXY

Anand Bhattacharya

Materials Science Division, Argonne National Laboratory, IL, UNITED STATES OF AMERICA

Interfaces in complex oxide heterostructures present new opportunities to tailor novel magnetic properties. Using molecular beam epitaxy based approaches, we seek to create model systems where we can explore the effects of interfacial charge transfer, electronic reconstructions and exchange interactions on magnetic order in these systems - and ultimately tailor novel magnetic states by design. I will present some recent results on non-collinear magnetism and spin transport across oxide interfaces. A central question regards the role of defects in the magnetic properties of these interfacial systems, particularly in light of what we understand about exchange interactions, which are sensitive to the coordination between nearest neighbors. In this talk I will try to frame the question, and point to experiments that constrain possible answers.

TWO-INCH, HIGH TRANSPARENCY ALUMINUM NITRIDE SINGLE CRYSTAL GROWTH FOR COMMERCIAL APPLICATIONS

Leo J. Schowalter, Robert Bondokov, Jianfeng J. Chen, Murugesu Yoganathan, Takashi Suzuki, Shailaja Rao, Toru Kimura, Keisuke Yamaoka

Crystal IS, Inc., UNITED STATES OF AMERICA

Aluminum nitride (AlN) crystals are used by Crystal IS, Inc., to make single crystal AlN wafers which are then used in the commercial manufacturing of UVC LEDs. The AlN crystals are grown using a proprietary physical vapor transport (PVT) method where a sublimation-recondensation approach is utilized. The AlN source material sublimes and decomposes into Al atoms and N_2 molecules. These species are then transported to the AlN seed where they incorporate into the growing crystal along the c-axis. Increasing the crystal dimensions demands careful thermal gradients tailoring in order to lower the thermally induced stresses. Currently, AlN single crystals with diameters > 2 inch are grown using the method described above and larger diameters are possible with appropriate furnace design. The accessibility of AlN single-crystal material will continue to drive further development of novel electronic and opto-electronic applications due to its distinctive semiconductor, thermo-physical, and mechanical properties. Large diameter, bulk AlN crystals could also be beneficial for production of non-polar and semi-polar substrates which are used to reduce the internal electric fields due to polarization in some novel applications. The wafers show excellent quality as measured by XRD rocking curves with FWHM < 30 arcsec. These wafers are then used to fabricate high performance, long lifetime UVC LEDs for air purification, water disinfection, and environmental sensing. Commercially available SMD product (Klaran™) achieve germicidal power outputs up to and exceeding 30 mW at a nominal wavelength of 265nm with drive currents up to 400 mA. While IQE and current injection efficiency are important factors in device efficiency; the wall plug efficiency in our devices is now dominated by the photon extraction efficiency and the substrate transparency is a key part of the photon extraction efficiency. The substrate purities and growth regimes are linked to high UV transmission. In particular, reducing the peak in the absorption at 265nm requires low carbon concentration while oxygen impurities also need to be tightly controlled to reduce UV absorption below 300nm. However, the thermal treatment of the crystal boule also changes the UV absorption dramatically. For instance, rapid cooling of the boule causes a UV absorption band between 300 and 350 nm due to an increase in the point defect concentration at the higher cooling rate [1]. Thus, the absorption of the AlN substrates can be changed to match the application by varying the cooling profile. [1] S. B. Schujman, et al., US patent 9,447,519.

SUBLIMATION GROWTH AND CHARACTERIZATION OF ERBIUM NITRIDE CRYSTALS

Hayder A. Alatabi, Balabalaji Padavala, James H. Edgar

Kansas State University, UNITED STATES OF AMERICA

Erbium nitride (ErN) is a transition metal nitride notable for its magnetic and optical properties. Here we report on its growth a non-native substrate, tungsten foil, via physical vapor transport, and characterization. The source material was erbium metal that was converted to ErN by heating in nitrogen. Subsequently, it was sublimed to form the ErN crystals. The operating conditions were 1600^{o}C-1780^{o}C and 150-510 torr in pure nitrogen. The growth rate increased exponentially with temperature with an activation energy of 508 KJ/mol, and inversely with pressure. X-ray diffraction revealed the ErN preferentially adopted a (100) orientation, the same as the dominant orientation of the tungsten sheet. The lattice constant was 4.853 Å. The crystal shapes and sizes were dependent on the temperature, as revealed by SEM and optical microscopy. The ErN crystals were highly faceted, bound by (100) and (111) crystal planes. Nitrogen-rich conditions produced transparent crystals.

FROM X-RAYS TO NEUTRONS (AND BEYOND): CASE STUDIES OF COMPLEX VANADATES GROWN FROM MICRONS TO CENTIMETERS (AND BEYOND)

Colin Mcmillen[1], Vasile O. Garlea[2], Michael A. Mcguire[2], Liurukara Sanjeewa[1], Joseph Kolis[1]

[1]Clemson University, SC, UNITED STATES OF AMERICA, [2]Oak Ridge National Laboratory, UNITED STATES OF AMERICA

The definition of “crystal growth” varies greatly among different members of the scientific community. To a crystallographer, crystals “grown” to the order sub-millimeter sizes can produce a wealth of structural information. To the physicist studying the magnetic structures of single crystals, crystal growth may entail reaching multi-millimeter sizes. For certain physical properties measurements or device prototyping the definition of crystal growth, well, grows. Regardless of what one identifies as the target size for a crystal, it usually requires a concerted and rational scientific effort to reach, while for some systems, just preparing any crystals at all can be quite a feat. This presentation will highlight several case studies of complex vanadate crystals where hydrothermal crystal growth has been used to systematically obtain large single crystals. Achieving certain crystal growth benchmarks in these systems has been a critical step enabling the detailed study of structure-property relationships. The vanadates display a diverse structural chemistry, sometimes including polar structures, triangular magnetic lattices and phase transitions. This study begins to clarify the approach needed to identify interesting structural features and then advance from initial synthesis to bulk crystal growth.

POSSIBLE PRESENCE OF AL-GA COMPLEX IN THE $CA_3TA(GA,AL)_3SI_2O_{14}$ MELT AND ITS PARTITIONING DURING GROWTH FROM THE MELT

Satoshi Uda, Shuhei Sakano, Chihiro Koyama, Junpei Okada

Tohoku University, JAPAN

$Ca_3TaGa_3Si_2O_{14}$ (CTGS) is a langasite-type crystal with $A_3BC_3D_2O_{14}$ structure. It has been remarked as a promising candidate for the high-temperature pressure sensor installed in the cylinder engine of automobiles. This is because CTGS is an ordered crystal and the addition of Al into CTGS is beneficial to achieving larger piezoelectric constant and lower electronic conductivity at the operating temperature higher than 400 ˚C. In this paper, we discuss the possible presence of an octahedral structure in the melt in association with the partitioning of Al into CTGS. Al could enter either B, C or D sites when simply taking account of its ionic radius. Consequently, Al would replace Ga and Si simultaneously and its distribution in the crystal might not be homogeneous. However, by considering the possible occupation of Al in crystal sites of CTGS, which satisfies the non-negatvie degrees of freedom [1] in each site, C site is found to be the only space for Al to enter by replacing Ga. Al could entirely replace Ga. Then Al-doped crystals with $Ca_3Ta(Ga_{1-x}Al_x)_3Si_2O_{14}$ (CTGAS) were grown via a μ-PD method by varying x from 0.0 to 1.0 and consuming the whole melt. Growths with $x \geq 0.8$ were not successful. Distributions of all five elements in these crystals ($0<x<0.8$) were measured with an EPMA along the growth axis. All of them show constant through the whole crystal and their values are equal to those of the source materials, indicating that their effective partition coefficients, k_{eff}, are unity. Since the growth rate was 5mm/h, which was not large enough for the solutes to become saturated at the interface to make their k_{eff} unity, their equilibrium partition coefficients, k_0, including those of Al and Ga need to be unity regardless of the Al/Ga ratio in C site (Figure 1). On the other hand, the melting temperature rises with the Al content, indicating that k_0 of Al is larger than unity. This inconsistency will be solved when thermodynamically considering the possible presence of a 'C-site like' structure in the melt lumping Al and Ga together. This 'C-site like' structure may be partitioned into crystal with its k_0 of unity to become C-site in CTGS (Figure 2). [1] S. Uda, Chapter 4 in Handbook of Crystal Growth, Vol. IA, 2nd Ed. (Elsevier, 2014), T. Nishinaga Ed.

GROWTH OF CORUNDUM CRYSTALS FOR CALIBRATION STANDARDS USED IN DETERMINING GEOGRAPHICAL ORIGIN OF NATURAL RUBIES AND SAPPHIRES

Zachary Cole[1], Jennifer Stone-Sundberg[2], Randy W. Equall[1], Tim Thomas[3], John Emmett[4]

[1]FLIR - Scientific Materials, UNITED STATES OF AMERICA, [2]Crystal Solutions, OR, UNITED STATES OF AMERICA, [3]PDX Photonics, OR, UNITED STATES OF AMERICA, [4]Crystal Chemistry, WA, UNITED STATES OF AMERICA

Corundum, like many other transparent gemstones, is inherently colorless if pure. Isovalent and aliovalent transition and alkaline earth metal impurities that substitute for Al^{3+} into the lattice during geologic formation are key in producing the resulting color and vary from one geographic location to another. Having accurate quantitative information on the levels of these impurities within the lattice is essential to correctly ascribe cause of color, and can serve as a chemical 'fingerprint' correlating directly to a specific geographic origin. Here we report on the Czochralski crystal growth of corundum doped with multiple transition and alkaline earth metals, developed as laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) calibration standards to aid in determining the geographic origin of natural rubies and sapphires. Simultaneous and predictable incorporation of Mg, Ti, V, Cr, Fe and Ga was achieved, but complicated by charge compensation dynamics, multiple allowed valence states, and evaporation of Fe and Ga. Distribution coefficients are reported for Mg, Ti, V, and Cr.

PROPERTY MODIFICATION OF RELAXOR-PT CRYSTALS BY ACCEPTOR AND DONOR DOPANTS

Jun Luo[1], Sam Taylor[1], Fei Li[2], Shujun Zhang[3], Tom Shrout[2], Wes Hackenberger[1]

[1]TRS Technologies, Inc., UNITED STATES OF AMERICA, [2]Material Research Lab, Pennsylvania State University, UNITED STATES OF AMERICA, [3]Australian Institute of Innovative Materials, University of Wollongong, AUSTRALIA

Relaxor-PT (relaxor-$PbTiO_3$) ferroelectric single crystals have attracted much attention since later 1990s. It was found that these crystals exhibit extremely high electromechanical performance when they lie near the morphotropic phase boundary (MPB) composition in the rhombohedral phase and are poled along the non-polar, [001] orientation. Sponsored by the Office of Naval Research (ONR), TRS has commercialized PMN-PT ($Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$) and PIN-PMN-PT ($Pb(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$) crystals and the 100mm diameter crystals are currently in production. The motivation of adding either acceptor or donor dopants into these crystals is to enhance their performance for curtain types of applications. For the ceramic counterparts of these crystals, PZT ($PbZrO_3$-$PbTiO_3$) piezoelectric ceramics, the different types of dopants successfully made the materials either “harder” (reduced dielectric and mechanical loss by adding acceptors) or “softer” (increased dielectric constant and elastic compliance by adding donors). In this work, TRS grew a series of doped relaxor-PT crystals by a multi-crucible vertical Bridgman method to develop “harder” and “softer” piezoelectric crystals. For the high-power transduction and actuation applications, acceptors, such as Mn, Mn+F, Co, Fe, Ni, Al, K, Cu etc, were added into PIN-PMN-PT crystals. Systematic property measurement indicated that Mn has the strongest “hardening” effect while Fe, Co and Ni may also have “hardening” effect but far less significant. TRS has also identified a donor-type dopant recently, which may dramatically increase dielectric constant of both PMN-PT and PIN-PMN-PT crystals for the transduction applications where either crystal composites or arrays are desirable for the devices. In this presentation, Bridgman growth and property measurement of the above doped relaxor-PT crystals will be discussed in details.

BASIC AMMONOTHERMAL GROWTH OF BULK GAN IN MOLYBDENUM CAPSULES

Siddha Pimputkar[1], James S. Speck[2], Shuji Nakamura[2]

[1]Lehigh University, PA, UNITED STATES OF AMERICA, [2]University of California, Santa Barbara, CA, UNITED STATES OF AMERICA

Gallium nitride (GaN) is a wide bandgap semiconductor which has received widespread attention as it has enabled the development of short wavelength (UV, blue) optical emitters and promises a new generation of highly efficient power electronic devices for power conversion. A common desire in the III-N community is the widespread availability of low defect density substrates of arbitrary orientation to improve on optoelectronic emitters and enable higher breakdown voltage electronic devices. The ammonothermal method [1] is a bulk, single crystal growth method which has already demonstrated growth of high structural quality boules greater than 2 inches in diameter, though with insufficient growth rates to make it truly economically viable. Basic ammonothermal growth of GaN benefited from the use of a silver capsule to improve purity and growth rates.[2] As part of the quest to determine the origin of growth rate improvements, pure molybdenum capsules were fabricated as they were found to be stable under typical ammonothermal conditions.[3] Development of molybdenum capsules lead to growth of high purity GaN of comparable purity to silver capsule growths,[4] with indications of possible oxygen gettering effects by the capsule (Fig. 1). The transparent crystals (Fig 2.) exhibit broadband, sub-bandgap optical absorption due to phonon assisted free carrier absorption [5], though visually lack the characteristic orange or yellow coloration due to hydrogenated gallium vacancies [6] suggesting a reduction in their concentration. Growth rates were not enhanced over unlined NiCr superalloy autoclave growths as was observed for silver capsule growths. Possible explanations are provided by analyzing the chemical composition of the supercritical ammonia solution. **Fig 1.** Oxygen impurity levels as determined by SIMS for GaN boules based on growth zone. Grey bar represents levels measured in the GaN source. **Fig 2.** Transmitted light images of as-grown boules: a) (11-22) and b) (0001) oriented boules. Total thickness 0.8 mm and 0.6 mm, respectively. [1] D. Ehrentraut, M. Bockowski, Handbook of Crystal Growth - Bulk Crystal Growth, Elsevier, 2015: pp. 577–619. [2] S. Pimputkar, et al., *J. Cryst. Growth*. **403** (2014) 7–17. doi:10.1016/j.jcrysgro.2014.06.017. [3] S. Pimputkar, et al., *J. of Supercritical Fluids*. **110** (2016) 193–229. doi:10.1016/j.supflu.2015.10.020. [4] S. Pimputkar, et al., *J. Cryst. Growth*. **456** (2016) 15–20. doi:10.1016/j.jcrysgro.2016.07.034. [5] S. Pimputkar, et al., *J. Cryst. Growth*. **432** (2015) 49–53. doi:10.1016/j.jcrysgro.2015.09.016. [6] S. Suihkonen, et al., *Appl. Phys. Lett.* **108** (2016) 202105. doi:10.1063/1.4952388.

THE SODIUM FLUX TECHNIQUE FOR BULK GALLIUM NITRIDE

Paul M. Von Dollen[1], Mohammed Abo Alreesh[2], Siddha Pimputkar[3], Hamad Albrithen[4], Shuji Nakamura[1], James S. Speck[1]

[1]University of California, Santa Barbara, CA, UNITED STATES OF AMERICA, [2]University of California, Santa Barbara, UNITED STATES OF AMERICA, [3]Lehigh University, PA, UNITED STATES OF AMERICA, [4]King Adbulaziz City for Science and Technology, SAUDI ARABIA

Though there are several demonstrated techniques to produce bulk crystals of gallium nitride (GaN), none has proven capable of large-scale industrial implementation. The sodium flux method, [1-3] which involves precipitation of GaN from a sodium-gallium melt supersaturated with nitrogen, offers relatively mild process conditions while maintaining high crystal quality. Typical sodium flux growth pressures (<6 MPa) enable use of low-cost and scalable reactors while elemental precursors obviate the need for a discrete feedstock production process. Current major challenges for the sodium flux method include control of GaN nucleation as well as low growth rates. Our approach has sought to address these challenges through a novel internally-heated reactor and capsule system. Two features of this design are the ability to control the corrosive sodium vapor[4] and development of method to monitor growth *in situ* via the gas phase (Figure 1)and "fingerprint" events such as widespread GaN polynucleation on the crucible walls.[5] Recent sodium flux crystal growth results using our novel system and carbon as an additive for polynucleation suppression[6] include +*c* plane growth rates in excess of 50 μm/hr (Figure 2) and measured oxygen impurity levels <10^{18} atoms/cm^3. These

results indicate our system and approach are capable of producing high quality GaN.

References 1. Yamane, H., et al., *Preparation of GaN Single Crystals Using a Na Flux.* Chemistry of Materials, **9**(2): p. 413-416. (1997) 2. Mori, Y., et al., *Growth of GaN Crystals by Na Flux Method.* ECS Journal of Solid State Science and Technology, **2**(8): p. N3068-N3071. (2013) 3. Kawamura, F., et al., *Study of the Metastable Region in the Growth of GaN Using the Na Flux Method.* Journal of Crystal Growth, **311**(22): p. 4647-4651. (2009) 4. Von Dollen, P., et al., *A New System for Sodium Flux Growth of Bulk GaN Part I: System Design.* Journal of Crystal Growth, **456**: p. 58-66. (2016) 5. Von Dollen, P., et al., *A New System for Sodium Flux Growth of Bulk GaN Part II: in situ Growth Processes.* Journal of Crystal Growth, **456**: p. 67-72. (2016) 6. Kawamura, F., et al., *Effect of Carbon Additive on Increases in the Growth Rate of 2in GaN Single Crystals in the Na Flux Method.* Journal of Crystal Growth, **310**(17): p. 3946–3949. (2008)

IN-SITU GROWTH MODE CONTROL OF ALN ON SIC SUBSTRATE BY SUBLIMATION CLOSED SPACE TECHNIQUE

Daichi Dojima, Koji Ashida, Tadaaki Kaneko

Kwansei Gakuin University, JAPAN

The engineering of the relaxation mechanism by hetero-epitaxy of lattice mismatch system at the interface has been a critical issue to grow high quality single crystal. In the case of the high temperature sublimation growth of AlN on SiC (0001) substrate (1800-2300°C), the relatively large lattice mismatch and thermal expansion coefficient of 1% and 23%, respectively, induce a massive distortion in the grown AlN lattice planes. It results in the formation of a large number of misfit dislocations and even cracks in the grown layer. In order to inhibit the propagation of the dislocations and the formation of the cracks, a hetero-interface engineering has been proposed to relax the strain by controlling a growth mode shifting to epitaxial lateral overgrowth (ELO) to take place on a mesa-patterned substrate, which has been proved by Hydride Vapor Phase Epitaxy (HVPE) at 1200-1500°C [1]. For the sublimation growth of AlN requiring a higher growth temperature than that of HVPE, it is more difficult to obtain the ELO-like growth mode control because of another necessity in the growth mode for suppressing the thermal decomposition of SiC substrate. Therefore, there are two conditions to be satisfied in the engineering of the hetero-epitaxy of AlN: a suppression of an inhomogeneous SiC thermal decomposition at the interface, and an increment of the AlN lateral growth rate to promote the coalescence of the AlN layers grown on each mesa-top. In this study, in order to optimize the growth condition for the maskless ELO process by sublimation method, the dependence of a temperature gradient and growth ambient pressure on the AlN growth mode is examined. The experiment was performed in a graphite-free furnace in order to reduce the impurity incorporation into the AlN layer. AlN was grown on the 4H-SiC (0001) on-axis substrate with mesa structures in the temperature range 1600-2100℃ in 50kPa of N_2 and N_2/Ar ambient. As a result, a sharp interface was obtained at the temperature gradient of ~7℃/mm. In addition, the strong dependence on the ambient gas was also observed. A continuous AlN *c*-plane growth was observed in the N_2/Ar ambient, whereas *a*-plane growth was dominant in the pure N_2 ambient. It was also confirmed that these growth modes were controllable *in-situ* by changing the ambient gas, suggesting the possibility of the maskless ELO by sublimation method. [1] D.

S. Kamber *et al*. *Appl. Phys. Lett.* **90**, 122116 (2007).

IMF GROWTH OF GASB ON V-GROOVED SI WITH ASPECT RATIO TRAPPING

Billy Lai, Qiang Li, Kei M. Lau

Hong Kong University of Science and Technology, HONG KONG PRC

GaSb holds promise for applications in long wavelength devices such as the infrared light emitting diode, the interband cascade laser, and the infrared photodetector. Commercially available GaSb substrates are costly and limited in size and quality. An effort to improve the availability of GaSb-based devices has led to the development and integration of GaSb on Si. In this work, we grew GaSb on nanopatterned V-grooved Si by using a thin GaAs buffer layer to accommodate the large lattice mismatch between GaSb and Si. Without the need for thick metamorphic buffer layers, an interfacial misfit (IMF) array, consisting of a 2-dimensional network of misfit dislocations, provides instantaneous strain relief caused by the lattice mismatch between GaAs and GaSb. We first tuned the growth temperature, the V/III ratio, and the As desorption time for GaSb growth based on GaAs substrates. Taking advantage of IMF growth in conjunction with aspect ratio trapping, we further explored the improvement in crystalline quality on V-grooved (001) Si. GaSb growth, characterized using x-ray diffraction (XRD), exhibited good crystalline quality when compared to GaSb grown on Si substrates by molecular beam epitaxy (MBE). Our 1 um GaSb growth on V-grooved Si resulted in an omega rocking curve full-width-at-half-maximum of 318 arcsec while the best reported MBE grown GaSb on planar Si, requiring precise tuning of an AlSb buffer, yielded a full-width-at-half-maximum of 347 arcsec [1]. Also, different thicknesses of GaSb grown on V-grooved Si were referenced using GaSb grown on GaAs substrates [Fig. 1(a-b)]. A thickness dependent lattice relaxation fitting was performed using the relative separation of the omega-2 theta peaks obtained from XRD; 250nm and 1um coalesced GaSb film on V-grooved Si resulted in a relaxation of 99.4% and 100.8%, respectively. We investigated the heterointerface between GaAs and GaSb as well as the misfit dislocations along the (111) facets and the bottom of the V-groove using cross-sectional transmission electron microscopy (X-TEM) [Fig. 1(c)]. Photoluminescence measurements were carried out to further substantiate the crystalline quality. Additional optimization of GaSb and exploration of possible heterostructure growth is in progress. Fig. 1. X-TEM images of (a) uncoalesced GaSb grown between SiO_2 stripes on V-grooved Si, (b) coalesced GaSb film on V-grooved Si and, (c) GaSb/GaAs heterointerface near the bottom of the V-groove. References: [1] J. Rodriguez et al., J. of Cryst. Growth, 439 (2016) 33-39.

OMVPE GROWTH OF STRAIN-COMPENSATED $GAAS_{1-Y}P_Y$/$GAAS_{1-X}BI_X$ QUANTUM WELL ACTIVE REGION LASERS

Honghyuk Kim[1], Yingxin Guan[2], Thomas F. Kuech[3], Luke J. Mawst[1]

[1]Department of Electrical and Computer Engineering, University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA, [2]Department of Material Science and Engineering, University of Wisconsin Madison, WI, UNITED STATES OF AMERICA, [3]Department of Chemical and Biological Engineering, University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA

$GaAs_{1-x}Bi_x$ quantum well (QW) active regions are an alternate approach to dilute-nitride QWs for achieving lasers in the telecom wavelength regions (λ~1.3-1.55μm) on GaAs substrates. *Ludewig et al* first reported the successful operation of $GaAs_{0.978}Bi_{0.022}$ single quantum well laser with low threshold current densities, J_{th}=1.56kA/cm^2 and a lasing wavelength of 946nm [1]. However, the device quality OMVPE growth of the metastable $GaAs_{1-x}Bi_x$ has remained challenging because of its required low growth temperature affecting the effective V/III ratio and incorporation of carbon impurities. In addition, surface-segregated Bi affects the growth rate and surface morphology. Here we report on the use of *in situ* optical reflectance monitoring during the OMVPE growth of $GaAs_{1-x}Bi_x$ QWs, along with *ex situ* high resolution x-ray diffraction and room temperature photoluminescence, which can provide valuable feedback for the optimization of the material growth conditions. The OMVPE growth of the $GaAs_{1-x}Bi_x$ films were carried out in a close-coupled showerhead reactor with a rotating susceptor using a continuous feed of Triethyl-gallium (TEGa), tertiarybutyl-arsine (TBAs) and trimethyl-bismuth (TMBi) as Ga, As and Bi precursors respectively. In addition, we implemented the use of tensile-strained $GaAs_{1-y}P_y$ as a QW barrier material, providing carrier confinement as well as potential for strain-balancing. Laser structures employing either 5nm or 7nm thick single $GaAs_{0.965}Bi_{0.035}$ quantum wells (SQW) and double quantum wells (DQW) with $GaAs_{0.75}P_{0.25}$ barriers were grown on (001) GaAs substrates. Ridge waveguide lasers, 27μm-wide ridge, were fabricated and characterized under pulsed current conditions at room temperature. The threshold current densities (J_{th}) for 3mm long cavity length was 5.73kA/cm^2 and 8.02kA/cm^2 for the 5nm and 7nm thick SQW devices respectively, with lasing wavelengths of 974nm and 1006nm. These data represent the longest emission wavelengths reported for OMVPE grown GaAsBi QW lasers, operating at room temperature. While threshold currents are relatively high, no post growth thermal annealing was performed on these laser materials. Thermal annealing studies, including the relative improvement in QW luminescence and its effects on laser device parameters, will be presented. [1] Ludewig, P., Knaub, N., Hossain, N., Reinhard, S., Nattermann, L., Marko, I. P., and Volz, K. 2013. *Appl. Phys. Lett.*, *102*(24), 242115.

THERMODYNAMIC STABILITY ANALYSIS OF BI-CONTAINING III-V QUATERNARY ALLOYS AND THE EPITAXIAL STRAIN EFFECTS

Yingxin Guan, Guangfu Luo, Dane Morgan, Thomas F. Kuech

University of Wisconsin Madison, UNITED STATES OF AMERICA

Bi-containing III-V ternary and quaternary alloys have been proposed as alternative candidates for near and mid-infrared optoelectronic applications in recent years, due to the bandgap energy reduction and other band structure changes arising from Bi addition. However, the Bi incorporation into the III-V matrix is difficult due to the subsequently considerable distortion of the elemental bonding in the crystal lattice, which results in a large enthalpy of mixing and destabilizes the alloy system with regard to phase decomposition. This lack of solubility leads to the Bi surface segregation which has been encountered in many growth studies on Bi-containing III-V alloys. Since Bi incorporation exceeding the thermodynamically determined limit has been achieved, these Bi-containing III-V alloys are referred to as ‘metastable alloys’. While several studies of thermodynamic stability and phase relationships have been presented for the Bi-containing ternary alloys, the thermodynamic stability analysis of the Bi-containing quaternaries, either in the bulk or the strained pseudomorphic state, has not been systematically reported. In this study, the delta lattice parameter (DLP) model is applied to analyze the thermodynamic stability of the Bi-containing III-V quaternaries by calculating the binodal and spinodal isotherm contours for the bulk and pseudomorphic $In_{1-y}Ga_yAs_{1-x}Bi_x$ and $GaAs_{1-x-y}P_yBi_x$ systems. The results of the DLP model are also compared with density functional theory (DFT) calculations. The DFT and DLP calculations showed remarkably good agreements over selected compositions within the quaternary $In_{1-y}Ga_yAs_{1-x}Bi_x$ and $GaAs_{1-x-y}P_yBi_x$ systems. In general, pseudomorphic strain reduces the critical temperature and stabilizes the alloy over a broader compositional range for both quaternary systems. It was also found that elemental mixing on the cation sublattice for $In_{1-y}Ga_yAs_{1-x}Bi_x$/InP destabilizes the system leading to a reduced Bi solubility, while the addition of P into the $GaAs_{1-x-y}P_yBi_x$/GaAs matrix stabilizes the alloy. This work broadens the DLP model to a wider elemental range of quaternary semiconductor alloys and elucidates the thermodynamic stability dependence for Bi-containing quaternary alloys on the epitaxial strain and composition, which can provide a guideline for the alloy growth to obtain relatively high Bi concentration as well as maintain high crystalline quality.

GROWTH AND CHARACTERIZATION OF INXGA1-XSB METAMORPHIC BUFFER LAYERS BY METAL-ORGANIC VAPOR PHASE EPITAXY ON THE GASB SUBSTRATE

Yingxin Guan[1], Aaron Tan[2], Susan E. Babcock[3], Luke J. Mawst[4], Thomas F. Kuech[3]

[1]University of Wisconsin Madison, UNITED STATES OF AMERICA, [2]University of Wisconsin Madison, WI, UNITED STATES OF AMERICA, [3]University of Wisconsin-Madison, WI, UNITED STATES OF AMERICA, [4]University of Wisconsin-madison, WI, UNITED STATES OF AMERICA

Compositionally graded metamorphic buffer layer (MBL) growth has been proposed as a practical approach to bridge the large lattice-mismatch between the commercially available substrates and the desired heterostructures for III-V optoelectronic device applications. Through the alloy composition control and the intentional introduction of misfit dislocations within the compositionally graded region, MBLs can provide adjustable lattice constants for the sequential thin film growth and thus offer more freedom for the heterostructure design to achieve a wider range of bandgap energies. The metal-organic vapor phase epitaxy (MOVPE) of As-based and P-based MBL structures on GaAs and InP substrates have been studied for the growth of near to mid-wavelength infrared lasers and solar cells. However, at this moment, the Sb-based MBL on the GaSb substrates is less explored by MOVPE, which has the potential to support the $InAs_{1-y}Sb_y$ growth for mid- to long-wavelength infrared detector applications. The related MOVPE growth challenges may include the essential surface treatment for the de-oxidation of the GaSb substrate, the exploration of the narrow growth window of the gas-phase V/III ratio, as well as the control for the alloy composition and strain-relaxation during the compositionally graded III-Sb alloy growth. In this work, we have demonstrated the MOVPE growth of the step-graded $In_xGa_{1-x}Sb$ MBLs on the GaSb substrate at the temperature of 550ºC. The composition of the $In_xGa_{1-x}Sb$ buffers was graded to x=40-50% over 9 $In_xGa_{1-x}Sb$ layers with the total thickness of 3-5 μm. The top buffer layers achieved an in-plane lattice constant with a 2.2-2.5% lattice-mismatch to the GaSb substrate and a strain-relaxation of ~90%. Conventional crosshatch features were also observed on the MBL surface, which were effectively reduced after the chemical mechanical planarization (CMP) process. Besides, the dislocation distribution as well as any other microstructure defects in the MBL samples will be analyzed by the transmission electron microscopy study. The exploration for the MOVPE grown $In_xGa_{1-x}Sb$ MBLs may offer the solution for the bulk $InAs_{1-y}Sb_y$ growth on the GaSb substrate for long-wavelength infrared optoelectronic applications.

HIGH PRESSURE OXYGEN SPUTTER DEPOSITION OF PEROVSKITE OXIDE METALS AND SEMICONDUCTORS

Chris Leighton[1], Jeff Walter[1], Koustav Ganguly[1], Palak Ambwani[1], Shameek Bose[1], Peng Xu[1], Abhinav Prakash[1], Greg Haugstad[1], Jaume Gazquez[2], Neven Biskup[2], Maria Varela[2], Jong Seok Jeong[1], Andre Mkhoyan[1], Bharat Jalan[1]

[1]University of Minnesota, MN, UNITED STATES OF AMERICA, [2]Universidad Complutense de Madrid, SPAIN

This presentation will review recent progress at the University of Minnesota in the use of high pressure oxygen sputter deposition for the epitaxy of perovskite oxide metals, magnets, and semiconductors. Reactive sputter deposition from compound ceramic targets is a versatile approach to the epitaxy of perovskite oxides, but oxygen-ion-induced resputtering is a serious issue that often necessitates off-axis geometries and/or high accompanying Ar pressure. This can lead to low growth rates, in addition to other limitations. In high pressure oxygen sputtering the sources are redesigned to enable stable operation in pure O_2 at pressures *over 1 Torr*. This creates a highly oxidizing plasma where the oxygen ions are thermalized by collisions, essentially eliminating oxygen-induced resputtering. Typical source-to-substrate distances of only 2-3 cm are employed, leading to average growth rates of 10-15 Å/min for conductors (DC excitation), and 2-3 Å/min for insulators (RF excitation). A system based on this technology has been commercialized by Forschungszentrum Jülich and is now in use in a handful of labs around the world, where high quality epitaxy of oxide superconductors, magnets, metals, and insulators has been demonstrated. In this talk I will illustrate the capabilities of this technique *via* a discussion of the epitaxy and properties of the perovskite oxide ferromagnetic metal $La_{1-x}Sr_xCoO_3$, the archetypal perovskite oxide semiconductor $SrTiO_3$, and the high room temperature mobility perovskite semiconductor $BaSnO_3$. The technique will be shown capable of the growth of: $La_{1-x}Sr_xCoO_3$ films with physical properties competitive with any others reported; rigorously stoichiometric $SrTiO_3$; and La-doped $BaSnO_3$ (on mismatched substrates, with no buffer layer) with 60 $cm^2V^{-1}s^{-1}$ mobility. Strengths and limitations of the growth method will be discussed. Various aspects of this work were supported by the DOE through the University of Minnesota Center for Quantum Materials (DE-SC-0016371, DE-FG02-06ER46275), and by the NSF through the University of Minnesota MRSEC (DMR-1420013) and DMR-1507048.

GROWTH OF HIGH QUALITY EPITAXIAL LAALO3 ON SRTIO3 ON (001) SI VIA MOLECULAR-BEAM EPITAXY

Zhe Wang, Darrell G. Schlom

Cornell University, NY, UNITED STATES OF AMERICA

We report the *in-situ* integration of epitaxial $LaAlO_3$ on silicon using a 5 unit-cell (u.c.) thick $SrTiO_3$ buffer layer. Both $LaAlO_3$ and $SrTiO_3$ films were grown with molecular-beam epitaxy (MBE). Strontium and titanium molecular beams were generated using a conventional effusion cell and a Ti-Ball^{TM} titanium sublimation pump, respectively. Lanthanum and aluminum beams were generated via conventional effusion cells. The 5 u.c. thick $SrTiO_3$ buffer layer was grown using the so-called epitaxy-by-periodical-annealing method, which we have perfected to yield $SrTiO_3$ films with rocking full width at half maxima (FWHM) narrower than 0.02° for $SrTiO_3$ films up to 300 nm thick. To ensure the stoichiometry of the $LaAlO_3$ film, lanthanum and aluminum fluxes were calibrated by codeposition of $LaAlO_3$ for stoichiometric reflection high-energy electron diffraction (RHEED) patterns and also by observing the RHEED oscillations for the growth rate. After the calibration, $LaAlO_3$ was grown by codeposition with an oxygen partial pressure of ~ Torr at the substrate temperature of ~590 °C. *In-situ* RHEED images showed both the $SrTiO_3$ and $LaAlO_3$ films were smooth. *Ex-situ* X-ray diffraction (XRD) θ-2θ scan shows only *00l* reflections of $LaAlO_3$, indicating the film is epitaxial. A ø scan shows the $LaAlO_3$ layer on silicon to have a cube-on-cube epitaxial orientation relationship. The rocking curve of the $LaAlO_3$ layer shows a single peak with a full width at half maximum (FWHM) of 0.02°, which is comparable to single crystal $LaAlO_3$ substrates and is the narrowest $LaAlO_3$ rocking curve ever reported for the growth of $LaAlO_3$ on silicon. Using MBE, our *in-situ* growth yields a high quality epitaxial $LaAlO_3$ film on (001) Si, which could find its applications in serving as a twin-free template for multi-functional oxide integration on silicon.

GROWTH OF DEFECT MITIGATING, METASTABLE $(SRTIO_3)_N(BATIO_3)_MSRO$ SUPERLATTICES

Natalie M. Dawley[1], Megan E. Holtz[1], Gerhard H. Olsen[1], Xifeng Lu[2], Nathan D. Orloff[2], Che-Hui Lee[1], Jingshu Zhang[1], James C. Booth[2], Craig J. Fennie[1], David A. Muller[1], Darrell G. Schlom[1]

[1]Cornell University, UNITED STATES OF AMERICA, [2]NIST, UNITED STATES OF AMERICA

The Ruddlesden-Popper (RP) superlattice series, $(ABO_3)_nAO$, has been identified as a defect mitigating structure via a proposed mechanism in which the $(AO)_2$ layer accommodates the local non-stoichiometry of the crystal by changing its area. This allows the rest of the material to remain stoichiometric. In the strained $(SrTiO_3)_nSrO$ thin film phase we recently demonstrated record tunable dielectric performance at gigahertz frequencies, a region where point defects significantly contribute to dielectric loss. We use oxide molecular-beam epitaxy (MBE) as a controlled way to fabricate these metastable epitaxial thin films via precise atomic layering. In this work we use MBE to grow related RP phases containing $BaTiO_3$. In bulk form, no RP phases containing $BaTiO_3$ are known. Nonetheless, using MBE we synthesized the $(SrTiO_3)_n(BaTiO_3)_mSrO$ structures shown in figure 1, in hopes of making thicker films of this new type of low-loss tunable dielectric to achieve devices with higher tunability. Thicker films are achieved by lowering the epitaxial strain due to $BaTiO_3$'s smaller mismatch with the (110) $DyScO_3$ substrate, while still maintaining the ferroelectric instability needed to be a tunable dielectric. Precise layering is obtained from reflection high-energy electron diffraction shuttered

oscillations and source flux matching.

Figure 1 Schematic of the unit cell crystal structure of $(SrTiO_3)_n(BaTiO_3)_mSrO$ Ruddlesden-Popper phases for m=1, n=1-5. The first five members of this RP homologous series, m=1, n=1-5, have been grown on (110) $DyScO_3$ using MBE and characterized by x-ray diffraction. We use scanning transmission electron microscopy (STEM) and electron energy-loss spectroscopy (EELS) to identify barium and $(SrO)_2$ fault placement, and find high quality films with 1-3 atomic layers of barium interdiffusion. Density function theory (DFT) calculations were preformed to examine the ground state and strained structures, and their ferroelectric distortions. In-plane measurements of the dielectric constant have been made as a function of temperature and frequency in the gigahertz frequency regime.

EPITAXIAL GROWTH OF EXTREME-MOBILITY OXIDES

Jon-Paul Maria

North Carolina State University, NC, UNITED STATES OF AMERICA

Thanks to sustained and growing interest in light-matter interaction at infrared (IR) energies, transparent conducting oxides (TCOs) command considerable attention from the photonics and plasmonics communities. This attention originates from optical properties that are smoothly tunable though a large spectral window connecting the short and long wave energy bands. This large window is accessible because electron concentrations can span 10^{18} to 10^{21} cm^{-3} in a single material by doping. Matching this range in either metals or covalent semiconductors is a fundamental challenge. Recently, our group developed an approach to engineer the defect equilibrium in doped CdO that enables carrier densities between mid 10^{18} cm^{-3} and mid 10^{20} cm^{-3} while retaining mobility values between 300 cm^2/Vs and 500 cm^2/Vs. To date, CdO is the only material that can host this combination of mobility and carrier density. In this presentation, we describe CdO thin film synthesis and Fermi level control of point defect populations. Materials prepared by molecular beam deposition and sputtering will be discussed, with a variety of donors on both cation and anion sublattices. We will also demonstrate how carrier density can be used to tune plasma oscillation through the IR spectrum; this will be shown for surface plasmon polariton and epsilon-near-zero oscillation modes. We also highlight how CdO can be used to visualize the evolution of SPP modes, to coupled-supermodes, and to the limiting case of ENZ oscillations. The discussion will focus on specific aspects of CdO deposition for epitaxial and non-epitaxial conditions. Particular attention will be given to sputtering with a pulsed dc plasma, which allows for very high ionization fractions of oxygen and metal cations. We show how these conditions lead to superior control of oxygen stoichiometry, which directly relate to enhanced control of transport and optical properties.

HIGH PRESSURE FLOATING ZONE GROWTH OF CORRELATED ELECTRON TRANSITION METAL OXIDES

John F. Mitchell, Junjie Zhang, Hong Zheng, Michael Norman, Daniel Phelan, Antia Botana

Argonne National Laboratory, IL, UNITED STATES OF AMERICA

The optical floating zone technique has been established for more than three decades as a powerful and effective way to grow complex oxide crystals of high purity and sufficient size for condensed matter physics, and in particular neutron scattering. Thus, it has been a tool for the physics community to advance. The recent innovation of adding high pressure of either inert or reactive gases adds a new level of versatility to this technique, allowing the crystal grower (a) to move phase lines to allow growth of 'impossible to grow' crystals, (b) to uncover new compounds, or (c) to extend doping ranges into high metal formal oxidation states. In this talk, I will describe the underlying advantages of this approach, illustrated by examples of each of these capabilities in the area of correlated electron transition metal oxides. Specifically, I will discuss discovery of the previously unknown brownmillerite Ca2Co2O5, discovery of charge and spin stripes in layered nickelates, and the appearance of magnetism in highly doped 2D manganese oxides.

EFFECT OF MOLTEN-ZONE INSTABILITY ON THE IMPURITY PARTITIONING DURING FZ GROWTH

Satoshi Uda, Yutaroh Takehara, Chihiro Koyama

Tohoku University, JAPAN

Growth by floating zone (FZ) method has characteristics that the composition of growing crystal in steady sate is equal to that of the source material. However, there are not reasonable reports available that precisely demonstrate such a compositional equality. In fact, the compositional mismatch between these two are sometimes observed, which is often attributed to the mass loss of a volatile solute from the high-temperature melt. On the other hand, a solute increment in grown crystal is also observed for some FZ growth. Thus, it is important to examine the solute partitioning during FZ growth. Here we investigate the mass conservation condition on impurity during FZ growth of an impurity-doped crystal, which is predominated by the molten-zone instability and then we set up the differential equation for the mass conservation of which solution is more suitable to represent the impurity partitioning during FZ growth. The impurity concentration profile analyzed by Pfann [1] assumes that the molten zone length (volume) is constant during growth and that there is no difference in density and diameter between the source rod and the growing crystal. In our model both density and diameter are not the same. We developed the impurity profile equation for two cases; the melt quantity in the molten zone is constant during growth (Model-I), and the melt quantity monotonously changes with the growth (Model-II). Model-I basically follows the Pfann's equation and the impurity concentration of the growing crystal in steady state is equal to that of the source material. In contrast Model-II yields either less or more impurity in the growing crystal depending on the ratio of the crystallized mass to the dissolved mass. We grew TiO_2 crystals doped with Nb_2O_5. Both TiO_2 and Nb_2O_5 are not volatile at the growth temperature. The equilibrium partition coefficient of Nb_2O_5 is around 0.6. Nb_2O_5 distributions in grown crystals were surveyed with various growth conditions and they were attempted to optimize with Pfann's equation as well as Model-II to see which model is more suitable to employ. A comparison example is given in Figure 1 illustrating the initial transient to the steady- state region of Nb_2O_5-doped TiO_2 crystal, which clearly shows that Model-II represents the Nb_2O_5 profile better.

[1] Pfann, W. G., *J. Metals,* **4,** 747 (1952).

SEARCHING FOR IDEAL BI-SYSTEM TOPOLOGICAL INSULATOR, PB-SYSTEM TOPOLOGICAL CRYSTALLINE INSULATOR AND THEIR TOPOLOGICAL SUPERCONDUCTOR

Genda Gu

Brookhaven National Laboratory, NY, UNITED STATES OF AMERICA

The discovery of 3D topological insulator materials and topological superconductor open up a new research field in the condensed matter physics. In order to search for the ideal topological insulator, topological crystalline insulator and topological superconductor, we have grown a large number of the single crystals of Bi-system and Pb-system (Pb-Sn-In-Te) topological crystalline insulator and their topological superconductor . We have measured the physical properties on these single crystals by various techniques. We have studied the effect of crystal growth condition, impurity and composition on the bulk electrical conductivity of these single crystals. We try to find out which composition and crystal growth condition is the best for the ideal topological insulator, topological crystalline insulator and topological superconductor. We have got the bulk topological superconductor with Tc=5K.

GROWTH OF 8-HYDROXYQUINOLINE SINGLE CRYSTAL BY MODIFIED CZOCHRALSKI GROWTH TECHNIQUE AND CHARACTERIZATION

Sonu Kumar, Binay Kumar

Crystal Lab, Department of Physics & Astrophysics, University of Delhi, Delhi-7, India, INDIA

Large sized 8-Hydroxyquinoline single crystal was grown by modified low temperature Czochralski growth technique [1,2]. A suitable low temperature CZ system was developed and a crystal of diameter 0.5 cm and length 4 cm was grown in Ar-atmosphere. The structural parameters were determined by powder X-ray diffraction method. The functional groups were confirmed by FITR spectrum. Thermal transitions at various temperatures were measured by TG/DTA analyses. The dependent dielectric properties of the grown crystal were studied with the variations of temperature as well as frequency. The grown crystal can be used for the fabrication of microstrip patch antenna because it’s low value of dielectric constant [3]. The grown crystals are piezoelectric as confirmed by d_{33} coefficient =3pC/N thus, it can used in piezoelectric applications. UV-vis analysis was used for transmittance and band gap measurement. Vicker’s microhardness indenter was used to evaluate the hardness of the sample. References H. Yadav, N. Sinha, B. Kumar, Journal of Crystal Growth 450 (2016) 74–80. K. Aravinth, G. Anandha Babu, P. Ramasamy, J Therm Anal Calorim 110 (2012) 1333–1339 H. Yadav, N. Sinha, B. Kumar, CrystEngComm 16 (2014) 10700.

GROWTH, INTERNAL STRUCTURE AND MECHANICAL PROPERTIES OF PLATINUM FIBER CRYSTALS BY ALLOY-MICRO-PULLING-DOWN METHOD

Takayuki Nihei[1], Yuui Yokota[2], Akihiro Yamaji[1], Yuji Ohashi[2], Shunsuke Kurosawa[3], Kei Kamada[2], Akira Yoshikawa[2]

[1]Institute for Materials Research, Tohoku University, JAPAN, [2]NICHe, Tohoku University, JAPAN, [3]Department of Physics, Yamagata University, JAPAN

Platinum group metals and alloys such as Pt and Ir have high melting points and high oxidation resistances, and therefore they have been used for various applications in the industrial field. However, the material loss at forming processes originated from the difficult workability affects the product cost. We have developed an alloy-micro-pulling-down (A-μ-PD) method as a new molding technology that can fabricated metals and alloys with close to the product shape and reported the growth of the Ir and Pt fibers by the A-μ-PD method. In this study, the microstructure of the Pt fiber crystal grown by the A-μ-PD method was observed by the electron backscattered diffraction (EBSD) measurement and the mechanical properties were evaluated. Pt pellets (99.99% purity) were prepared as a starting material and they were set in a ZrO_2 crucible with a hole of f 1 mm at the bottom. The Pt pellets were heated up to the melting point (1768°C) by high frequency induction heating under N_2 gas. After the Pt pellets were melted, the Pt melt was pulled down at 1 mm/min growth rate using a commercially available Pt wire produced by wire-drawing process. The growth rate gradually increased every 100 mm. The growth of Pt fiber was stable at the growth rate from 1 to 110 mm/min and the shape didn't change during crystal growth while the shape control became unstable at 120 mm/min. Figure shows crystal orientation maps of the Pt fiber grown by the A-μ-PD method at 50 mm/min and the commercial Pt wire. In Fig. (a), grain boundary was clearly observed in the grown Pt fiber. The size of the crystal grains was the almost same as or larger than the fiber diameter, and the grain boundary is connected from one side of the fiber surface to the other side. In contrast, the commercial Pt wire was composed of many small grains elongated along to the longitudinal direction. The results revealed that the domain structure of the Pt fiber grown by the A-μ-PD method was completely different from that of the commercial Pt wire.

Details of the microstructure observation and their mechanical properties will be reported.

INFLUENCE OF CARRIER CONCENTRATION ON BULK LIFETIME IN CZ-SI CRYSTAL

Koichi Kakimoto

Research Institute for Applied Mechanics, Kyushu University, JAPAN

Long lifetime of carrier is required to realize a power device with high performance or a solar cell with high conversion efficiency. The lifetime of Czochralski (CZ) grown silicon crystals has been reported to be affected by oxygen precipitates and related defects. Furthermore, a light element of carbon degrades the lifetime [3]. In this study, we investigated the effect of light elements of oxygen and carbon atoms on lifetime of carrier in a CZ grown silicon single crystal. The results show that lifetime in CZ silicon crystal is not determined by carbon concentration, but carrier concentration. We performed growth experiment to obtain n-type crystals with 3 inches diameter by phosphorous doping. Resistivity, concentrations of oxygen and carbon, and lifetime were measured by four-point, Fourier Transformation Infrared spectroscopy and eddy current (Sinton BLS-1) methods, respectively. Crystals named “High-Cs” contain higher carbon concentration of more than 1 x 1016 atoms/cm3, while crystals named “Low-Cs” have concentration less than 2 x 1015 atoms/cm3. Oxygen concentrations of the crystals are 6 to 8 x 1017 atoms/cm3 (JEITA). The measured bulk lifetime was in the range from 10 to 20 msec. The experimental results show that the dependence of carbon concentration on lifetime is small and that we can obtain silicon crystals with high lifetime of 10 msec even with high concentrations of carbon. Lifetime of Low-Cs and High-Cs lie on a straight line. We concluded that lifetime in CZ silicon crystal is not determined by carbon concentration, but dopant concentration. We also grow two non-doped crystals with 3-inch diameter, named crystal A and B, using the same condition as the Low-Cs crystal growth. The carrier concentration decreases from the top to the bottom. Those carriers are thought to originate from boron and phosphorous impurities in the quartz crucible. Lifetime of crystal A and B are in the rage from 14 to 16 and from 15 to 18, respectively. The lifetime increases from the top to the bottom. The results show a curvilinear relationship between lifetime and carrier concentration, even if they contain 1016 /cm3 of carbon or they have donor-accepter compensation.

SIC CRYSTAL GROWTH AND SUBSTRATE TECHNOLOGY FOR DEVICE MANUFACTURING

Robert T. Leonard, Yuri Khlebnikov, Michael Paisley, Simon Bubel, Jyothi Ambati, Eugene Deyneka, Ian Currier, Valeri Tsvetkov, Jeff Seaman, Adrian Powell, Mike O'Loughlin, Edward Van Brunt, Al Burk, Elif Balkas

Cree, Inc., NC, UNITED STATES OF AMERICA

The integration of silicon carbide (SiC) power devices into many applications over the last several years has been driven by superior device and system performance enabled by the favorable physical properties of SiC. These demonstrations have led to a wider adoption of SiC based devices into many applications, driving substantial commercial growth and maturation of the technology. The SiC technology maturation is visible in three ways. First, there is an accelerating drive to increase the quality of the SiC material by reducing defects necessary to increase device yield and performance. Crystalline defects of hollow-core screw dislocations, or micropipes (MP), have been reduced to typical densities of much lower than 1 cm^{-2}, and substrates with zero MPs [1] are available in 100 mm and 150 mm diameters. After achieving these results, the quality improvement focus has shifted to dislocations. SiC crystals exhibit several dislocation types including basal plane dislocations (BPDs) and threading screw dislocations (TSDs). Effective and automated characterization techniques for rapid feedback to crystal growth processes were utilized to reduce the BPD and TSD densities in SiC substrates [2]. Second, there is the continuing drive to increase substrate diameter to gain efficiencies of scaling and reduced cost. Following the physical vapor transport (PVT) methods of Tairov and Tsvetkov [3], SiC substrate diameters have increased from near 1 inch in the early 1990’s to 200 mm in 2015, while the MP and dislocation densities continue to decrease. Third, there is the drive to optimize and improve the substrate physical characteristics to streamline device fabrication processing. Developing methods to control the substrate thickness, resistance, surface, and geometrical shape are vital to producing a controlled device processing environment. Our current work focuses on performance improvements on our 150 mm diameter substrates to enable better integration and lower cost for device manufacturing. This work is being done primarily through improvements to our crystal growth technologies and processing the grown crystals into substrates. Parallel R&D efforts focus on 200 mm substrate at the same or better quality as 150 mm. We will discuss the challenges to maintain low defect densities as it applies to PVT SiC growth, and the methods used to characterize the substrates and growth process. [1] R.T. Leonard et al., Mat Sci Forum, Vols. 600-603(2009), pp. 7-10. [2] J.J. Sumakeris, et al., Mater. Sci. Forum 858 (2016) p. 393. [3] Tairov & Tsvetkov, J. Cryst. Growth 43, (1979), pp.209−212.

OMVPE GROWTH OF AL-RICH ALGAN ALLOYS FOR POWER ELECTRONICS

Andrew Allerman, Mary Crawford, Greg Pickrell, Andrew Armstrong, Robert Kaplar, Jeramy Dickerson, Brianna Klein, Michael King, Michael Van Heukelom

Sandia National Laboratories, NM, UNITED STATES OF AMERICA

As the performance of GaN- and SiC-based power devices becomes limited by fundamental material properties, semiconductors with larger bandgaps are appealing due to their projected higher critical electrical field. Thus, diodes employing ultra-wide bandgap semiconductors are expected to operate at higher breakdown voltages with thinner and more heavily-doped drift regions, leading to lower resistive losses. AlGaN alloys with their much larger bandgap compared to SiC and GaN are thus appealing for high voltage pn diodes and transistors. Additionally, the utilization of polarization fields in AlGaN heterostructures offer design options not possible for devices based on materials such as SiC and diamond. Here we report on the growth and current-voltage (IV) characteristics of pn diodes fabricated from $Al_{0.30}Ga_{0.70}N$ (Eg = 4.1 eV) and $Al_{0.74}Ga_{0.26}N$ (Eg=5.3eV) alloys, illustrating the potential for AlGaN alloys as a viable material for next-generation power diodes. Quasi-vertical, homojunction pn diodes consisting of $Al_{0.30}Ga_{0.70}N$ epilayers were grown by metalorganic vapor phase epitaxy. Devices with drift layers from 4.3 to 11 µm thick exhibited breakdown voltages from 1600 to 3000 V in reverse bias and had a forward turn-on voltage of 6 – 8 volts. To our knowledge, this is the first AlGaN-based pn diode exhibiting a breakdown voltage in excess of 1 kilovolt. We have also investigated quasi-vertical pn diodes consisting of $Al_{0.74}Ga_{0.26}N$ epilayers to exploit the expected higher critical electric field in higher aluminum mole fraction alloys. The combination of thick AlN buffer and $Al_{0.74}Ga_{0.26}N$ layers resulted in x-ray diffraction linewidths of 164-197 (237–284) arc seconds for the (0002) and (10-12) reflections for the drift layer, respectively. By optimizing the growth conditions used for the drift layer, the density of electron compensating defects can be reduced to ~ $1x10^{16}$ cm^{-3} — a level reported for GaN pn diodes. Unlike pn diodes based on $Al_{0.30}Ga_{0.70}N$ epilayers, simple homojunction pn diodes are not practical in Al-rich AlGaN alloys due to the very deep acceptor level. Consequently, other approaches were considered for hole transport. We will report on the forward and reverse IV characteristics of pn heterojunction diodes where a Mg-doped p-type $Al_{0.30}Ga_{0.70}N$ layer is grown on the n-type $Al_{0.74}Ga_{0.26}N$ drift layer. Additionally, the current-voltage characteristics of pn diodes where holes are generated in the p-region by field ionization of Mg acceptors will also be presented.

PULSED OMVPE GROWTH STUDIES OF INN FOR INTEGRATION IN INGAN ACTIVE REGION

Ioannis Fragkos, Wei Sun, Damir Borovac, Renbo Song, Jonathan J. Wierer, Jr., Nelson Tansu

Lehigh University, PA, UNITED STATES OF AMERICA

In virtue of its narrow bandgap of ~ 0.7 eV, indium nitride (InN) is an important semiconductor material for optoelectronic applications including solar cells, THz generation and high-speed electronic devices. Furthermore, InN can be used in conjunction with the InGaN-based technology to form nano-engineered active region applicable for red and near-infrared light emitters. By inserting an ultrathin (delta-like) InN layer in a conventional InGaN-based QW, the electron-hole wavefunction overlap will increase dramatically in the active region with emission wavelengths covering from red up to near-infrared spectral regime. However, the challenges for integrating InN delta-layer in InGaN active region via OMVPE still exists, attributed to 1) large difference in the optimized growth conditions for these two alloys, and 2) narrow optimized growth condition of InN limited by low ammonia (NH_3) dissociation and In-metallic formation. Our recent work by using the pulsed OMVPE technique has shown the growth of metallic-free InN with bandgap of 0.77 eV. In this work, the pulsed OMVPE method was employed to synthesize InN for insertion into InGaN-based active region. The InN layers were grown on GaN/sapphire templates with TMIn and NH_3 as the In- and N- precursors respectively. In the pulsed OMVPE technique, the NH_3 was constantly flown into the reactor with pulsing of TMIn. A comprehensive study on the effects of the pulsing period (T) and the pulsing duty cycle of the growth mode is carried out under a growth temperature of 540 ^{o}C, a growth pressure of 200 torr, and V/III ratios of 4.86-6.48 x 10^5. The XRD measurements revealed the presence of metallic In (101) in the InN films grown under low V/III ratio of 4.86 x 10^5. By decreasing the pulsing period (T) from T=72 sec to T=18 sec, the FWHM of the corresponding XRD peak of metallic In (101) was increased from 0.05 to 0.09 degrees, while the peak intensity of metallic (101) peak disappeared. This observation indicated that the metallic In deposition can be removed by optimizing the pulsing period. Furthermore, under higher V/III ratio of 6.48 x 10^5, by increasing the duty cycle of the pulse from 35% to 75% the crystallinity of the InN films is increased as reflected from the reduction in the FWHM of the corresponding InN (002) XRD peak. Strategies on incorporation of InN into InGaN QW by using pulsed OMVPE growth method will be presented and analyzed.

PROPERTIES OF GAN ON HIGH QUALITY ALN SAPPHIRE TEMPLATE BY USING METALORGANIC CHEMICAL VAPOR DEPOSITION

Akira Mishima[1], Yuji Tomita[1], Guanxi Piao[1], Yoshiki Yano[2], Toshiya Tabuchi[2], Koh Matsumoto[2]

[1]Taiyo Nippon Sanso corporation., JAPAN, [2]Taiyo Nippon Sanso, JAPAN

[Introduction] GaN-based electron devices have been studied as high-frequency, high-breakdown voltage and high-temperature operation devices. In order for the high performance electron device, GaN on a high quality AlN template is a promising candidate for its high thermal conductivity and high resistivity. Usually GaN with good crystallinity can be grown by carrying out two-dimensional growth after three-dimensional growth. [1] However, Three-dimensional growth incorporates much oxygen and forms a leakage path. In this study, we have prepared a high quality AlN template by high temperature metal organic chemical vapor deposition (MOCVD) at 1340 ºC. We have conducted two-dimensional growth of GaN on high quality AlN on sapphire, and investigated the crystal quality and electrical properties. [Experimental] 3-mm-thick AlN template was grown on a 2 inch sapphire substrate using MOCVD tool (SR4000HT, Taiyo Nippon Sanso). The full width at half maximum (FWHM) of the XRC of the (0002) plane was 286.3 arcsec, and that of the (10-12) plane was 501.7 arcsec. The growth temperature, V/III ratio, and growth pressure for GaN on AlN template were 1110 ºC, 3044 and 100 kPa, respectively. The growth rate was 2.7 mm/h and the thickness was 2.7 mm. Crystallinity of the GaN was evaluated by the FWHM of the X-ray rocking curve (XRC), the relaxation rate was evaluated by Reciprocal Space Mapping (RSM) and sheet resistance of the GaN was evaluated by eddy current. [Result] A mirror-like and smooth surface was obtained after GaN growth on AlN template. The FWHM of the XRC of GaN (0002) plane was 236.2 arcsec, and that of GaN(10-12) plane was 379.6 arcsec. The sheet resistance was more than 3000 ohm / sq, which was measurement limit of eddy current tool. The relaxation rate of the GaN was 77.2% estimated by RSM. From these results, it was confirmed that GaN on a high quality AlN template can be obtained with high crystallinity and high resistance. By applying this technique for electron devices, improvement of thermal properties and high breakdown voltage can be expected. [1] S. Nitta et al., J. Cryst. Growth 272, 438 (2004).

DELTA DOPING AND BIASED ENHANCED GROWTH DIAMOND BY HOT FILAMENT CVD TECHNOLOGY

Gary L. Harris[1], Aaron Jackson[1], Amber Wingfield[1], James Griffin[1], Crawford Taylor[1], Marko Loncar[2]

[1]Howard University, DC, UNITED STATES OF AMERICA, [2]Harvard University, MA, UNITED STATES OF AMERICA

Low intrinsic nucleation density of diamond grown on foreign substrates has limited the material performance. In this, paper we report on the heteroepitaxial grown of diamond using bias enhanced nucleation (BEN) in a hot filaments chemical vapor high vacuum deposition reactor. The BEN is an efficient mechanism to increase the nucleation density. This BEN process in conjunction with our seeding process produces an oriented nucleation over areas. The Raman spectrum of thin film grown on monocrystal diamond was characterized by a sharp line at 1332.5 cm^{-1} with a full width at half maximum (FWHM) of 2 cm^{-1} with a flat background. The large grain oriented diamond films grown on silicon and silicon carbide were characterized by sharp line at 1334.5 cm^{-1} with a FWHWH of 11 cm^{-1} and a low level graphitic characteristic peak at 1531 cm^{-1}. The growth rate as high as 10μm/hour have been obtained. We also will present delta doping results of diamond films using both the BEN and normal hot-filament CVD techniques with nitrogen, silicon, and germanium deep colors centers. We have been able to place this color center within 10 nm of the surface. This type of doping control is required for such devices as quantum registrars, and quantum keying applications. This work was supported by the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319 and a grant from Northrop-Grumman Corporation.

DOPED, HIGH MOBILITY CADMIUM OXIDE FILMS FOR TUNABLE PLASMONICS

Evan L. Runnerstrom[1], Jon-Paul Maria[2]

[1]North Carolina State University, UNITED STATES OF AMERICA, [2]North Carolina State University, NC, UNITED STATES OF AMERICA

Heavily doped semiconductors, particularly transparent conductive oxides (TCOs), are a particularly promising class of plasmonic materials with optical properties that can be tuned over much of the near- and mid-infrared (IR). This enables light manipulation over broad spectral regions and provides the opportunity to match plasmonic excitations to other optical transitions to enable new modes of molecular sensing, hot carrier injection, etc. However, TCOs are subject to ionized impurity scattering and suffer optical losses as a result. When large numbers of impurities are present, the electronic mobility and associated plasmon quality factors are greatly reduced. In 2015, our group showed that cadmium oxide (CdO), particularly when doped with dysprosium, is an excellent materials platform for low-loss, tunable mid-IR plasmonics, with very high free carrier mobility and low damping enabled by suppressed ionized impurity scattering. Here, we explore additional degrees of freedom for the CdO system, including thickness, substrate, and dopant choice, which afford additional tunability in carrier concentration, plasmonic properties, and epsilon-near-zero modes, while maintaining high carrier mobilities and low optical losses. We utilize a relatively new physical vapor deposition technique, high power impulse magnetron sputtering (HiPIMS), which combines the advantages of magnetron sputtering (high deposition rates and scalability) with the advantages of molecular beam epitaxy (very smooth and dense films). Through the judicious use of dopants, including Ag^+, Y^{3+}, In^{3+}, and F^-, we access more than two orders of magnitude in carrier concentration combined with maximum electronic mobilities over 480 $cm^2/V \cdot s$. In the particular case of fluorine-doped CdO, we also explore doping using a gas-phase precursor, CF_4, as opposed to using a second sputtering source or alloyed target. Gas-phase doping offers additional flexibility and scalability for the synthesis of plasmonic doped metal oxides. This contribution will detail the properties of our plasmonic CdO thin films synthesized with various dopants, as well as the advantages of HiPIMS as a versatile and high quality fabrication technique for plasmonic oxide thin films.

MAESTRO: A SYNCHROTON BEAMLINE FOR ELECTRONIC STRUCTURE DETERMINATION OF IN-SITU GROWN OXIDES AND 2D MATERIALS

Eli Rotenberg

Lawrence Berkeley National Laboratory, CA, UNITED STATES OF AMERICA

MAESTRO, the Microscopic and Electronic Structure Observatory, is a new synchrotron based facility for the study of *in situ* prepared materials, including oxides, 2D van der waals material, semiconductors, metals, and surfaces. This experimental system fuses powerful sample preparation tools (glovebox, MBE, PLD) with state of the art photoemission end stations (µARPES, PEEM, nanoARPES) -- all of which are connected through an automated UHV transfer system. A particularly novel feature of MAESTRO is its nanoARPES setup. This technique mates the merits of state of the art angle resolved photoemission (ARPES) with spatial resolution presently less than 120 nm, with an eventual goal of less than 50 nm, bringing *k* - and energy resolved electronic contrast on the nano- and mesoscale within reach. This talk will review recent studies of the electronic structure of *in situ* grown oxides such as CuO, VO_2, TiO_2. Although these studies are on (nominally) homogeneous systems, prospects for new results from inhomogeneous systems when studied with nano-probe ARPES will be discussed. As an example I will show very recent results on the spatially-resolved electronic structure of hybrid systems composed of monolayers of 2D chalcogenides mechanically transferred onto TiO_2 or STO.

IN SITU X-RAY STUDIES OF EPITAXIAL OXIDE NANOCOMPOSITE FORMATION

Matt Highland[1], Dillon Fong[1], Hua Zhou[2], Carol Thompson[3], Peter Baldo[1], Jeffrey Eastman[1], Paul Fuoss[1]

[1]Materials Science Division, Argonne National Lab, IL, UNITED STATES OF AMERICA, [2]X-ray Science Division, Argonne National Lab, IL, UNITED STATES OF AMERICA, [3]Department Of Physics, Northern Illinois University, UNITED STATES OF AMERICA

Oxide materials exhibit a wide variety of scientifically interesting and technologically useful properties. Recently there has been significant interest in combining the intrinsic properties of multiple materials, as well as engineering new emergent properties, through the formation of phase-separated oxide nanocomposites. In such composite materials, the lattices of two or more separated phases influence one another. This gives rise to unique interfaces and strain states that can be used to manipulate and enhance the properties of a material. The synthesis processes that govern the formation of these materials depend on phase solubility, polarity, strain and synthesis conditions. To better understand these complex processes we utilize in-situ x-ray scattering to probe synthesis in real-time. Our aim in utilizing *in-situ* studies to elucidate, both qualitatively and quantitatively, the models used to describe film growth and suggest new pathways for the synthesis of materials. In this talk, results from *in-situ* studies of the synthesis of In_2O_3:CeO_2 on different crystallographic orientations of YSZ will be discussed. Doped In_2O_3 has been extensively studied and utilized as a transparent conductor and gas sensing material. Nanocomposites of In_2O_3 and doped CeO_2 have recently been reported to exhibit enhanced ionic conductivity. These properties make In_2O_3:CeO_2 an interesting system in which to study the fundamentals of nanocomposite formation. We will describe how misfit strain can influence pattern formation and how the microstructure of these materials can be used to template and guide the composite formation process. We will discuss how these results suggest new strategies for controlling nanocomposite formation both in this material system and oxides in general. This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.

ISLAND GROWTH DYNAMICS IN PULSED LASER DEPOSITION OF $SRTIO_3$

Gyula Eres

Oak Ridge National Laboratory, TN, UNITED STATES OF AMERICA

Heteroepitaxial thin films fabricated by pulsed laser deposition (PLD) often exhibit intriguing thickness dependent behavior manifested by a critical thickness for example, for two-dimensional conductivity at the $LaAlO_3/SrTiO_3$ interface, and metal-insulator transition in ruthenates and nickelates. The thickness dependent behavior is related to intrinsic or extrinsic factors such as substrate overlayer interactions, film growth inhomogeneities, or both. However, the exact mechanisms have been difficult to pinpoint obscuring the fundamental physical phenomena of interest. In this talk I discuss the observation of thickness dependent behavior in the absence of substrate overlayer interactions. Such thickness dependence was observed in the island growth dynamics during high perfection homoepitaxial growth of a model perovskite, $SrTiO_3$. The island size distributions were extracted from real-time measurements of the surface x-ray diffraction diffuse scattering intensity during PLD growth. The analysis was performed by power law plots of the diffuse scattering correlation length describing the island size distribution as a function of time. The analysis shows two distinctly different island growth regimes revealed by a change in the slope of the power law plots. The power law exponent change from $n=1/3$ to $n=1/2$ shows that following nucleation, island growth initially occurs by diffusion limited kinetics, which after 2-3 unit cell growth crosses over to attachment-detachment limited growth. The existence of these two regimes was confirmed by direct measurement of the island size evolution just below and just above the thickness corresponding to the cross over. Theoretical modeling of the island growth kinetics exploring the role of different island growth mechanisms shows that the occurrence of such cross over in the island growth regime signifies a change in the atomic surface transport mechanisms. Importantly, these experiments reveal that in the attachment limited regime the island sizes during the dwell time between successive laser shots remain frozen, which indicates absence of thermally driven Ostwald ripening that is the main mechanism of surface smoothing in thermal film growth. The absence of thermal ripening implies that island growth occurs only during the arrival of the laser plume by non-thermal mechanisms involving collisional relaxation of the superthermal growth species delivered by the laser plume. The significance of the thickness dependent island growth dynamics for heteroepitaxy is that it can affect the evolution of both structure and composition near the interface, which must be considered for understanding interface related thickness dependent phenomena.

DETACHED MELT AND VAPOR GROWTH OF INI IN SUBSA FURNACE

Aleksandar Ostrogorsky[1], Vladimir Riabov[1], Martin Volz[2], Lodewijk Van Den Berg[3], Arne Cröll[4]

[1]Illinois Institute of Technology, IL, UNITED STATES OF AMERICA, [2]NASA Marshall Space Flight Center, AL, UNITED STATES OF AMERICA, [3]Constellation Technology, FL, UNITED STATES OF AMERICA, [4]NASA MSFC, AL, UNITED STATES OF AMERICA

InI is a promising wide energy band gap nuclear detector material. It is ideal for space experiments because it is non-toxic, and has a relatively low melting point of only 351 C. However, it has been established, that melt grown crystals contain a large amount of second phase inclusions/precipitates. Typical size of inclusion is 1 to 27 μm in diameter, while the volume fraction of all sizes is 300 to 600 ppm. The SEM-EDS analysis of the inclusions has revealed that they all contain oxygen and some contain carbon. At present, under sponsorship of NASA and CASIS (Center for the Advancement of Science in Space) we are conducting ground-based experiments with indium iodide (InI) in preparation for the “flight experiments” to be conducted in the SUBSA (Solidification Using a Baffle in Sealed Ampoules) furnace in the Microgravity Science Glovebox at the International Space Station, planned for the summer/Fall of 2017. The experiments conducted on earth (i) include melt growth, (ii) vapor growth experiments conducted in the SUBSA ground unit, (ii) measurements of the volumetric expansion coefficient of the melt and (iv) wetting angle of molten InI. Finite element modeling is conducted, to optimize the design of the flight ampoules, i.e. the Sample Ampoule Assembly (SAA). Alloying with Tl and Ga has given promising results.

EFFECT OF POWER HISTORY ON THE SHAPE AND THE THERMAL STRESS OF LARGE SIZE SAPPHIRE CRYSTAL DURING THE KYROPOULOS PROCESS

Tran Phu Nguyen, Jyh-Chen Chen, Hsiao-Tsun Chuang, Chieh Hu

National Central University, TAIWAN

In this study, the effect of power history on the shape of sapphire crystal and the thermal stress during the Kyropoulos process are numerically investigated. The simulation results show that the shape of crystal and the thermal stress are strongly dependent on the power history. The thermal stress distributions in crystal for all growth stages with different power histories are also studied. The results indicate that maximum thermal stress occurs at the crystal-melt interface, and the value significantly increases as the crystal expands in the crown of crystal. After that, maximum thermal stress reduces as the crystal length gets longer. There is a remarkable enhancement in the maximum von Mises stress when the crystal-melt interface is close to the bottom of the crucible. Different power histories are considered in order to optimize the process with the lowest thermal stress in crystal.

LATEST PROGRESS IN GALLIUM OXIDE EPITAXIAL GROWTH TECHNOLOGIES FOR POWER DEVICES

Masataka Higashiwaki[1], Yoshiaki Nakata[1], Man Hoi Wong[1], Keita Konishi[2], Takafumi Kamimura[1], Ken Goto[3], Kohei Sasaki[3], Akito Kuramata[3], Shigenobu Yamakoshi[3], Hisashi Murakami[2], Yoshinao Kumagai[2]

[1]National Institute of Information and Communications Technology, JAPAN, [2]Department of Applied Chemistry, Tokyo University of Agriculture and Technology, JAPAN, [3]Tamura Corporation, JAPAN

Gallium oxide (Ga_2O_3) has excellent material properties especially for power electronics represented by the extremely large breakdown electric field of 8 MV/cm due to its large band gap of 4.5 eV. It is also attractive from an industrial viewpoint since large-size, high-quality wafers can be manufactured from a single-crystal bulk synthesized by melt-growth methods. These two features have drawn much attention to Ga_2O_3 as a new wide bandgap semiconductor. In this talk, following a short introduction of material properties and bulk melt growth of Ga_2O_3, we will discuss the recent progress in our development on molecular beam epitaxy (MBE) and halide vapor phase epitaxy (HVPE) technologies for Ga_2O_3 thin films, as well as device processing and characterization of lateral metal-oxide-semiconductor field-effect transistors and vertical Schottky barrier diodes fabricated with MBE- and HVPE-grown epitaxial wafers, respectively. MBE has been most popular approach among Ga_2O_3 epitaxial growth techniques. Its main advantage is the precise control over growth parameters and impurity incorporation in epitaxial films. Two types of oxygen sources used for MBE growth are oxygen radicals generated by an RF-plasma cell and ozone. The typical growth temperature range of 500~800°C is similar to MBE growth of GaAs- and GaN-based materials. HVPE is the most promising technique for future mass production of Ga_2O_3 epitaxial wafers, because it can offer high-speed growth of high-quality and thick Ga_2O_3 films with well controlled electrical conductivity. From thermodynamic analysis, GaCl and O_2 were selected as precursors for Ga_2O_3 growth. $SiCl_4$ dopant gas is simultaneously supplied for growing n-type Ga_2O_3. The typical growth temperature is 1000°C, and the highest growth rate without degradation of electrical and material properties of Ga_2O_3 films is about 20 μm/h. Excellent structural and electrical properties have been confirmed for unintentionally-doped Ga_2O_3 thin films that have an extremely low residual carrier concentration of less than 1×10^{13} cm^{-3}. The electron concentration is controllable in the range of 10^{15}~10^{18} cm^{-3} by Si doping. This work was partially supported by "The research and development project for innovation technique of energy conservation" of the New Energy and Industrial Technology Development Organization (NEDO), and Council for Science, Technology and Innovation (CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), Next-generation power electronics (funding agency: NEDO).

FAST CVD CRYSTAL GROWTH OF 4H-SIC FOR POWER DEVICES

Hidekazu Tsuchida, Isaho Kamata, Masahiko Ito, Tetsuya Miyazawa, Norihiro Hoshino

Central Research Institute of Electric Power Industry (CRIEPI), JAPAN

This paper reports our recent achievements in fast 4H-SiC CVD crystal growth, aiming to produce high-quality epilayers with high-throughput and bulk crystals with a low production cost for high-voltage power devices. Toward high-throughput production of high-quality 150 mm-diameter 4H-SiC epilayers, we developed a new single-wafer vertical reactor equipped with a high-speed wafer rotation system. The total time for heating and cooling the wafer between the transfer and growth temperatures (1600-1650ºC) is less than 15 min, which allows production of a 10 um-thick epilayer within 30 min when the growth rate is ~50 um/h. Excellent thickness uniformity of ±2.3% and the doping uniformity of ±6.5% were obtained simultaneously for a 150 mm-diameter 4H-SiC epilayer at a growth rate of 54 um/h. Low densities of downfall and 3C defects, in-grown stacking faults and BPDs were also demonstrated using the reactor. Fast bulk crystal growth of 4H-SiC using a gas-source method was attempted at a seed temperature of 2350-2550ºC using an H_2-SiH_4-C_3H_8-N_2 gas system in a home-made vertical CVD reactor. By adjusting process parameters to improve the trade-off between growth rate and crystal quality, fast 4H-SiC crystal growth at a growth rate exceeding 3 mm/h was achieved while maintaining the low dislocation density (threading screw dislocations: $\sim 2.5\times10^{2}$ cm^{-2}) of the seed crystal.

GROWTH AND CHARACTERIZATION OF SIC

Balaji Raghothamachar, Michael Dudley, Yu Yang, Jianqiu Guo

Stony Brook University, NY, UNITED STATES OF AMERICA

The application of wide band gap semiconductors such as silicon carbide (SiC), aluminum nitride (AlN), gallium nitride (GaN) and related alloys in high power devices in extreme environments is of particular interest in the energy economy. Among the wide bandgap semicondutors, SiC is the most promising semiconductor for efficient and reliable electrical energy conversion and power management. Low defect density active layers are essential and consequently low defect density native substrates are necessary for these applications. The physical vapor transport (PVT) method is used for bulk single crystal growth of SiC. Currently, micropipe defects in bulk SiC material have been effectively eliminated and threading screw dislocations (TSDs) are present at levels of about 10^2 – 10^3 cm^{-2} which propagate into the subsequently grown epitaxial layers. Basal plane dislocations (BPD) densities are at about 10^2 – 10^3 cm^{-2} and threading edge dislocations (TEDs) at 10^4 - 10^5 cm^{-2}. TEDs directly propagate into epitaxial layers while BPDs mostly convert to TEDs during epitaxial growth. These crystal defects prevent the development of cost-effective and reliable high-voltage SiC power devices. Continued reduction in defect content relies on analysis of defect configurations and correlation with growth processes and thermal modeling to optimize the growth process. In this presentation, a comprehensive overview will be presented of PVT growth of bulk SiC and CVD growth of SiC homoepitaxial layers with defect characterization by synchrotron X-ray topography. A complete analysis of the distribution, character and origins of grown-in c-axis screw dislocations, deformation induced basal plane dislocations (BPDs), grown-in threading edge dislocations and stacking fault formation in PVT-grown substrates will be discussed. In addition, dislocation behavior during homo-epitaxy on offcut substrates will be presented. Correlations with thermal modeling will be discussed. Insights from these analyses to achieve elimination of or minimizing specific defects will be demonstrated. Further the impact of these defects on stress relaxation of epilayers and device failure will be revealed through in situ synchrotron studies.

UNDERSTANDING THE MICROSTRUCTURES OF TRIANGULAR DEFECTS IN 4H-SIC HOMOEPITAXIAL LAYERS GROWN BY CVD METHOD

Jianqiu Guo[1], Yu Yang[1], Jungyu Kim[2], Tae Jin Kim[1], Balaji Raghothamachar[1], Michael Dudley[1]

[1]Stony Brook University, NY, UNITED STATES OF AMERICA, [2]LG Chem, KOREA, REPUBLIC OF

Unique properties of silicon carbide (SiC) especially 4H-SiC have enabled many successful applications in the field of power electronics under harsh environment such as high-power, high frequency and high temperature. Despite the rapid development, there remains several issues which limit the performance of these SiC devices. The existence of triangular defects in the active layers for p-n junction diodes, for example, has been reported to reduce the device breakdown voltage for over 65%. [1] Understanding the origin and microstructure of this type of defect becomes very crucial in order to eliminate them or to reduce its density as much as possible. We have recently characterized a 150mm 4H-SiC homoepitaxial wafer using synchrotron X-ray topography and Normaski optical microscopy and observed a significant number of triangular defects in it. The epitaxy growth was carried out by chemical vapor deposition (CVD) method on a 150mm 4H-SiC commercial substrate from Cree. Inc. Optical images and X-ray topographs show that these defects are typical 3C triangular inclusions with the apex in the up-step side while the triangles open towards the down-step direction, which agrees with previous investigations. [2, 3] However, the morphologies of these defects we observed seem to be fairly complex, which indicates their complicated microstructures. Raman spectroscopy mapping and cross-sectional transmission electron microscopy (TEM) has been carried out on selected triangular defects. Raman mappings over these defects have confirmed their nature as 3C-SiC inclusions but more than one orientation is involved as different regions within one triangular defect have distinct Raman peak intensities. High resolution TEM results reveal the existence of double positioning twin boundaries inside the triangle defects, which agrees very well with the optical morphologies of the defects as well as the Raman maps. Further TEM studies underway to understand the formation mechanism for the observed triangle defects will be discussed. [1] T. Kimoto, N. Miyamoto, and H. Matsunami, IEEE Transactions on Electron Devices, 46(3), 471-477 (1999). [2] C. Hallin, A.O. Konstantinov, B. Pecz, O. Kordina, and E. Janzen, Diamond and Related Materials, 6, 1297-1300 (1997) [3] W. Si, M. Dudley, H. Kong, J. Sumakeris, and C. Carter, Jr, Journal of Electronic Materials, 26(3), 151-159 (1997)

REFRACTORY METALS - MATERIAL OF CHOICE FOR SINGLE CRYSTAL GROWTH

Heike Larcher

Plansee SE, AUSTRIA

Molybdenum and Tungsten are widely used in single Crystal growth due to their outstanding properties like high temperature strength, high melting point and low chemical reactivity. Motivated by the strongly increased usage of single crystal materials like Sapphire in the last years, material properties have been investigated in depth and optimized by new production technologies. In the presentation, an overview about newly developed alloys, their properties as well as due to adapted production routes will be shown. Topics in the presentation will be for example new materials for high temperature heaters, new production route for pressed sintered Moly and W crucibles and the , influence of different sheet quantities to Shaper performance.

IMPROVED CARBON AND GRAPHITE MATERIALS FOR CRYSTAL GROWTH

Chong Chen, Helen K. Mayer

GrafTech Advanced Graphite Materials LLC, OH, UNITED STATES OF AMERICA

In the fabrication of crystal growth equipment, carbon/graphite materials play an important role due to their unique properties from thermal to mechanical. One of the most unique property is its high temperature stability at as high as ~3000 °C in the inert atmosphere. Depending on the structure of starting material and process selected, the materials can be tailored to be either a thermal conductor or an insulator. The Coefficient of Thermal Expansion (CTE), porosity and permeability as well as mechanical properties can also be modified to suit the applications through the manufacturing process. The talk will cover the effect of the carbon/graphite structure on their properties, and the impact of product properties to the crystal growth applications. The wide range of carbon/graphite products offered by GrafTech Advanced Graphite Materials suitable for the crystal growth applications will also be introduced and discussed.

APPLICATION OF HEATER MAGNET MODULE FOR IMPROVED CRYSTAL GROWTH OF SEMICONDUCTORS

Christiane Frank-Rotsch[1], Iryna Buchovska[1], Natasha Dropka[1], Radoslaw Zwierz[1], Peter Rudolph[2], Frank M. Kießling[1]

[1]Leibniz Institute for Crystal Growth, GERMANY, [2]Crystal Technology Consulting, GERMANY

The benefit of magnetic fields in crystal growth is well-known since many years, but up to now mostly steady magnetic fields are applied in industrial scale. Compared to steady magnetic fields the application of travelling magnetic fields (TMF) is also very promising since similar effect in the melt can be obtained already by a significantly lower induction. The idea to use the heater itself in a modified configuration to generate a suitable TMF in the melt was put in practice at the Leibniz Institute for Crystal Growth (IKZ). This KRIST*MAG*® technology was developed in close cooperation with industrial and academic partners, within several related projects. The developed so-called heater magnet module (HMM) combines the simultaneous operation with direct current (dc) and alternating current (ac) that enables decoupled generation of heat and TMF. The generated Lorentz forces ensure the control of melt flow. They can be used to improve the crystal quality by: (i)- control of the melt mixing, (ii)- shaping the solid/liquid interface, and (iii)- damping possible temperature oscillations at the growing interface. The direction and magnitude of the TMF can be adjusted by the variation of ac/dc ratio, frequency and phase shift between the heater coils. The suitable parameter field is estimated with the help of numeric simulations and according to the desired growth conditions. On this some selected results will be shown. HMM´s have been designed and realized in various geometries and scales and were built from laboratory to industrial scale. Outgoing from an overview about the already realized heater magnet modules for numerous growth techniques and materials like Czochralski [1], vertical gradient freeze [2], directional solidification [3] the results of recent developments at IKZ will be presented [4]. Results of the positive impact of the KRIST*MAG*® technology on crystal quality, such as enhanced homogeneity of electrical parameters, reduced defect content, improved solid-liquid interface morphology and increased crystallization rates due to TMF melt flow controlling, will be illustrated on basis of selected examples.Thereby the main focus will be on recent growth results of VGF GaAs single crystals and mc-Si grown in HMM´s. [1] P. Rudolph et al., J. Cryst. Growth 318 (2011) 249–254. [2] Ch. Frank-Rotsch et al., J. Cryst. Growth 401 (2014) 702–707.

[3] Ch. Kudla et al., J. Cryst. Growth 365 (2013) 54–58. [4] N. Dropka et al., Patent description WO2014/202284A1.

TEMPERATURE UNIFORMITY OF INDUCTION-HEATED OMVPE SUSCEPTORS AT HIGH TEMPERATURE

Kuang-Hui Li, Hamad S. Alotaibi, Xiaohang Li

King Abdullah University of Science and Technology (KAUST), SAUDI ARABIA

Induction heaters have been employed for OMVPE since early stage of the OMVPE due to its low cost and high reliability.[1] The OMVPE processes of III-V alloys and the later-emerging GaN alloys generally operate at moderate temperatures (<1100 °C). Also, the induction heater was gradually replaced by the resistive heater which provided more precise temperature control. Thus, the temperature uniformity of the induction-heated susceptor at higher temperatures has yet been studied. AlN is crucial for UV optoelectronics. High temperatures >1600 °C have been shown desirable for AlN growth by improving adatom mobility and reducing impurity incorporation.[2] Yet, common resistive heaters could have reliability issue at this temperature range. Consequently, the induction coil has been utilized.[3,4] Since any temperature non-uniformity can be amplified at high temperatures causing varying growth rates and bowing, it is critical to investigate it for high temperature OMVPE reactors. In this work, the temperature uniformity of two conventional designs of induction-heated susceptors has been studied. The first is a pancake induction coil beneath the susceptor (Design-1) [Figure 1(a)]. The second design is a solenoid induction coil around the susceptor outside the reactor (Design-2) [Figure 1(b)]. In the modeling, the target substrate temperature is set to be ~1900 °C. We found that the temperature non-uniformity is severe in Design 1 and acceptable in Design 2, where differences across the 2"-wafer substrates are 55 and 11 °C, respectively, as shown in Figure 2(a) and 2(b). For Design-1, the pancake induction coil has better coupling with outer zone than inner zone of the susceptor, causing the V-shape temperature profile. For Design-2, the solenoid induction coil couples with the outer zone of the susceptor and the heat transfers from the side to the center. However, the susceptor in Design-2 is thicker than the susceptor in Design-1, which serves as a thermal buffer and improve the uniformity. Although Design-2 offers better uniformity, however, it needs twice input power (~40 kW) to reach the target temperature than Design-1 (~20 kW), indicating low heating efficiency. This is because the space between the susceptor and induction coil in Design-2 renders part of magnetic flux useless. Based on this study, we proposed a novel design to minimize the non-uniformity and improve the heating efficiency. More details will be discussed in the conference presentation.

1. Dupuis, APL (1977). 2. Imura, APL (2006). 3. Creighton, JCG (2016). 4. http://agnitron.com/.

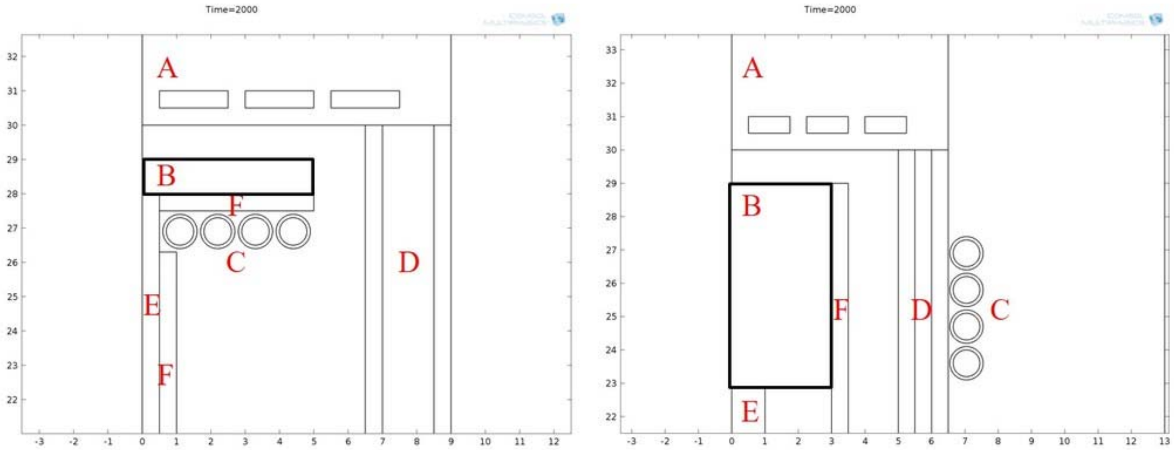


Figure 1. (a) Design-1 with a 22 kW induction heater built beneath of the susceptor. (b) Design-2 with a 40 kW induction heater built around the susceptor, where A, B, C, D, E, and F represent showerhead, susceptor, induction coil, double quartz wall, supporter, and thermal insulator, respectively.

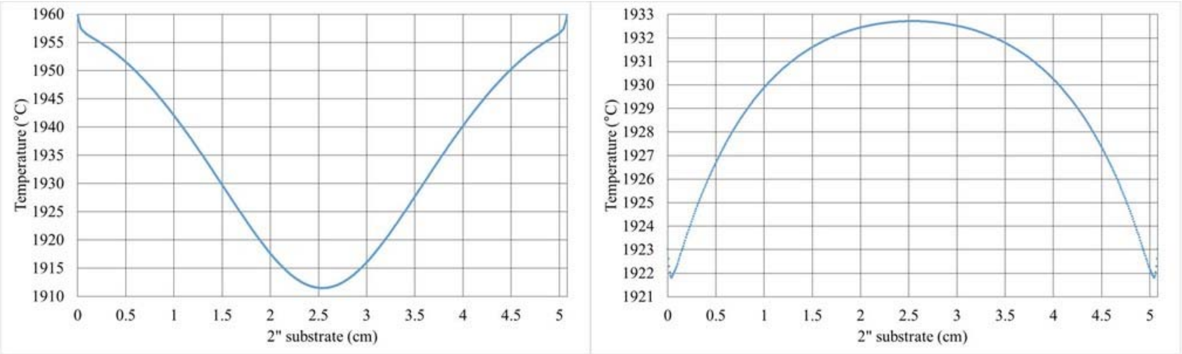


Figure 2. (a) Temperature profile across a 2” substrate in Design-1. (b) Temperature profile across a 2” substrate in Design-2.

A SMALL BUSINESS PERSPECTIVE ON INDUSTRIAL CRYSTAL GROWTH

Candace Lynch, Thomas Caughey, Sergey Selin, Tony Inzalaco

Inrad Optics, Inc., NJ, UNITED STATES OF AMERICA

In this talk we will give one view of the challenges and benefits of conducting industrial bulk crystal growth in a small business setting. At Inrad Optics, we currently grow potassium dideuterium phosphate (KD*P), barium borate (BBO), lithium niobate, stilbene, potassium hydrogen phthalate (KAP), and two varieties of ultraviolet filters. For each material, we will discuss considerations for production crystal growth, post-growth fabrication, and assembly; some applications will also be highlighted. Insights will be shared from recent successes in leveraging government small business innovation research (SBIR) funding to develop new commercial products.

INSIGHTS INTO THE MATERIALS SCIENCE OF COLLOIDAL CRYSTALS FORMED BY DNA-FUNCTIONALIZED PARTICLES

Talid Sinno, Ian Jenkins, Mehdi B. Zanjani, John C. Crocker

University of Pennsylvania, UNITED STATES OF AMERICA

The self-assembly of colloidal crystals from micro- or nano-particles has long been studied as a potential avenue for making novel materials with unique optical and/or structural properties. A diverse range of ordered configurations have now been demonstrated using self-assembling particles driven by one or more of a number of strategies, including external fields, depletion, and functionalized particles. One particularly versatile approach is to functionalize particles with brushes of single-stranded DNA oligomers that are designed to partially hybridize with strands on other particles. These hybridization events collectively create an interaction potential between particles, similar to those that exist between atoms. Careful design of the DNA oligomer sequence allows for the creation of distinct ‘elements’ and the spontaneous assembly of a diverse range of multicomponent crystalline structures. The numerous experimental demonstrations notwithstanding, it is now increasingly clear that a rigorous understanding of the ‘materials science’ governing the kinetics and thermodynamics of crystallization is required in order to fully take advantage of this powerful route for assembling interesting ordered configurations. In this work we employ a combination of computational techniques such as Monte Carlo, Brownian dynamics simulations, and free energy calculations to study the nucleation and growth of colloidal crystals in several vignettes. First, we describe how intentional control of size mismatch between crystals may be used to create ‘floppy’ structures with interesting degrees of freedom. Next, a study of heterogeneity in the interactions between particles is presented that shows how a seemingly detrimental aspect of the DNA-functionalization process can in fact increase crystallization robustness. Finally, we briefly describe how more complex structures may be assembled by creating clusters of particles that exhibit directional bonding.

DIRECT CALCULATION OF SOLID-LIQUID INTERFACIAL FREE ENERGIES FROM EQUILIBRIUM MOLECULAR DYNAMICS SIMULATIONS.

Luis A. Zepeda-Ruiz

Lawrence Livermore National Laboratory, CA, UNITED STATES OF AMERICA

Using expressions for equilibrium thermodynamic potentials of closed heterogeneous systems containing solid and liquid phases in coexsistence, we determine liquid-solid interfacial free energies directly from molecular- dynamics (MD) simulations. This is within the larger context of MD simulations of a system undergoing solidification, where individually-prepared spherical (and cylindrical) solid particles of different sizes grow while surrounded by liquid until they reach a steady state. The resulting equilibrium shapes possess the full structural details expected for solids with anisotropic surface free energies; analysis of the MD during these later times using the simplifying assumption of spherical shapes allows us to extract the orientatationally-averaged quantities needed for coarse-grained, but atomistically-informed, models of solidification kinetics. This work is performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

ANALYSIS OF RE-MELTING PROCESS OF SILICON GROWN BY TRANSVERSE MAGNETIC FIELD APPLIED CZ METHOD

Koichi Kakimoto

Research Institute for Applied Mechanics, Kyushu University, JAPAN

A three-dimensional (3D) analysis was carried out to study re-melting process of silicon crystals at the interface during CZ-Si crystal growth in a transverse magnetic field (TMCZ). A three-dimensional (3D) global model was used in this study. It was found that the interface deflection changes from non-uniformity in the azimuthal direction to an axisymmetric distribution with increasing crystal rotation rate. The mechanism of this effect is mainly attributed to the spatial fluctuations of local growth rate, which is derived as a function of crystal rotation rate and non-uniformity of interface deflection in the azimuthal direction. It contributes to the formation of the shape of the melt–crystal interface through the heat transfer of solidification at the melt–crystal interface. When crystal rotation rate is small local growth rate fluctuations are noticeable and play an important role in the re-melting process and impurity segregation at the melt–crystal interface.

CRYSTALLIZATION BY PARTICLE ATTACHMENT OF METASTABLE NANOPARTICLES IN PULSED LASER DEPOSITION

David B. Geohegan

Oak Ridge National Laboratory, TN, UNITED STATES OF AMERICA

The formation of nanoparticles and their incorporation dynamics during nanosecond-laser PLD has never been well understood. Here we report the intentional formation of ultrasmall amorphous nanoparticles (UANPs) by gas-phase condensation in PLD plumes, and demonstrate their advantages when deposited as metastable “building blocks” for the catalyst-free growth of crystalline nanostructured films of different morphology and phase by the process of crystallization by particle attachment (CPA). Temporally- and spatially-resolved gated-ICCD imaging and ion probe measurements are employed as in situ diagnostics to understand and control the plume expansion conditions for the synthesis of nearly pure fluxes of ultrasmall (~3 nm) amorphous TiO_2 nanoparticles in background gases and their selective delivery to substrates. These amorphous nanoparticles assemble into loose, mesoporous assemblies on substrates at room temperature, but dynamically crystallize by sequential particle attachment at higher substrate temperatures to grow nanostructures with different phases and morphologies. Molecular dynamics calculations are used to simulate and understand the crystallization dynamics. This work demonstrates that non-equilibrium crystallization by particle attachment of metastable ultrasmall nanoscale “building blocks” provides a versatile approach for exploring and controlling the growth of nanoarchitectures with desirable crystalline phases and morphologies. This process appears quite general, and although we concentrate on the formation of anatase, B-phase, and rutile (as well as ‘black anatase’) TiO_2 nanostructures and films, we will show the formation and integration of other oxide nanostructures (e.g. MgO, SnO_2) as well as atomically-thin 2D materials (e.g. GaSe, $MoSe_2$) by PLD of UANP precursors. Research sponsored by the U.S. Dept. of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Div. (synthesis science) and Scientific User Facilities Div. (characterization science).

ENGINEERING DEFECT FORMATION IN FUNCTIONAL OXIDE THIN FILMS AND HETEROSTRUCTURES

Regina Dittmann[1], Felix Gunkel[2], Felix Hensling[1], Chencheng Xu[1]

[1]Forschungszentrum Jülich GmbH, GERMANY, [2]Institut f˙ur Werkstoffe der Elektrotechnik II, RWTH Aachen University, GERMANY

The functional properties of complex transition metal oxides are very sensitive on the details of the electronic structure and are thereby strongly influenced by the elemental composition and the lattice disorder. Although device materials typically require unparalleled levels of purity and perfection, the presence of point and extended defects in oxides have been identified to be advantageous for a variety of applications. Therefore, the precise control over the defect configuration is one of the key challenges for the oxide thin film growth community. Defect formation during pulsed laser deposition growth can be either governed by the defect equilibria at the given growth conditions or by the plume dynamics or growth kinetics. We will present detailed studies on selected prototypical oxide thin film systems such as $SrTiO_3$, $SrRuO_3$ and $SrTiO_3/LaAlO_3$ which enabled us to disentangle the different factors influencing the formation of both, oxygen and cation vacancies. By investigating the early stage of growth by in situ AFM and RHEED we could reveal the complex interplay between non-stoichiometry, growth mode and the formation of extended defects such as antiphase boundaries and Ruddlesden-Popper-type of defects. We will furthermore give examples how defect engineering can be employed to fabricate thin film heterostructures and devices with tailored functional properties.

TUNING THE SUPERCONDUCTIVITY IN SINGLE-LAYER FESE/OXIDES BY INTERFACE ENGINEERING

Haichao Xu, Rui Peng, Donglai Feng

Fudan University, CHINA

The discovery of high T_c superconductivity in single-layer FeSe films has enormous implications for both searching new high Tc superconductors and exploring the important factors for high temperature superconductivity. In this talk, I will show our angle-resolved photoemission studies on various FeSe-based heterostructures grown by molecular beam epitaxy. We systematically studied the electronic structures and superconducting properties of FeSe with varied strain, different interfacial oxide materials, different thicknesses, and controlled carrier doping. We found that the electronic correlations and superconducting gap-closing temperatures could be tuned by interfacial effects. We exclude the direct relation between superconductivity and tensile strain, or the energy of an interfacial phonon mode, and demonstrate the crucial and non-trivial role of FeSe/oxide interface on the high pairing temperature. By tuning the interface, superconducting pairing temperature reaches up to 75K in FeSe/Nb:$BaTiO_3$/$KTaO_3$ with the in-plane lattice of 3.99Å, which sets a new superconducting-gap-closing temperature record for iron-based superconductors, and may pave the way to more cost-effective applications of ultra-thin superconductors. In extremely tensile-strained single-layer FeSe films, we found that the Fermi surfaces consist of two elliptical electron pockets at the zone corner, without detectable hybridization. The lifting of degeneracy is clearly observed for the first time for the iron-based superconductors with only electron Fermi surfaces. Intriguingly, the superconducting gap distribution is anisotropic but nodeless around the electron pockets, with minima at the crossings of the two pockets. Besides, using K-dosing on FeSe surface, we revealed an exotic phase diagram of FeSe as a function of electron doping and obtained superconductivity around 46 K in an FeSe layer under electron doping without interfacial effects. Our results provide important experimental foundations for understanding the interfacial superconductivity and the pairing symmetry puzzle of iron-based superconductors, and also provide clues for further enhancing Tc through interface engineering.

RAPID-ANNEAL SOLID PHASE EPITAXY OF ATOMICALLY FLAT HIGH SURFACE ENERGY RUO_2(001) FILMS

Paul C. Snijders[1], Yang Wang[1], Yang Song[1], Rui Peng[1], Andreas Herklotz[1], Matthew F. Chisholm[1], Zili Wu[1], Thomas Z. Ward[1], Hanno H. Weitering[2]

[1]Oak Ridge National Laboratory, UNITED STATES OF AMERICA, [2]University of Tennessee, TN, UNITED STATES OF AMERICA

The functional design of nanoscale transition metal oxide heterostructures depends critically on the growth of atomically flat epitaxial thin films. Often, improved functionality is expected for heterostructures and surfaces with orientations that do not have the lowest surface free energy. For example, crystal faces with a high surface free energy, such as rutile (001) planes, frequently exhibit higher catalytic activities but are correspondingly harder to synthesize due to energy-lowering faceting transitions. Here we propose a broadly applicable rapid-anneal solid phase epitaxial synthesis approach for the creation of atomically flat, high surface free energy oxide heterostructures. This approach takes advantage of the fast heating and cooling capabilities of an in-situ laser heater. We demonstrate its efficacy *via* the synthesis of atomically flat, thin epitaxial RuO_2(001) and TiO_2(001) films. We monitor the growth using reflection high energy electron diffraction, we use in situ scanning tunneling microscopy, and ex situ atomic force microscopy, x-ray diffraction, and scanning transmission microscopy to evaluate the quality of the film and shed light on the growth mechanism. Moreover, we demonstrate that the RuO_2(001) surface has a superior oxygen evolution activity, quantified by their lower onset potential and higher current density, relative to that of more common RuO_2(110) films that were grown by conventional molecular beam epitaxy. This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

LOW COST III-V PHOTOVOLTAICS BY HYDRIDE VAPOR PHASE EPITAXY

Kevin L. Schulte[1], John Simon[1], Nikhil Jain[1], John Mangum[2], Corinne E. Packard[2], Brian P. Gorman[2], Aaron J. Ptak[1]

[1]National Renewable Energy Laboratory, CO, UNITED STATES OF AMERICA, [2]Colorado School of Mines Department of Metallurgical and Materials Engineering, CO, UNITED STATES OF AMERICA

III-V photovoltaics (PV) offer significant advantages over commercial Si such as higher conversion efficiency, reduced weight, flexibility, and the ability to easily form multi-junction stacks. III-Vs are ideal for distributed applications where high efficiency and low weight are required, such as rooftop PV, space power, unmanned aerial vehicles (UAVs), and portable power. High manufacturing costs have generally limited their penetration to niche markets, however. Typically these materials are grown by metalorganic vapor phase epitaxy (MOVPE), which is an expensive batch process. Hydride vapor phase epitaxy (HVPE) offers the benefit of higher throughput, as well as reduced input costs by substitution of metalorganic reagents with metal chlorides generated *in situ* from elemental metals and HCl. As a consequence of the high growth rates and *in situ* reactant generation, however, the formation of abrupt heterointerfaces fundamental to the designs of modern semiconductor devices, such as high efficiency PV, has traditionally been problematic. Using our custom HVPE reactor design, which contains two growth chambers between which the substrate is transferred dynamically, we demonstrate the formation of PV devices with abrupt, high quality heterointerfaces featuring combinations of multiple different III-V materials. We have achieved a 23.8% efficient single-junction GaAs cell with GaInP passivation layers, as well as 18.7% efficient 1.7 eV GaInAsP cells, which are desirable for tandems with silicon. As a path to 30% efficiency, progress towards an all-HVPE-grown GaInP/GaAs tandem will be demonstrated. We demonstrate the growth and characterization of thick GaInP layers free of extended defects, and incorporate them into simple GaInP p-n junction solar cells for the first time using HVPE. The effect of cell parameters such as emitter thickness and base doping on cell performance is discussed. Optical modeling is performed to understand the performance of the devices in context of the ultimate limit of this specific design. We show that our devices are limited by the presence of deep level defects, and elucidate the relationships between growth parameters, such as growth temperature and V/III ratio, and defect concentrations. Using this understanding we demonstrate a 12.8% efficient GaInP device measured under the AM1.5G solar spectrum by employing an optimized V/III ratio, despite a lack of surface passivation. As another step towards an HVPE-grown tandem, the development of the first HVPE grown tunnel diode is demonstrated with peak tunneling current > 8 A/cm^2, equivalent to more than 500 suns concentration. A pathway to 30% efficiency HVPE-grown tandem devices is discussed.

FIRST BIFACIAL GROWTH AND BIFACIAL EPITAXIAL LIFT OFF (B-ELO) OF 3J SOLAR CELLS ON 6 INCH GAAS SUBSTRATES

Kamran Forghani, Andree Wibowo, Chris Stender, Joshua D. Wood, Noren Pan

MicroLink Devices Inc., IL, UNITED STATES OF AMERICA

Multijunction III-V solar cells have the highest conversion efficiencies among competing photovoltaics due to the ability to provide absorption at multiple energy gaps across the solar spectrum. Of these, III-V inverted metamorphic (**IMM**) solar cells are technologically attractive, as they have projected efficiencies of beyond 50% with increasing junction number. However, the production cost remains a major hurdle to commercialize them for consumer market applications. We report bifacial growth and epitaxial lift-off of large (6” or 150mm) GaAs substrates. An IMM solar cell structure with three junctions (3J: GaInP/GaAs/GaInAs) was grown on GaAs substrates using an Aixtron 2800 MOVPE reactor equipped with LayTec’s *in situ* stress, reflectance, and temperature monitoring. After the first growth, the GaAs substrates were flipped over, and we repeated the growth, growing a second 3J solar cell on the GaAs/3J structure. The GaAs substrates with 3J solar cell devices on either side went through MicroLink’s proprietary epitaxial lift off (**ELO**) process. Two ELO 3J foils, one per growth side, lifted off the GaAs substrate. This is the first successful demonstration of a concurrent bifacial epitaxial lift off (**B-ELO**) from the 6-inch GaAs. The substrates can be repolished for further MOVPE growth runs. We present a comparison of the devices grown on both faces of the substrates. Bifacial CVD growth combined with B-ELO offers huge opportunities for (opto-)electronics, photovoltaics and hybrid devices, and some of these device concepts will be discussed in this presentation. The potential advantages and challenges to this method will also be presented.

ELECTRON CHANNELING CONTRAST IMAGING OF GAINP/GAAS/SI SOLAR CELLS

Ryan France[1], Markus Feifel[2], Jens Ohlmann[2], David Lackner[2], Frank Dimroth[2]

[1]National Renewable Energy Laboratory, UNITED STATES OF AMERICA, [2]Fraunhofer Institute for Solar Energy, GERMANY

Multiple research groups have now demonstrated APB-free epitaxy of III-V material on Si substrates, paving a pathway towards low-cost III-V/Si multijunction solar cells with over 30% efficiency. However, solar cells require large-area analysis of other structural defects such as dislocations and stacking faults, for which electron channeling contrast imaging (ECCI) is well-suited. Here, we discuss recent progress that has led to high efficiency III-V on Si triple junction solar cells and analyze the device components using ECCI. The directly-grown III-V on Si multijunction solar cell relies on multiple recent advances: 1) APB-free III-V material on Si substrates via low-temperature pulsed-growth MOVPE, 2) SiN-based diffusion barriers that protect the Si minority carrier lifetime during growth and 3) a metamorphic GaAsP buffer to translate the lattice constant between the Si substrate and the III-V subcells. Using these techniques, a GaInP/GaAs/Si triple junction solar cell with 19.7% efficiency is demonstrated, showing the realistic potential of III-V/Si solar cells. However, nearly identical GaInP/GaAs dual junction cells grown on GaP substrates have higher subcell voltages, implying additional non-radiative recombination on the Si platform. ECCI of the metamorphic GaAsP buffers shows that the threading dislocation density is nearly an order of magnitude higher on Si substrates than GaP substrates. To investigate the source of the dislocation density difference, thin layers of GaP on Si were grown and imaged. Both stacking fault pyramids and pits are observed at densities of 1e6 cm^{-2} to 5e7 cm^{-2}. Furthermore, these defects are observed to either generate or block gliding dislocations, and thus contribute to the increased dislocation density of the metamorphic GaAsP buffer on GaP/Si templates. We find that the stacking fault pyramid density is related to the pulsing sequence of the III-V nucleation, and the pits are formed during the deoxidation step of the III-V regrowth on GaP/Si templates. Optimizing the pulsing sequence and regrowth procedure using ECCI and AFM characterization leads to GaP/Si templates that are structurally perfect enough for large area devices.

GROWTH OF GAASPN P-I-N JUNCTIONS ON SI SUBSTRATES WITH LATTICE MATCHING CONDITIONS FOR MONOLITHIC III-V/SI MULTI-JUNCTION SOLAR CELLS

Keisuke Yamane, Kento Sato, Masaya Goto, Kenjiro Takahashi, Hiroto Sekiguchi, Hiroshi Okada, Akihiro Wakahara

Toyohashi University of Technology, JAPAN

GaAsPN quaternary alloys are essential candidates of materials for subcells of dual junction solar cells on Si substrates due to their perfect lattice matching to Si with satisfying the ideal bandgap energy of 1.7 eV. However fundamental researches on GaAsPN have been mainly performed on GaP substrates due to the difficulties on growth of III-V-V-V materials and by mismatches of polarity. Recently we have successfully achieved doping controls of *p*-and *n*-types GaAsPN alloys by precisely tuning the growth condition and performing a post growth annealing. In this work, we demonstrate GaAsPN *p-i-n* junctions on Si substrates with lattice matching conditions by using and high quality GaP/Si heteroepitaxy technique. GaAsPN *p-i-n* samples were grown on 2-inch vicinal Si (001) substrates by using molecular beam epitaxy apparatus. After a thermal treatment of Si substrate, a 30-nm-thick GaP layer was grown at 440°C by modified MEE methods followed by MBE of GaAsPN *p-i-n* layers at 550°C. The MBE-grown layers were consisted of 20-nm-thick p^+-GaP / 30-nm-thick *p*-GaAsPN / 900-nm-thick *i*-GaAsPN (undoped) / 100-nm-thick *n*-GaAsPN. The As and N compositions were 19% and 6 %, respectively, which is almost Si-lattice matching condition with bandgap energy of 1.7 eV. From the start of the MEE growth to the end, a 1×1 streaked patterns were changed to a 2×4 streaked one. The 2×4 patterns maintains during the growth of GaAsPN *p-i-n* structure, meaning that two dimensional growth was proceeded. As a result, crack free and mirror surface was obtained. The symmetrical 2θ-ω HRXRD profiles of the samples were collected, together with a dynamical simulation of the grown-layers without relaxation. The 2θ angles of $GaAs_{0.75}P_{0.19}N_{0.06}$ and GaP layers were in good agreement with the simulation, indicating that all layers were coherently grown on the Si substrate. The FWHM value of 004 XRC was 11 arcsec, which is comparable to that of the Si substrate. A TEM image showed that defect-free layers were successfully grown on Si. Finally, in order to measure the electrical properties of the samples, AuZn and AuSb electrodes were fabricated as front and back contacts, respectively. A current voltage characteristic shows typical rectifying curve with ideal factor of 1.9 and series resistance of 8.9 mΩcm^2 .The reverse saturation current of the device was estimated to be in the order of 1 nA/cm^2 which is indicative of high crystallinity of the device layer.

SELECTIVE AREA GROWTH OF GAAS ON SI FOR PHOTOVOLTAIC APPLICATIONS

Michelle Vaisman[1], Nikhil Jain[2], Qiang Li[3], Kei M. Lau[3], Emily Makoutz[2], William E. Mcmahon[2], Jeramy D. Zimmerman[4], Adele C. Tamboli[2], Emily L. Warren[2]

[1]Yale University, CT, UNITED STATES OF AMERICA, [2]National Renewable Energy Lab, CO, UNITED STATES OF AMERICA, [3]Hong Kong University of Science and Technology, HONG KONG PRC, [4]Colorado School of Mines, CO, UNITED STATES OF AMERICA

Growth of III-V materials directly on Si has been a long-standing goal of the epitaxial community for applications in optoelectronics. In particular, heteroepitaxy is a promising approach to mate the high-efficiency of III-V multijunction photovoltaics with the low-cost enabled by large-area Si substrates. The incompatibility of these materials introduces growth challenges, such as material polarity, lattice mismatch, and a difference in thermal expansion coefficient. To achieve material quality sufficient for device operation, current epitaxial approaches utilize expensive, thick graded buffers that undermine commercial viability. Here, we use selective area growth (SAG) and aspect ratio trapping as a means to achieve high quality GaAs grown directly on Si without the use of thick graded buffers. We investigate a two-step GaAs growth process: the SAG of GaAs to nucleate in V-grooved (100) Si that is patterned with SiO_2 stripes, followed by the removal of the SiO_2 and bulk GaAs growth, as described previously [1]. These CMOS-compatible on-axis GaAs/Si templates are free of antiphase domains, and have a threading dislocation density of just 4×10^7 cm^{-2}. We demonstrate a functional GaAs solar cell on these templates, with preliminary devices exhibiting an efficiency of 6.3% [Fig. 1(a)]. We furthermore investigate an approach that uses nano-imprint lithography (NIL) of sol-gel as a low-cost patterning technique for SAG on offcut Si. We are able to grow GaAs islands within various nano-features along with coalesced films on patterned Si [Fig. 1(b-c)]. Nucleation density can be controlled as a function of feature size. Our results are a promising step towards the realization of low-cost, high-quality III-V on Si

growth for both photovoltaic and CMOS applications.

Fig. 1. (a) Current-voltage characteristics for a p-on-n GaAs solar cell grown directly on V-grooved Si (green) and homoepitaxially on a GaAs substrate (red) without the use of a graded buffer. (b) Planar and (c) cross-sectional SEM of a coalesced film of GaAs grown via SAG on Si patterned with lines with NIL.

[1] Q. Li, K. W. Ng, and K. M. Lau, “Growing antiphase-domain-free GaAs thin films out of highly ordered planar nanowire arrays on exact (001) silicon,” *Appl. Phys. Lett.*, vol 106, p. 072105, 2015.

SINGLE-CRYSTAL-LIKE THIN FILM III-V MATERIAL DIRECTLY GROWN ON HASTELLOY TAPE FOR FLEXIBLE SOLAR CELLS

Jae-Hyun Ryou[1], Venkat Selvamanickam[2], Sara Pouladi[2], Mojtaba Asadirad[2], Monika Rathi[2], Seung Kyu Oh[2], Devendra Khatiwada[2], Pavel Dutta[2], Shahab Shervin[2], Yao Yao[2], Yongkuan Li[2], Jie Chen[2]

[1]University of Houston, TX, UNITED STATES OF AMERICA, [2]University of Houston, UNITED STATES OF AMERICA

There is a fast increasing demand for thin film solar cells (SCs) in the photovoltaics industry due to their several advantages including light-weight, mechanical flexibility, low cost, wide range of applications, and easy scalability. III-V compound semiconductor materials are the top candidates for thin-film SCs as they have high absorption coefficients which enable them to provide a SC with complete photon absorption of the entire terrestrial solar spectrum within a few micron thickness of the material. III-V wafer based SCs have showed the state-of-the-art photon conversion efficiency. However, their applications have been limited mainly due to the high-cost of initial materials, inflexible and brittle wafer substrate. In this study, we develop a technology that can provide high-quality epitaxial semiconductor thin films on low-cost metal foils bypassing expensive wafer substrates while also offering scalability and flexibility. The epitaxial (Al)GaAs semiconductor thin films are grown on the biaxially textured Ge thin film which is grown on the polycrystalline metal tape through crystallinity-transitional buffer layers from poly- to single-crystalline-like material, consisting of biaxially textured oxide layers. A 2-dimentioal numerical simulation has been employed to evaluate this photovoltaic technology. The simulation result has showed that a single junction SC based on single-crystalline-like (Al)GaAs thin films has the potential to offer ~17% conversion efficiency. The single-crystal-like thin-film (Al)GaAs device structure layers are developed to the flexible SJ GaAs SC with front illumination geometry due to the presence of insulating buffer layers. The photovoltaic characteristics of the proof-of-concept flexible SJ GaAs SC under AM 1.5G 1-Sun illumination are promising. The GaAs SC shows the photon conversion efficiency of ~5% with open circuit voltage of 330 mV, short circuit current of J_{sc} of 21 mA/cm^2 and fill factor of 73%. Further improvement in epitaxial material quality, device design and fabrication process optimization would improve the device performance. This approach offers a new technology platform which has the potential for next-generation low-cost high efficiency flexible SCs.

THREE-DIMENSIONAL, HIGH ASPECT RATIO GAN NANOSTRUCTURES BY TOP-DOWN ETCHING

George T. Wang[1], Benjamin Leung[1], Miao-Chan Tsai[2], Changyi Li[2], Ganesh Balakrishnan[2]

[1]Sandia National Laboratories, NM, UNITED STATES OF AMERICA, [2]The University of New Mexico, NM, UNITED STATES OF AMERICA

Chemical etch processes for GaN materials and devices are significantly underdeveloped due to its apparent inertness to common wet etchants. For the processing and fabrication of optical structures and devices, wet anisotropic (crystallographic) chemical etching is a key process technology for the fabrication of semiconductor devices. Thus, to fully realize the potential of the III-nitrides in new optical and electronic devices, such as in optical nano- and microcavity lasers, more complete knowledge and development of techniques with anisotropic etching are needed. Here, we explore the etch characteristics of GaN using the general geometric principles of crystallographic dissolution processes to enable the prediction of facet-determined etch structures. Significant etch rates albeit with extremely high crystallographic anisotropy are observed in KOH-based etchants. Fabricating novel GaN based devices requires understanding the consequences of this extremely high etch rate anisotropy for the resulting etch geometries. For silicon, full knowledge of orientation-dependent etch rates and geometry evolution has enabled design of silicon MEMS structures. Here, we use the same framework (Wulff-Jaccodine method) for understanding and predicting the geometry of the facet evolution and final structure, and apply it to GaN. We perform the first complete orientation-dependent etch rate measurements, clearly showing fast a-plane etch rate relative to m-plane, and use them to predict the faceting of pillar structures with good agreement with experiment. Finally, we use these developments in GaN wet etching to go beyond the current paradigm of bottom-up grown hexagonal nanowires to fabricate functional optical nanowire and microcavity structures with controlled three-dimensional cross-sectional shapes, where faceting enables smooth sidewalls for a high-quality cavity structure. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

EFFECT OF ALGAN UNDERLAYER ON REVERSE-LEAKAGE CURRENT REDUCTION IN GAN/INGAN CORE-SHELL NANOSTRUCTURE LIGHT-EMITTING DIODES

Mohsen Nami, Ashwin Rishinaramangalam, Darryl Shima, Ganesh Balakrishnan, Steve Brueck, Daniel Feezell

University of New Mexico, Center for High Technology Materials, UNITED STATES OF AMERICA

Group III-Nitride family is the most widely used material system to fabricate visible optoelectronic devices. GaN based light-emitting diodes (LEDs) grown on conventional polar c-plane sapphire substrates suffer from high internal polarization-related electric fields, resulting in spatially separated electron-hole wave functions and reduced radiative efficiency. Furthermore, the radiative efficiency is further reduced at longer wavelengths (also known as green gap) and high current densities (efficiency droop). Alternately, bottom-up GaN/InGaN core-shell nanostructure LEDs grown on c-plane GaN are promising candidates to mitigate efficiency droop due to their larger surface area to volume ratio and to improve radiative efficiency via access to various nonpolar and semipolar orientations with lower polarization-related electric fields. Despite numerous reports related to the growth of bottom-up core-shell nanostructures, there have been limited reports of high-performance electrically-injected nanostructured devices. The most significant challenge in obtaining these devices is achieving efficient p-type doping in the nanostructures that is easily hindered by the compensation of magnesium acceptors with donor-type. In this work, we present a simple technique to improve the performance of GaN nanostructured LEDs using a thin n-type AlGaN underlayer. The effects of various MOCVD growth techniques, AlGaN layer thickness and trimethylaluminum (TMAl) flow rates during the n-type AlGaN underlayer growth on the reverse-leakage current are studied and a significant reduction of reverse-leakage current is demonstrated for electrically injected nanostructure LEDs with the underlayer. Secondary ion mass spectroscopy (SIMS) profiles indicate lower O and Si concentrations in samples with the underlayer, when compared to samples without the n-AlGaN underlayer. Additionally, LEDs with an underlayer exhibit enhanced Mg incorporation for the same gas-phase flow rates.

POLARITY INVERSION IN EPITAXIAL ALN: NEW INSIGHTS IN OBTAINING SELECTIVE AREA EPITAXY OF GA-POLAR GAN-ON-SILICON

Kris Bertness, Matt Brubaker, Alexana Roshko, Joel Weber, Todd Harvey, Paul Blanchard, Bryan Spann, Norman Sanford

NIST, CO, UNITED STATES OF AMERICA

Crystallographic polarity plays a central role in the synthesis of III-N materials, including selective area growth (SAG) of epitaxial GaN nanostructures. We have previously demonstrated that it is possible to obtain both polarity configurations on Si (111) substrates by controlling the V/III ratio during growth of an intermediary AlN layer [Brubaker, et al., Cryst. Growth Des., 16 (2016), 596]. However, the exact nature of this effect has yet to be determined. Additionally, inversion domains are sometimes observed for Ga-polar SAG, resulting from a mixed polarity growth mode. To address these issues, we have studied the mechanism for AlN polarity inversion, using a combination of reflection high energy electron diffraction (RHEED) and cross-sectional scanning transmission electron microscopy (STEM). STEM indicates that polarity inversion occurs from N- to Al-polarity. RHEED patterns obtained as growth proceeds through the inversion layer show the emergence of Al-polar surface reconstructions, corroborating the STEM measurements, and further reveal a simultaneous transition from streaky-to-spotty diffraction patterns. The latter observation signifies an unintentional transition from Al- to N-rich growth conditions that is coincident with the polarity inversion. The emerging variation in V/III ratio is possibly related to increased output of the nitrogen plasma during warmup. These observations suggest that polarity inversion does not proceed through an abrupt impurity layer, but rather is triggered by the onset of N-rich growth conditions. It was also found that, once completed, polarity inversion was irreversible and Al-polarity persisted despite changes to the V/III ratio. In this manner, the V/III ratio and polarity are decoupled post inversion, allowing Al-polar AlN growth to be performed under stoichiometric flux conditions more amenable to high-quality AlN growth. Using these conditions, buffer layers for SAG were prepared using a process that allowed for complete AlN polarity inversion. Subsequent regrowth by SAG on these optimized buffer layers produced nanostructures with uniform Ga-polar characteristics.

QUANTUM SIZE CONTROLLED ETCHING OF INGAN QUANTUM DOTS

George T. Wang[1], Benjamin Leung[1], Xiaoyin Xiao[1], Arthur J. Fischer[1], Daniel D. Koleske[1], Ping Lu[1], Miao-Chan Tsai[2], Michael E. Coltrin[1], Jeffrey Y. Tsao[1]

[1]Sandia National Laboratories, NM, UNITED STATES OF AMERICA, [2]The University of New Mexico, NM, UNITED STATES OF AMERICA

III-nitride quantum dots (QDs) have significant potential for single-photon sources or gain media for low threshold and high efficiency visible and UV lasers, among others. “Bottom-up” Stranski− Krastanov growth is widely used, however both the size distribution and densities are difficult to precisely control. Here, we show that a top-down fabrication process that itself can be controlled by the properties of the nanostructures being fabricated. This process, called quantum size controlled photoelectrochemical (QSC-PEC) etching, uses laser excitation at a selected and narrowband wavelength to control the final sizes of the QDs through an etch that self-terminates when the QD band gaps increase due to quantum confinement effects until they exceed the energy of the incident photons. Beginning with epitaxially grown InGaN films, we examine the etch process from large to quantum-scale nanostructures with AFM, TEM, and photoluminescence measurements. Quantitative analysis of size and density of the ensemble are made after image-post processing techniques and deconvolution of the AFM tip and QD. We further investigate the passivation of the QDs through regrowth of AlGaN and GaN capping layers, as well as fabrication of multilayers of QDs from multiple-quantum well structures. These results show the potential for a combination of unprecedented uniformity and density towards InGaN QD devices. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04–94AL85000.

SELF-ASSEMBLED GROWTH OF GAN NANOWIRES ON METALLIC SUBSTRATES

Lutz Geelhaar

Paul-Drude-Institut für Festkörperelektronik, GERMANY

Epitaxy in the form of free-standing vertical nanowires allows the combination of dissimilar materials in high crystalline quality, because strain induced by structural mismatch can elastically relax at the free sidewalls, and dislocation lines are likely to terminate there. An extreme example for this conceptual advantage are single-crystalline GaN nanowires on metallic substrates. In plasma-assisted molecular beam epitaxy, GaN nanowires grow by self-assembly on various substrates, with Si being the most popular one. The formation of these nanowires is not induced by a droplet or particle but takes place spontaneously. Strikingly, these single-crystalline nanowires elongate perpendicularly to a smooth substrate even without any epitaxial relation. These properties inspired us to pursue their growth on metallic substrates, i.e. substrates that differ not only in lattice constant but also in chemical bonding. Metallic substrates are very interesting for applications because of their high electrical as well as thermal conductivity and optical reflectivity. The first considered case are single-crystalline Ti films sputtered onto sapphire. Upon exposure to reactive nitrogen, these films are converted into TiN, which is also a metal. On this surface, vertically oriented GaN nanowires form that exhibit an epitaxial relationship to the substrate. Low temperature photoluminescence spectroscopy reveals excitonic transitions whose energy, line width, and decay time are essentially the same as for state-of-the-art GaN nanowires grown on Si. Hence, the crystalline quality of the nanowires grown on TiN is equivalent. A detailed growth study shows that due to differences in adatom diffusion, on TiN nanowire ensembles can be fabricated with much lower number density than on Si. Thus, the coalescence of neighboring nanowires can be avoided up to a greater height. As an even more drastic example, we employed as substrate flexible, polycrystalline Ti foils. Also in this case, GaN nanowires grow that are in the vast majority oriented vertically. Again, their photoluminescence demonstrates a high crystalline perfection. Very importantly, the room temperature photoluminescence spectrum does not change upon bending of the foil, which indicates that the nanowires are well anchored to the substrate. In addition, we have investigated as substrate epitaxial graphene layers synthesized on SiC. GaN nanowires grow epitaxially with vertical orientation and in high structural quality. At the same time, our study shows that graphene is slowly etched by the N plasma. Thus, continuous graphene layers are found below the GaN nanowires and connecting them only if multi-layer graphene is used as the starting surface.

PHASE FIELD MODELING OF GRAIN STRUCTURE EVOLUTION DURING DIRECTIONAL SOLIDIFICATION OF MULTI-CRYSTALLINE SILICON SHEET

Chung-Wen Lan, H.K. Lin

Dept. of Chem. Eng., National Taiwan University, TAIWAN

Evolution of grain structures and grain boundaries (GBs), especially coincident site lattice (CSL) GBs, during directional solidification of multi-crystalline silicon sheet are simulated by using a phase field model for the first time. Since CSL GBs, having lower mobility, tend to follow their own crystallographic directions despite thermal gradients, the anisotropic energy and mobility of GBs are considered in the model. Three basic interactions of GBs during solidification are examined and they are consistent with experiments. The twinning process for new grain formation is further added in the simulation by considering twin nucleation. The effect of initial distribution of GB types and grain orientations is also investigated for the twinning frequency and the evolution of grain size and GB types.

OPTIMIZATION OF HEAT TRANSFER DURING THE DIRECTIONAL SOLIDIFICATION PROCESS OF 1600 KG SILICON FEEDSTOCK CAPACITY

Hu Chieh[1], Jyh-Chen Chen[1], Thi Hoai Thu Nguyen[1], Hou Zhi Zhong[1], Chun Hung Chen[2]

[1]Department of Mechanical Engineering, National Central University, TAIWAN, [2]Research and Development Division, GlobalWafers Co., Ltd., TAIWAN

In this study, we have performed a series of transient global numerical simulations to optimize the heat transfer during the directional solidification (DS) process of 1600 kg silicon feedstock capacity. The hot zone in an industrial DS furnace and the growth conditions are modified to improve the quality of crystals and enhance the energy saving. The power ratios between the side and the top heaters and the raise velocity of the side insulation are designed to control the thermal field which is able to produce the 1600 kg multi-crystalline silicon ingot with a good quality. The optimization is estimated by analyzing the shape of the crystal-melt interface, the growth time and the heating power consumption during the solidification process. Moreover, the evolution of temperature gradient reflecting the thermal stress distribution in the crystal are also discussed. Adjusting the power ratios and the raise velocity of the side insulation may produce the flatter crystal-melt interface shape and the lower temperature gradient in the crystal.

CONTROL OF CRUCIBLE MOVEMENT ON MELTING PROCESS AND CARBON CONTAMINATION IN CZOCHRALSKI SILICON CRYSTAL GROWTH

Xin Liu, Xuefeng Han, Satoshi Nakano, Koichi Kakimoto

Research Institute for Applied Mechanics, Kyushu University, JAPAN

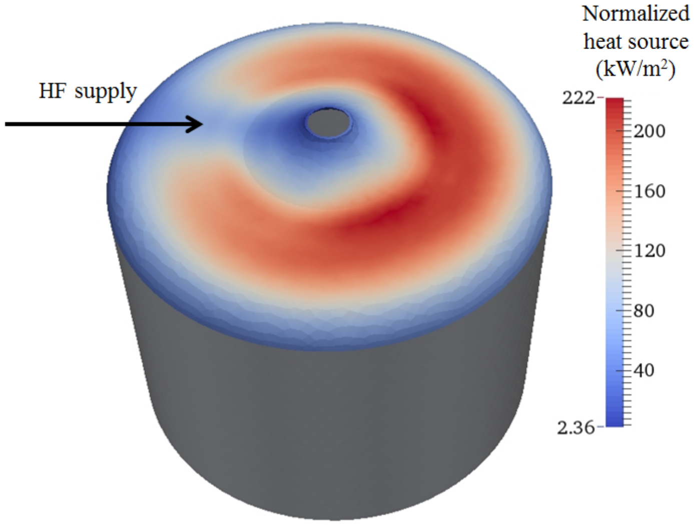
The bulk lifetime of Czochralski silicon (CZ-Si) crystal is shortened by the oxygen (O) precipitates, which are enhanced by the carbon (C) contamination. Reduction of C contamination in the grown crystal is required for the production of Si wafer with long carrier lifetimes. Contamination of C in Si crystal mainly originates from carbon monoxide (CO) generation on the graphite component, which is triggered from the preheating stage and reaches the maximum during the melting stage. Therefore, it is essential to control the CO generation and C incorporation from the preheating to the tailing stage. The packed Si chunks experience the collapsing and volume shrinking during the melting process. Axial movement of the crucible is generally applied to adjust the level of Si feedstock. Melting process, as well as the species transport, must be modeled by transient global simulation according to the crucible movement and the Si volume change.

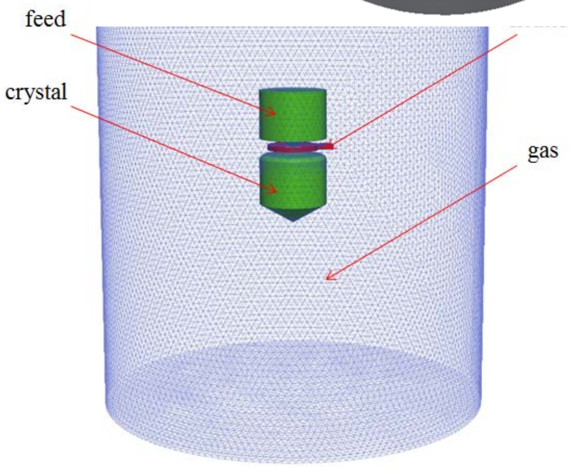
Due to the porosity of packing Si chunks, the heat transport modeling should take into account the effective thermal conductivity (ETC) of Si feedstock. The ETC model proposed by IAEA was applied in the transient global simulation of the melting process. Axial movements of the crucible and the melting of Si feedstock in CZ-Si crystal growth lead to the dynamic thermal and flow field, as well as the affected species transport. To study the effect of crucible movement control on the melting process and C contamination, the fixed and lifting crucible cases were investigated by the transient global simulation with dynamic mesh. The gap width between the gas-guide and the top surface of Si feedstock was kept constant during the crucible lifting process. Heat and impurity transport and accumulation of C in Si feedstock were compared for the static and dynamic crucible cases. Comparison of C accumulation for the fixed and lifting crucible cases indicate that the lifting crucible case resulted in higher C contamination than the fixed crucible case. Furthermore, different gap width cases with the lifting crucible were also investigated to clarify the control strategies of crucible movement on the melting process and C contamination in CZ-Si crystal growth.

3D GLOBAL MODELING OF INDUCTION HEATING OF SILICON IN THE FLOATING ZONE PROCESS

Xuefeng Han, Satoshi Nakano, Xin Liu, Koichi Kakimoto

Research Institute for Applied Mechanics, Kyushu University, JAPAN





Single crystal silicon grown by floating zone (FZ) is predominantly used in the power device due to its high level of working voltage [1].Considering expensive cost of experiments, numerical modeling is an efficient method to analyze heat transfer in the process. Many researchers have already developed 2D global model and 3D local model to investigate high frequency electromagnetic field and temperature distribution [2-4]. However, needle-eye inductor is not axis-symmetric, which results in asymmetric heating power distribution. So we developed a full 3D global model (Fig. 1) to calculate the heat generation rate (Fig. 2) and temperature distribution by solving quasi-steady time-harmonic electromagnetic field. Moreover, mass transfer and heat transfer including radiation in the gas phase are also included to better predict the temperature distribution. Fig. 1. 3D global model of floating zone process Fig. 2. Calculation result of heat source induced by inducting heating. [1] B. Nacke, A. Muiznieks, Numerical modelling of the industrial silicon single crystal growth processes,

GAMM-Mitteilungen, 30 (2007) 113-124. [2] A. Sabanskis, K. Surovovs, J. Virbulis, 3D modeling of doping from the atmosphere in floating zone silicon crystal growth, Journal of Crystal Growth, (2016). [3] M. Wünscher, R. Menzel, H. Riemann, A. Lüdge, Combined 3D and 2.5D modeling of the floating zone process with Comsol Multiphysics, Journal of Crystal Growth, 385 (2014) 100-105. [4] A. Sabanskis, J. Virbulis, Simulation of the influence of gas flow on melt convection and phase boundaries in FZ silicon single crystal growth, Journal of Crystal Growth, 417 (2015) 51-57.

ANALYSIS OF THE V/G CRITERION IN SI SINGLE CRYSTAL GROWTH

Francois Dupret

FEMAG S. A., BELGIUM

The *v/G* criterion [1] governs the behavior of point-defects in silicon single crystals. Depending on whether the ratio of the growth rate *v* over the thermal gradient *G* above the solid-liquid interface is higher or lower than a critical value C_{crit}, then the “surviving species” at some distance from the interface is the vacancy or the self-interstitial. Furthermore, *v/G* equals C_{crit} at a radial distance from the axis where the surviving point-defect concentrations are very low. The present paper proposes a method to determine the dependence of C_{crit} upon the point-defect material parameters at the melting temperature. Our approach is based on the development of a model problem where simplifications are introduced in order to capture the essence of the problem physics. The *v/G* criterion was the object of several publications [2, 3], while various expressions were proposed for C_{crit} as a function of the point-defect material parameters. However the proposed formulas for C_{crit} are only approximations and their validity limits are unclear. Also the effect of thermo-diffusion is insufficiently understood [4-7]. To address these issues the hypotheses of our model problem (similar to those of previous authors) are: (i) 1D problem; (ii) constant formation and migration enthalpies, and reduced heats of transport; (iii) infinite or finite recombination rate; (iv) steady problem; and (v) infinite crystal. In fact we are not interested in the crystal behavior “at infinity” but our technique consists in smoothly prolonging all fields in order to understand their behavior at some location where the point-defect concentrations reach their asymptotic values. With these hypotheses the mathematical problem is closed and provides a transcendental relationship linking C_{crit} to the defect material parameters. This relation can be approximated to the required precision by standard techniques (typically using rational approximants). [1] V. V. Voronkov, J. Crystal Growth **59**, 625 (1982). [2] T. Sinno, R.A. Brown, W. von Ammon and E. Dornberger, J. Electrochem. Soc. **145** No. 1, 302 (1998). [3] V. V. Voronkov and R. Falster, J. Appl. Phys. **86** No. 11, 5975 (1999). [4] N. Van Goethem, A. de Potter, N. Van den Bogaert and F. Dupret, J. Phys. Chem. Solids **69**, 320 (2008). [5] V. V. Voronkov and R. Falster, Mat. Sc. Engineer. B **159-160**, 138 (2009). [6] T.Y. Tan, Appl. Phys. Lett. **73** No. 18, 2678 (1998). [7] P. Pichler, Intrinsic Point Defects, Impurities, and Their Diffusion in Silicon, Springer-Verlag, Wien 2004.

COMPOSITION CONTROL AND STEP COVERAGE FOR ALD DEPOSITED PBTIO3 AND PZT THIN FILMS

Nick Sbrockey[1], Gary Tompa[1], Mark Fanton[2], Kathleen Trumbull[3], Robert Lavelle[3], David Snyder[2], Ronald Polcawich[4], Daniel Potrepka[4]

[1]Structured Materials Industries, NJ, UNITED STATES OF AMERICA, [2]Penn State Applied Research Laboratory, PA, UNITED STATES OF AMERICA, [3]Penn State University, UNITED STATES OF AMERICA, [4]U.S. Army Research Laboratory, UNITED STATES OF AMERICA

This presentation describes work to optimize the composition of atomic layer deposition (ALD) deposited lead-titanate ($PbTiO_3$) and lead-zirconium-titanate (PZT) thin films. A second objective was to demonstrate conformal step coverage into high aspect ratio trenches. The ALD precursors used were tetraethyl lead, tetrakis dimethylamino zirconium (TDMAZ) and tetrakis dimethylamino titanium (TDMAT). The Ti and Zr precursors could be easily reacted with a variety of oxidizers, including water, ozone and plasma dissociated oxygen. The Pb precursor was only successfully reacted using ozone. The composition of the films could be controlled by the relative number of Pb, Zr and Ti precursor doses during the ALD process. ALD processes to achieve stoichiometric $PbTiO_3$ and PZT films were demonstrated. The relative compositions of Pb, Zr and Ti in the films were found to be highly interdependent and not necessarily linear functions of the precursor dose ratios. In order to demonstrate step coverage of the films, substrates were prepared with deep vertical trenches of various aspect ratios. The starting materials were silicon on insulator (SOI) wafers, with 20 microns of silicon above the buried oxide layer. Vertical trenches were produced by reactive ion etching of the silicon, using the buried oxide layer as an etch stop. A platinum barrier layer was deposited on the exposed silicon and SiO_2 surfaces, to provide a uniform nucleation layer for the ALD films, and to prevent formation of lead silicide during the ALD process. The Pt layer was deposited by sputtering, which achieved a thickness on the trench sidewalls of about one half that on the wafer top surface. The optimized ALD processes were then used to deposit films of near stoichiometric $PbTiO_3$ and PZT, as well as TiO_2. Cross section SEM images were obtained to assess the step coverage and conformity of the films into the vertical trenches. In all cases, uniform films and complete coverage of the trench sidewalls and trench bottom were observed. The ability to deposit piezoelectric and ferroelectric films on vertical sidewalls and into deep trenches will enable future 3-D MEMS and high density FRAM devices.

EPITAXIAL GROWTH OF CAMN$_7$O$_{12}$ THIN FILMS BY BOTH OZONE-PLD AND OXIDE MBE

Amanda Huon[1], Ho Nyung Lee[2], Steven May[1]

[1]Drexel University, PA, UNITED STATES OF AMERICA, [2]Oak Ridge National Laboratory, TN, UNITED STATES OF AMERICA

We explore two thin film growth methods, ozone-assisted pulsed laser deposition (PLD) and molecular beam epitaxy (MBE) to synthesize the quadruple manganite $CaMn_7O_{12}$. $CaMn_7O_{12}$ is a quadruple perovskite that exemplifies the rich physics of complex oxides, exhibiting four phase transitions that induce charge-ordering (below 430 K), orbital-ordering (below 250 K), helical magnetic and ferroelectric ordering (below 90 K), and a second helical magnetic transition at 43 K. We achieved epitaxial films through a two-step O_2:O_3 post-growth anneal using oxide MBE. We find the films synthesized by this method are unstrained and exhibit bulk-like electronic and magnetic properties, including helical magnetism. By utilizing PLD in a dilute O_3 environment without a post-growth anneal, we observed epitaxial growth. We will discuss how the details of film growth affect electronic and magnetic properties of films on $YAlO_3$ and $SrLaAlO_4$ substrates. Harnessing the capability to epitaxially grow this quadruple manganite opens new opportunities in synthesis science, enabling the study of heterostructures based on quadruple perovskites. S.J.M. was funded through ARO grant # W911NF-15-1-0133. The PLD work at ORNL was supported by U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

SELF-TEMPLATED EPITAXIAL GROWTH OF LOW-SYMMETRY VANADIUM DIOXIDES ON PEROVSKITES

Xiang Gao, Shinbuhm Lee, Matthew F. Chisholm, Ho Nyung Lee

Oak Ridge National Laboratory, TN, UNITED STATES OF AMERICA

Bronze-phase VO_2(B) and TiO_2(B) are regarded as promising lithium electrode material owing to its high theoretical capacity, low cost, and abundant sources, as well as to their large open channels that are expected to enable rapid lithium ion diffusion and high rate capacity performance. In this work, pulsed laser epitaxy of VO_2(B) and TiO_2(B) on a perovskite substrates will be presented. Direct observations using state-of-the-art scanning transmission electron microscopy (STEM) unveil an intriguing interfacial bi-layer that enables epitaxial growth of a strain-free, monoclinic, bronze-phase VO_2(B) thin film on a perovskite $SrTiO_3$ (STO) substrate. We observed an ultrathin (2-3 unit cells) interlayer best described as highly strained VO_2(B) nanodomains combined with an extra (Ti,V)O_2 layer on the TiO_2 terminated STO (001) surface. By forming a fully coherent interface with theSTO substrate and a semi-coherent interface with the strain-free epitaxial VO_2(B) film above, the interfacial bi-layer enabled the epitaxial connection of the two materials despite their large symmetry and lattice mismatch. Furthermore, direct STEM observations found the single-crystalline VO_2(B) epitaxial films contain two high-coincidence internal domain boundaries. Atom arrangement at boundaries and their possible influence on Li-ion diffusion will be discussed. In addition, we will also show how the epitaxial growth of high crystalline TiO_2(B) thin films on STO is enabled by using a thin template layer of VO_2(B). 1 Gao, X. et al. Nanoscale self-templating for oxide epitaxy with large symmetry mismatch. *Scientific reports* **6**, 38168 (2016). 2 Lee, S., Ivanov, I. N., Keum, J. K. & Lee, H. N. Epitaxial stabilization and phase instability of VO2 polymorphs. *Scientific reports* **6**, 19621 (2016). 3 Lee, S. et al. Persistent Electrochemical Performance in Epitaxial VO2(B). *Nano letters*, doi:10.1021/acs.nanolett.6b04831 (2017). *This work was supported by the U.S. Department of Energy, Office of science, Basic Energy Sciences, Materials Sciences and Engineering Division.

MBE GROWN (LU1-XFEO3)M/(LU1-YMN(1/3)FE(2/3)O3)N SUPERLATTICES

Rachel Steinhardt[1], Julia Mundy[2], Megan E. Holtz[3], Charles Brooks[1], Darrell G. Schlom[1]

[1]Cornell University, NY, UNITED STATES OF AMERICA, [2]berkeley university, NY, UNITED STATES OF AMERICA, [3]Cornell University, UNITED STATES OF AMERICA

Hexagonal rare earth ferrites and manganites have a variety of useful properties ranging from ferroelectricity, to ferromagnetism and antiferromagnetism. In addition, with their similar structures and lattice constants, they can be combined epitaxially in interesting ways. Molecular beam epitaxy gives a unique way to create materials that are not stabile in bulk, or combine multiple structures to form superlattices that can have different properties from their layers individually. These techniques have been used to create Lutetium deficient $(Lu_{1-x}FeO_3)_m/(Lu_{1-y}Mn_{(1/3)}Fe_{(2/3)}O_3)_n$ superlattices by depositing Manganese and Iron without any additional Lutetium on top of stoichiometric $LuFeO_3$. The Lutetium is pulled out of the $LuFeO_3$ layer into the $Lu(MnFe)O_3$ layer. This creates a Lutetium deficiency not only in the $Lu(MnFe)O_3$ layers, but also in the $LuFeO_3$ layers. Normally $LuFeO_3$ compensates for Lutetium deficiency by forming $LuFe_2O_4$, but with this method no $LuFe_2O_4$ is created. The properties of these films are currently being investigated.

25 YEARS OF PROGRESS IN PEROVSKITE-TYPE SUBSTRATE CRYSTAL GROWTH AT THE LEIBNIZ INSTITUTE FOR CRYSTAL GROWTH

Christo Guguschev, Detlef Klimm, Reinhard Uecker, Mario Brützam, Isabelle M. Schulze-Jonack, Zbigniew Galazka, Rainer Bertram, Steffen Ganschow, Matthias Bickermann

Leibniz Institute for Crystal Growth, GERMANY

The growth of perovskite substrate single crystals in Berlin, Germany was intensified with the foundation of the Leibniz Institute for Crystal Growth (IKZ) in 1992. During more than 25 years of experience, technological and scientific aspects related to the growth of such bulk oxide crystals, with pseudocubic lattice parameters in the range of about 3.7 to 4.2 Å (Fig. 1), were explored. In shape of epi-ready substrates, the crystals served as fundamental basis for the discovery and development of advanced mixed oxide layers with interesting ferroelectric, ferromagnetic, multiferroic, or simply electronic properties. By growing these layers epitaxially on not completely lattice-matched substrates, the Gibbs free energy of the layers is influenced by a contribution of elastic distortion at the interface. Quite often, the structure of these epitaxially grown layers is orthorhombically distorted. Rare earth scandates $REScO_3$ (RE = Pr ... Dy) proved to be especially well suited as substrates, because they are orthorhombic from their high melting points near or beyond 2000°C down to room temperature and exhibit almost square (101) lattice meshes with spacings around 4 Å, which is close to the lattice parameters of many advanced perovskite oxides. The fruitful cooperation with the group of Prof. Darrell Schlom resulted in a pioneering work, which is recognized as cornerstone of the modern strain engineering of oxides: Haeni et al. (2004) [1] could shift the Curie temperature for the transition of ferroelectric (low T) to the paraelectric (high T) phase of $SrTiO_3$ from almost absolute zero to room temperature by epitaxial growth of 1% strained layers on $DyScO_3$ substrates. Depending on the epitaxial layer, the choice of appropriate substrates allows the adjustment of elastic strains stepwise, by the choice of proper RE ions. This talk will give an overview about important achievements in bulk single crystal growth, how solid solutions can extend the range of accessible substrate lattice parameters [2] and it will give insights into our recent crystal growth activities and technologies in the fascinating field of perovskites.

Fig. 1: Selection of perovskite-type substrate single crystals and their corresponding pseudocubic lattice parameters.

[1] J.H. Haeni et al., Nature, 430 (2004) 758-761. [2] R. Uecker at al., J. Cryst. Growth, 457 (2017) 137-142.

EFFECT OF WETTING ON THE TRANSITION FROM HOMOGENEOUS TO HETEROGENEOUS NUCLEATION OF DEUTERIUM

Luis A. Zepeda-Ruiz

Lawrence Livermore National Laboratory, CA, UNITED STATES OF AMERICA

Using Molecular Dynamics (MD) simulaitons we explore the effect of undercooling and wetting of deuterium (D2) by measuring the degree of supercooling required for liquid D2 to solidify below its triple point. The results show that for a given colling rate, higher degree of D2 wetting results in heterogeneus solidification at the liquid/wall interface, while for weak wetting, solidification is homogeneus at the bulk of liquid D2. This change in nucleation is accompanied by a transition from layer-by-layer growth to thress-dimensional island growth. In addition, we will show the effect of confinement on D2 solidification. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore Na- tional Laboratory under Contract DE-AC52-07NA27344.

ANALYSIS OF SILICON CARBIDE AND SILICON NITRIDE PARTICLE ENGULFMENT DURING MULTI-CRYSTAL SILICON GROWTH FOR PHOTOVOLTAICS

Yutao Tao[1], Jeffrey H. Peterson[1], Christian Reimann[2], Jochen Friedrich[2], Thomas Jauss[3], Tina Sorgenfrei[3], Arne Croell[3], **Jeffrey J. Derby**[1]

[1]University of Minnesota, MN, UNITED STATES OF AMERICA, [2]Fraunhofer IISB, GERMANY, [3]University of Freiburg, GERMANY

A major challenge for the growth of multi-crystalline silicon via directional solidification is the precipitation and growth of carbide and nitride (SiC and Si_3N_4) particles in the melt that are engulfed by the solidification front to form inclusions. These inclusions lower solar cell efficiency and can lead to wafer breakage and sawing defects. Minimizing the number of these engulfed particles will promote lower cost and higher quality silicon and will advance progress in commercial solar cell production. To better understand the physical mechanisms responsible for such inclusions during crystal growth, we have developed finite-element, moving-boundary analyses to assess particle dynamics during engulfment via solidification fronts. This numerical approach allows for an accurate representation of forces and dynamics previously inaccessible by approaches using analytical approximations. We present new results on the effects of carbon segregation at the interface on silicon carbide particle engulfment. Carbon changes the melting point of silicon, and the interaction of the particle with the rejected carbon at the growth interface redistributes the concentration in the liquid, affecting the shape of the solidification interface under the particle and the critical conditions for engulfment. We demonstrate that the rate of reaction at the particle surface has a profound effect on engulfment behavior. We also present initial computations for the case of silicon nitride particle engulfment in this system. Since both the thermal conductivity and the morphology of silicon nitride particles differ significantly from those of silicon carbide, we expect substantial differences in engulfment behavior. These computations will be compared with recent experiments on silicon nitride engulfment from experiments conducted by the ParSiWal (Partikeleinfang bei der Siliziumkristallisation im Weltall) project funded by the German DLR and involving the Fraunhofer IISB and the University of Freiburg. ---------------

This research was supported in part by the U.S. National Aeronautics and Space Administration, NNX10AR70G, and no official endorsement should be inferred.

ELECTRON-BEAM-INDUCED CURRENT IN GAAS/FE CORE-SHELL NANOWIRES

Mingze Yang, Simon Watkins, Karen Kavanagh

Department of Physics, Simon Fraser University, BC, CANADA

Electron-beam-induced current (EBIC) measurements were carried out in a scanning electron microscope (SEM) on GaAs-core/Fe-shell, free standing nanowires (NW). N-or p-type GaAs cores were grown by metalorganic vapour phase epitaxy (MOVPE) via the vapour-liquid-solid method using a Au catalyst. A thin layer of aluminum oxide (Al_2O_3) was deposited by atomic layer deposition to enable subsequent regrowth by MOVPE of an electrically-isolated top end. An epitaxial Fe shell was then electrochemically deposited to fabricate coaxial magnetic-metal injection barriers to the regrown GaAs core. In the SEM (field-emission - 5 keV or 10 keV), the metal was contacted by a tungsten tip with the GaAs substrate acting as the ground contact. The NWs were measured *in situ* without removal from the substrate, which was mounted perpendicular to the electron beam. EBIC was used to measure the radial minority current flow through the rectifying Fe/GaAs contact. Profiling as a function of beam energy, current, and dwell time, enabled a measurement of the axial variation in minority carrier collection along the length of the GaAs/Fe junction, as well as the influence of the oxide layer and interface state defects on recombination rates. In addition, small but reproducible oscillations in EBIC current are observed as the beam is scanned along the length of the NW, These oscillations, with a scale of around 30 nm, are independent of the beam scan direction along the NW, as well as the beam tilt angle away from the sample normal (which rules out channeling). These are therefore likely due to a lateral variation in the local interfacial state density at the epitaxial Fe/GaAs interface influencing the minority carrier recombination rates. Acknowledgements: Partial funding from NSERC, CFI, and BCKDF.

MOVPE OF INAS QDS ON INP EMITTING AROUND THE TELECOM C-BAND

Andrey B. Krysa[1], Joanna Skiba-Szymanska[2], Jan Huwer[2], Tina Müller[2], M. Felle[3], Brett Harrison[1], R.M. Stevenson[2], Jon Heffernan[1], Andrew Shields[2]

[1]EPSRC National Centre for III-V Technologies, Dept. of Electronic and Electrical Eng., University of Sheffield, UNITED KINGDOM, [2]Toshiba Research Europe Limited, UNITED KINGDOM, [3]Department of Engineering, University of Cambridge, UNITED KINGDOM

We have studied metalorganic vapour phase epitaxy of self-assembled InAs quantum dots (QDs) on InP in the regimes of Stranski-Krastanow (SK) growth and droplet epitaxy. The structures were examined by photoluminescence (PL) at room temperature (RT) and 4.2 K, optical polarized microscopy and atomic force microscopy (AFM). SK growth was performed at a temperature of 500 ^{o}C. A low growth rate of ~0.05 nm/s while restricting the nominal thickness of InAs to ~2 atomic monolayers was used to promote a low density QD growth. InP overgrowth was performed in two stages with a lower (~0.05 nm/s) and a higher (~0.43 nm/s) growth rates. The overgrown surface featured well resolved atomic terraces in AFM scans indicating that the preferred step-flow epitaxial regime was re-established after QD growth. A typical RT PL spectrum of SK QDs would contain the inhomogeneously broadened QD emission around the intended spectral band and an emission around 1.24 μm which we ascribe to the wetting layer. At 4.2K, the QD emission represents an ensemble of narrow emission lines. The alternative QD growth, droplet epitaxy, included formation of In droplets on the InP surface via pyrolysis of trimethylindium at 400 ^{o}C while withholding the supply of arsine to the growth chamber and then followed by InAs QD crystallization under arsine overpressure at 400-500 ^{o}C. The key differences between the PL spectra of droplet QDs in comparison to those grown in the SK regime were the absence of the emission from the wetting layer and a stronger QD emission. In both of the QD growth regimes, low QD densities ($<10^{9}$ cm^{-2}) were achieved which allowed optical access to individual QDs without additional fabrication steps. We have also developed distributed Bragg reflectors based on quarter wavelength layers of AlGaInAs and InP. The problem of the arsenic carry over at the As-P interface has been solved, and the resulting DBR surface was atomically flat. This allows growth of optical cavities incorporating InAs QDs for single-photon emitters operating around 1.55 μm.

LARGE AREA UNIFORM VLSI NANOWIRE GROWTH TOOL

Serdal Okur[1], Tom Salagaj[1], Nick Sbrockey[1], Gary Tompa[1], Jignesh Vanjaria[2], Ebraheem Azhar[2], Hongbin Yu[2]

[1]Structured Materials Industries, Inc., UNITED STATES OF AMERICA, [2]Arizona State University, UNITED STATES OF AMERICA

Photodetectors based on wide bandgap semiconductor materials operate in the ultraviolet (UV) spectral range and have wide range commercial, industrial, scientific and military applications. The use of nanowires enables much greater sensitivity and faster response time than possible with bulk or thin film materials. ZnO based nanowires also make the devices radiation hard, and compatible with high temperature operation. Although high sensitivity photodetection has been demonstrated using ZnO nanowires, the development of a practical nanowire growth technique to produce useable devices is still an issue. Most of present day nanowire growths are performed in horizontal tubes which have major composition, uniformity, and depletion effects limiting growth on large substrates. Using the traits of Vapour-Liquid-Solid (VLS) synthesis we developed an alternative method for the nanowire growth that also appears to be equally applicable to HVPE and sublimation techniques in general. The new system can deposit large areas (>100 mm) of doped/undoped nanowires. It is also unique in that it has been designed with thermal and flow modeling to present a large area growth surface at a uniform growth temperature to a uniform flux of precursors. The tool has multiple source stages and deposits nanowires on different size wafer up to 100 mm in diameter. It provides control of a wide range of process parameters including temperature, pressure, variable distance of the source materials, wafer, and oxidizer for the nanowire growth. We have grown Zn(Mg)O nanowires by varying the growth parameters, such as, pressure (3-200 Torr), substrate and source temperatures (500-1000 °C), and distance of the sources material and oxidizer. We have used Au and ZnO seed layers on Si wafers. A uniform ZnMgO nanowire growth was observed on Si wafers with Au seeds when the material source and wafer were separated by 50 cm apart and kept at 900 and 1000 °C, respectively, at 5 Torr chamber pressure. Proving a better control on many parameters of nanowire growth, the new tool also has the added value of being able to operate in CVD and HVPE modes for growths of materials such as: GaN, Ga_2O_3, MgB_2, and so on.

CHEMICAL SOLUTION SYNTHESIS OF EPITAXIAL THIN-FILM OXIDES

José Manuel Vila-Fungueiriño[1], Beatriz Rivas-Murias[2], Andrés Gómez[3], Jaume Gazquez[3], Marti Gich[3], Adrian Carretero-Genevrier[1], **Francisco Rivadulla**[2]

[1]Institut d´Électronique et des Systèmes (IES), FRANCE, [2]Universidad de Santiago de Compostela, SPAIN, [3]ICMAB, CSIC, SPAIN

Chemical solution methods of thin-film deposition are an affordable and versatile alternative to physical deposition techniques (PLD, Sputtering, MBE, etc.), which avoids the use of high-vacuum chambers, and are more suitable for coatings of large areas. However, a poorest control of the thickness and stoichiometry (particularly below »10-20 nm), along with larger interface and surface roughness, limited their applicability for the study of the subtle phenomena that occur at clean interfaces with a broken symmetry (spin, orbital, etc), or their use in highly demanding applications. In this regard, the introduction of water-based polymer assisted deposition (PAD) in 2004 by Jia et al.[1] was an important advance in the chemical methods for the synthesis of epitaxial thin-films. In this presentation I will demonstrate that an excellent control over the thickness, chemical, structural, electronic and magnetic homogeneity can be achieved by PAD on the synthesis of multicationic oxides, over areas of several cm^2. I will show that epitaxial oxide-heterostructures can be also prepared in this way, which constitutes an important step forward in the competitiveness of the chemical solution methods, compared with traditional physical deposition techniques. I will review the fabrication of complex functional oxides like $BiFeO_3$ and $Y_3Fe_5O_{12}$ (YIG). Finally, I will describe our attempts to combine this chemical solution technique with MBE for the synthesis of complex heterostructures on Silicon. Particularly, I will show how a large flexoelectric response can be obtained in relatively thick layers of BaTiO3, deposited over porous chemically-synthesized layers of LSMO, on STO/Si. [1] Quanxi Jia et al. Nature Materials 3, 529 - 532 (2004) [2] F. Rivadulla et al. Chem. Mat. 25, 55 (2013) [3] I. Lucas et al. ACS Appl. Mat. Interf. 6, 21279 (2014) [4] J. M. Vila-Fungueiriño et al.Chem. Mater. 26, 1480 (2014). [5] J. M. Vila-Fungueiriño et al., ACS Appl. Mat. Interf. (2015) [6] B. Rivas-Murias et al. Scientific Reports 5, 11889 (2015) [7] J. M. Vila-Fungueiriño et al. Frontiers in physics. 3, 38 (2015)

IN SITU OBSERVATION OF LAYER-BY-LAYER MEAN INNER POTENTIAL OSCILLATIONS AND PRECISE GROWTH CONTROL OF OXIDE INTERFACES

Yuefeng Nie

Nanjing University, CHINA

A variety of novel quantum phenomena have been discovered at oxide interfaces with technical advances in deposition techniques, especially with the application of *in situ* reflection high-energy electron diffraction (RHEED). One period of RHEED intensity oscillations typically corresponds to the growth of one atomic sublayer, however, the precise control of termination/interface is still challenging due to the rather complicated oscillation patterns in oxide growth and the lack of chemical information in RHEED. Here, we report the observation of layer-by-layer variations of the mean inner potential during the growth of epitixial $SrTiO_3$ films by reactive molecular beam epitaxy. A model including the effects of mean inner potential and surface roughness reveals the underlying mechanism of the complicated RHEED intensity oscillations in the growth of oxide films. As an example, atomic sharp $LaTiO_3$/$SrTiO_3$ interfaces and two dimensional electron gas (2DEG) were successfully fabricated on epitaxial $SrTiO_3$ films of any desired thickness. General rules were also proposed to guide the fabrication of ultimate precise interfaces for novel correlated quantum states.

ATOMICALLY ENGINEERED FERROIC LAYERS YIELD A ROOM-TEMPERATURE MAGNETOELECTRIC MULTIFERROIC

Julia A. Mundy

University of California, Berkeley, CA, UNITED STATES OF AMERICA

Materials that exhibit simultaneous order in their electric and magnetic ground states hold promise for use in next-generation memory devices in which electric fields control magnetism. Such materials are exceedingly rare, however, owing to competing requirements for displacive ferroelectricity and magnetism. Despite the recent identification of several new multiferroic materials and magnetoelectric coupling mechanisms, known single-phase multiferroics remain limited by antiferromagnetic or weak ferromagnetic alignments, by a lack of coupling between the order parameters, or by having properties that emerge only well below room temperature, precluding device applications. Here we present a methodology for constructing single-phase multiferroic materials in which ferroelectricity and strong magnetic ordering are coupled near room temperature. Starting with hexagonal $LuFeO_3$—the geometric ferroelectric with the greatest known planar rumpling—we introduce individual monolayers of FeO during growth to construct formula-unit-thick syntactic layers of ferrimagnetic $LuFe_2O_4$ within the $LuFeO_3$ matrix, that is, $(LuFeO_3)_m/(LuFe_2O_4)_1$ superlattices. The severe rumpling imposed by the neighbouring $LuFeO_3$drives the ferrimagnetic $LuFe_2O_4$ into a simultaneously ferroelectric state, while also reducing the $LuFe_2O_4$ spin frustration. This increases the magnetic transition temperature substantially—from 240 kelvin for $LuFe_2O_4$ to 281 kelvin for $(LuFeO_3)_9/(LuFe_2O_4)_1$. Moreover, the ferroelectric order couples to the ferrimagnetism, enabling direct electric-field control of magnetism at 200 kelvin. Our results demonstrate a design methodology for creating higher-temperature magnetoelectric multiferroics by exploiting a combination of geometric frustration, lattice distortions and epitaxial engineering.

Future Conferences

26th AACGE Western Section Conference on Crystal Growth & Epitaxy
Stanford Sierra Camp, Fallen Leaf Lake, CA
June 10-13, 2018

Past Session Topics included:

- Fundamentals
- Biomineralization, Bioinspired Materials and Self-assembly
- Energy Storage and Conversion
- Low dimensional materials

•The 25th AACGE Western Section Conference on Crystal Growth & Epitaxy will continue the tradition of a highly interdisciplinary program with emphasis on an understanding of the fundamental nanoscale physics and chemistry that are central to the growth of crystals for a wide array of technologies. The beautiful Fallen Leaf Lake Lodge is an intimate venue with nearby hiking and boating. Communal dinners and single session format allow time for both formal and informal discussion.

Visit www.crystalgrowth.org for the Call for Abstracts, registration information, and other announcements.

Conference sponsored

2019
ICCGE-19
Keystone, Colorado, USA
ISSCG-17 Colorado

The 19th International Conference on Crystal Growth and Epitaxy (ICCGE-19)

Keystone, Colorado, U.S.A. * July 28–August 2, 2019

and

The 17th International Summer School on Crystal Growth (ISSCG-17)

Colorado, U.S.A. * July 21–27, 2019 (Tentative)

You are invited to the beautiful mountains of Colorado for the 19th International Conference on Crystal Growth and Epitaxy (ICCGE-19) and the 17th International Summer School on Crystal Growth (ISSCG-17), to be convened over two weeks in July-August, 2019. ICCGE will be held at the Keystone Resort and Conference Center, featuring modern, comfortable accommodations and the largest conference center in the Rocky Mountains. ISSCG will take place at a companion location to be determined.

These triennial meetings, organized under the auspices of the International Organisation for Crystal Growth (IOCG), are the premier forums for the world's crystal growth communities. The International Summer School on Crystal Growth will feature world-renowned scholars delivering tutorials on the fundamentals and practice of crystal growth. The International Conference on Crystal Growth and Epitaxy will provide a forum for the presentation and discussion of recent research and development activities in crystal growth and will feature all aspects of bulk crystal and epitaxial thin film growth; sessions will integrate fundamentals, experimental and industrial growth processes, characterization, and applications.

The technical program will include both oral and poster sessions, as well as plenary and invited talks to provide a complete picture of the latest developments in the fields. The official language of the conference will be English. Conference proceedings will be reviewed and published in a special issue of the Journal of Crystal Growth.

The magnificent setting of the Rocky Mountains and the American West will provide multiple opportunities for recreation and enjoyment of nature for the conferees and their families before and after, as well as during the conference. There will be a full social program and vendor exhibit together with the technical sessions.

Organizing Committee:

ICCGE Co-Chair
Vincent Fratello
Quest Integrated, Inc.

ICCGE Co-Chair
Jeffrey Derby
University of Minnesota

Program Co-Chair
Christine Wang
Lincoln Laboratory, MIT (ret.)

Program Co-Chair
Peter Schunemann
BAE Systems

ISSCG Co-Chair
Thomas Kuech
University of Wisconsin

ISSCG Co-Chair
Joan Redwing
Penn State University

Inquiries: AACG@comcast.net * www.crystalgrowth.org

Organized under the auspices of the International Organisation for Crystal Growth

Coordinated by the American Association for Crystal Growth

aacg
AMERICAN ASSOCIATION FOR CRYSTAL GROWTH

Celebrating 50 years of Crystal Growth in the U.S.A., 1969-2019