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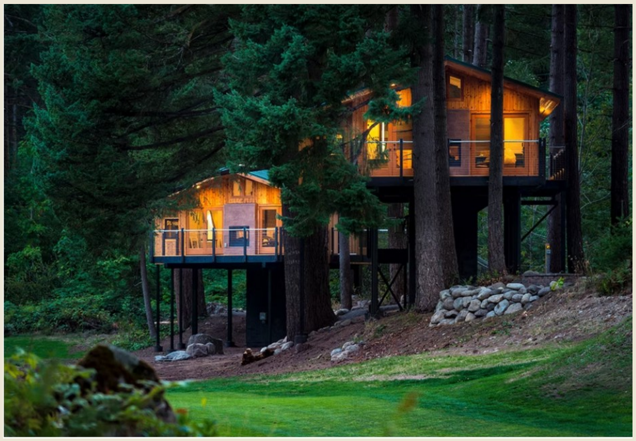
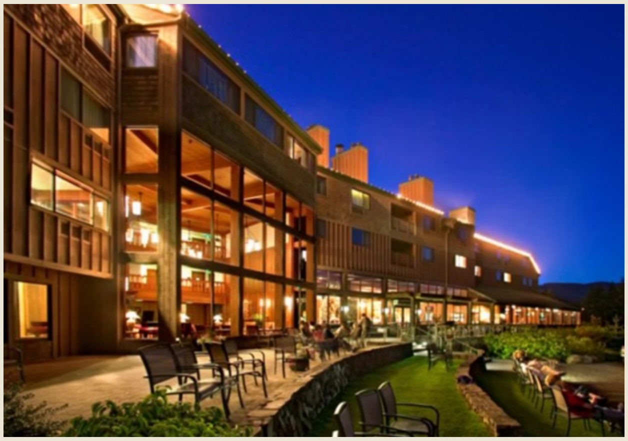
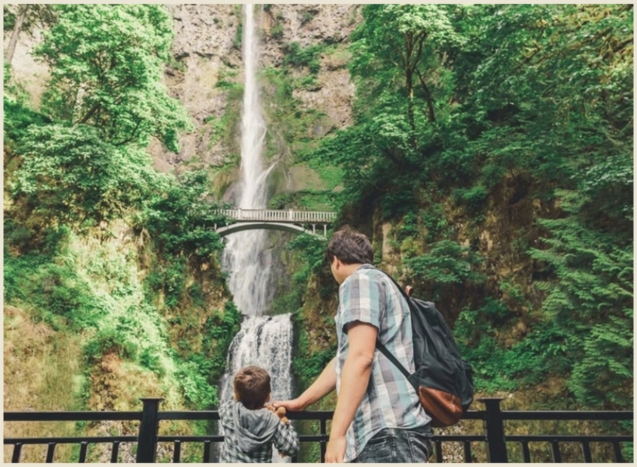


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SUPERCONDUCTING ND1-XEUXNIO2 (NENO) THIN FILMS USING IN-SITU MBE SYNTHESIS

Charles Ahn (Yale University)

The rare-earth nickelates display a broad range of phenomena, including functional behavior such as antiferromagnetism and superconductivity. The ability to synthesize heterogeneous epitaxial thin film structures out of nickelates enables one to control and modify these functional properties via the creation of atomically abrupt interfaces. Advanced synchrotron characterization can then be used to measure the resulting electronic and magnetic properties of these atomically engineered systems. Here, we discuss synchrotron characterization of the square-planar nickelates, which are a novel class of superconductors. We use in situ aluminum reduction of the perovskite nickelates to achieve superconducting Nd1-xEuxNiO2 (NENO) thin films grown by molecular beam epitaxy (MBE). Atomic structure is characterized using crystal truncation rod (CTR) analysis, and electronic structure is characterized using diffraction-based X-ray absorption near edge structure (dXANES). We also report on unusual superconducting transport properties of NENO films, including magnetic field enhanced superconductivity.

DIRECT HETEROGENEOUS INTEGRATION OF TRANSITION METAL DICHALCOGENIDES VIA SINGLE-SOURCE MOLECULAR CHEMISTRY

Zakaria Al Balushi (University of California, Berkeley)

Two-dimensional (2D) semiconductors, such as molybdenum disulfide (MoS2), are emerging as key materials for next-generation electronics, addressing challenges in the miniaturization of silicon-based technologies. Despite progress in scaling-up 2D materials, integrating them into functional devices remains challenging, particularly in the context of three-dimensional integration. In this talk, I will present a scalable method for growing high-quality mono- to few-layer MoS2 on large wafers using a spin-on precursor, molybdenum ethyl xanthate. This approach facilitates the formation of a metastable amorphous molybdenum trisulfide phase, which we can then be leveraged for direct heterogeneous integration. We thoroughly investigate the growth dynamics and associated versatile features using comprehensive characterization, reactive force-field molecular dynamics simulations, and Density Functional Theory. Our method allows precise control over film thickness, grain size, and defect density, yielding wafer-scale monolayer MoS2 with reliable optical properties comparable to as-exfoliated samples. Additionally, we achieve area-selective formation of MoS2 and the direct deposition of sub-5 nm high-k oxides using atomic layer deposition, without the need for seeding or surface functionalization. This process enables the fabrication of complex superlattice structures, top-gated FETs, and memristor devices, all from a single-source chemistry. Our findings highlight the versatility of spin-on metal xanthate chemistries for the synthesis and integration of transition metal dichalcogenides, paving the way for advanced nanoscale fabrication processes and enhancing the commercial viability of 2D materials in electronics.

DYNAMIC SURFACE POTENTIAL INDUCED BY COMPETITIVE ION ADSORPTION SWITCHES PARTICLE-ATTACHING FACETS

Yuna Bae (), Jim De Yoreo (Pacific Northwest National Laboratory), Dongsheng Li (Pacific Northwest National Laboratory)

The mechanism of facet selectivity during crystal growth by oriented attachment (OA) and its dependence on the structure and chemistry of the NP-electrolyte interface are poorly understood phenomena of mineral-fluid systems. The electrostatic forces associated with the facet-dependent surface charge is of NPs is expected to play a role, but whether — or when — it dominates over other factors, like hydration barriers or van der Waals interactions, is unclear. Here we investigate the formation of branched cubic Pt mesocrystals through OA in electrolyte solutions using advanced in situ imaging, surface characterization, and theoretical and computational modeling. We find that mesocrystal formation begins with aggregation of the NPs into a disorganized cluster within which subsequent OA events occur. During this process, the NPs are initially spatially separated in the clusters and become crystallographically coaligned before attachment. Attachment begins on the {100} facets of the inner particles, forming a cubic core, and later shifts to the {111} facets, leading to the growth of branched rods on the faces of cube. The transition from {100} to {111} attachments is driven by competitive ion adsorption and the resulting evolution of surface potential. This study demonstrates that anisotropic electrostatic interactions and resultant torques govern the directionality of OA, providing a deeper insight into how solution chemistry influences nanomaterial assembly and valuable guidance for designing complex nanostructures with tailored properties for diverse applications.

BRIDGMAN GROWTH OF SEMICONDUCTOR CRYSTALS FOR APPLICATION IN NON-LINEAR OPTICS

Pijush Bhattacharya (Azimuth Inc. A Core4ce company), MIcheael A Susner (2Materials and Manufacturing Directorate, Air Force Research Laboratory Wright-Patterson Air Force Base, Ohio 45433.)

The Airforce Crystal Growth Center (AFCGC) is engaged in focusing on synthesis of both 1) novel materials where fundamental structure-property relationships are being explored and 2) more mature materials for in-house requirements. This latter set of materials can encompass a large phase-space ranging from newer compounds where some fundamental properties are known but essential questions are yet unanswered to compounds that are well-established but are actively undergoing research in terms of optimizing size, purity, doping, etc. to unlock new opportunities for applications. In this talk, we will be discussing our overall approach to the development of mature materials as well as discussing a few recent cases where we have shown success including the growths low bandgap III-V semiconductors (both binary and ternary alloys) and more novel chalcogenide materials. The Bridgman technique is used to grow different low bandgap semiconductor crystals such as InSb, (In,Ga)Sb InAs and (In,Ga)As. We have also attempented Sn2P2S6 and In2Se3 semiconductors which exhibit attractively high non-linear properties. The charge materials for these crystal growths were synthesized using stoichiometric elemental materials with a purity of ~5N. The charge materials are sythesized from the stiochiometric amount of respetive crystals elements. The compositions and crystal structures of the grown crystals are verified using EDS and XRD measurements. The grown crysals show a very encouraging results and the feedback from characterisitions are underway to further improve the growth methods. We will discuss an overview of growth capabilities of the center; characterizations related to large-scale growth and plans for future.

CONTRAILS FROM FIRST PRINCIPLES

Rhys Bunting (Lawrence Livermore National Lab)

On a clear day, aviation contrails can be seen across the sky. Formation of these contrails depends on both the aviation soot formed and the external conditions; water vapor condenses on the soot and forms ice. Here, different experimentally sized soot particles (oxygen/sulfur lean/rich) are generated using a machine learned interatomic potential. The generated particles are then supersaturated in water. Heterogeneous ice cluster formation is analyzed using UMAP dimension reduction and k-means clustering. Key surface sites are found to dictate ice formations.

IMPACT OF DISLOCATION MOTION ON INTERDIFFUSION, STRUCTURING, AND THERMAL TRANSPORT AT GE-SI HETEROINTERFACE

Brandon Carson (Department of Materials Science and Engineering, University of California, Los Angeles, Los Angeles, California 90095, USA), Kenny Hunyh (Department of Materials Science and Engineering, University of California, Los Angeles, Los Angeles, California 90095, USA), Thomas Pfeifer (Department of Mechanical and Aerospace Engineering, University of Virginia, Charlottesville, Virginia 22904, USA), Xingxu Yan (Department of Materials Science and Engineering, University of California, Irvine, Irvine, California 92697, USA), Glenn Jernigan (U.S. Naval Research Laboratory, Washington, District of Columbia, 20375, USA), Karl Hobart (U.S. Naval Research Laboratory, Washington), Anna Mian (TESCAN Tempe, LLC.), Patrick Hopkins (Department of Mechanical and Aerospace Engineering, University of Virginia), Mark Goorsky (Department of Materials Science and Engineering, University of California, Los Angeles)

Interfaces play a critical role in determining the thermal performance of heterogeneous material stack ups. To investigate the effects of dislocations and interdiffusion on the structure and thermal properties of the Ge-Si heterointerface, transmission electron microscopy and x-ray diffraction were performed on epitaxial Ge thin films deposited on (001) Si using molecular beam epitaxy. Samples were characterized under various annealing conditions to understand the arrangement of dislocations at the interface. Dislocation motion was correlated to elemental corrugation at the interface, and the resulting thermal boundary resistance of the interface structure was characterized. Anneals were performed both in-situ and ex-situ in nitrogen, across temperatures ranging from 400-800 °C. Cross section transmission electron microscopy monitored the evolution of defects before and after different annealing treatments. High angle annular dark field scanning transmission electron microscopy revealed a strong correlation between dislocations and interdiffusion at the interface. The changes in broadening observed in x-ray diffraction reciprocal space maps support the microscopy data over macroscopic regions of the film, providing an accessible method to monitor the annealing process. The dominant interdiffusion driving forces of concentration gradient, stress gradient, and vacancy flux were simulated and corroborated with energy dispersive x-ray spectroscopy measurements. Thermal measurements were performed to extract the thermal boundary resistance of the various interface morphologies produced by each annealing condition. The results support that at the Ge-Si heterointerface, dislocation cores enhance interdiffusion by serving as vacancy sinks, resulting in a periodic nanoscale compositional corrugation. Although nanoscale interdiffusion and corrugation have been predicted to result in an improvement to thermal transport across the interface [1,2], our results show annealing increased the thermal boundary resistance and is largely attributed to alloy scattering becoming dominant as interdiffusion proceeds and without beneficial effects seen by the compositional corrugation.

[1] Z. Cheng et al., Nature Communications 12, 6901 (2021).
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CONTROLLING THE SHAPE OF SEMICONDUCTOR NANORODS USING HYDROTHERMAL GROWTH IN A CONTINUOUS FLOW REACTOR

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Recently, a large variety of semiconductor nanomaterials with tunable dimensions and morphologies have been prepared using various methods. While vapor-phase deposition techniques benefit from obtaining materials with defined composition, morphology, or properties, along with the advantage of in-situ monitoring, hydrothermal growth, on the contrary, emerges as an easy-to-implement and cost-effective approach for nanostructure synthesis with significant potential in the large-scale production in industry.

Traditionally, hydrothermal growth has been conducted in batch reactors, where reactants are mixed and the temperature and pressure are adjusted to control supersaturation. However, supersaturation changes over time as the growth units are consumed by both homogeneous and heterogeneous nanostructure growth and, essentially, there is only limited control over supersaturation as the growth proceeds. The decreasing supersaturation also leads to a reduction in the deposition rate over time, until the growth is terminated. Furthermore, time-dependent variation in supersaturation may inhibit changes in the growth mechanism.

Here, a simple method for growing nanocrystals using a continuous-flow reactor with the ability to design supersaturation over time is presented. This method enables control over the diameter of ZnO nanorods, starting with nanorods with sharp tips, then gradually increasing their diameters, and finally merging them into an array of packed nanorods. Using a mathematical model, we propose a possible explanation for the dependence of nanorod morphology on supersaturation. The use of a flow reactor for nanostructure preparation offers an innovative methodology that not only enhances the reproducibility and stability of nanostructure growth but also opens new possibilities for tailoring nanomaterials with desired morphological attributes for diverse applications.

TEXTURED PMN-PZT CERAMICS WITH EHANCED PIEZOELECTRIC PROPERTIES AND FATIGUE RESISTANCE

Yunfei Chang (Harbin Institute of Technology), Linjing Liu (Harbin Institute of Technology), Rui Lv (Harbin Institute of Technology), Hang Xie (Harbin Institute of Technology), Fei Li (Xi'an Jiaotong University)

Piezoelectric ceramics with high and fatigue-resisted piezoelectric properties are required for electromechanical applications such as ultrasonic transducers, high-precision actuators, and piezoelectric sensors. In this work, we fabricated highly [001]c-textured Pb(Mg1/3Nb2/3)O3-Pb(Zr, Ti)O3 (PMN-PZT) ceramics through templated grain growth process. The effects of texture engineering on unipolar fatigue behaviors of the ceramics were investigated in terms of dielectric, ferroelectric, and piezoelectric properties. The textured ceramics with Lotgering factor F001 ~98% exhibited about 230% enhanced piezoelectric coefficient d33∗ initially and substantially improved fatigue resistance during the entire unipolar cycling. Unipolar polarization Pmax and d33∗ were nearly maintained up to 1000000 unipolar cycles in the textured ceramics, while 19% and 14% degradations were respectively observed from non-textured counterparts. Besides, much lower bipolar strain asymmetry γs~4% was observed from the textured samples fatigued after 1000000 unipolar cycles. The mechanisms for enhanced fatigue resistance of textured PMN-PZT ceramics were also explored.

OXIDE SEMICONDUCTOR BASNO3 AS A NEW PLATFORM FOR PEROVSKITE OXIDE ELECTRONICS

Kookrin Char (Institute of Applied Physics, Seoul National University)

BaSnO3 perovskite oxide semiconductor system was found to possess high mobility at room temperature and stable surface/interface behavior. Such properties can provide a new platform to put together many interesting properties of various perovskite oxides and create new functions that have not been possible before.

In combination with the lattice matched polar perovskite oxide LaInO3, a high density 2DEG can be created. Its formation mechanism, namely the “interface polarization” created by the inversion symmetry breaking at the orthorhombic LaInO3 and the cubic BaSnO3 interface, is a very unique feature of perovskite oxides. The characteristics of the 2DEG at LaInO3/BaSnO3 interface were found to be very reliable even with the subsequent high temperature annealing. We have recently achieved a mobility of 2,000 cm2/V×sec by electric-double-layer gating the LaInO3/BaSnO3 2DEG.

When combined with the lattice matched and highly insulating SrHfO3, a complex multilayer structure such as double-gate FETs can be demonstrated. Such complex structure is possible due to the existence of degenerately doped La-doped BaSnO3 as the electrodes as well as the very low leakage current through the SrHfO3 used as the gate dielectric. In addition, the large conduction band offset between the BaSnO3 and SrHfO3 also enables 2DEG formation at the non-polar interface of SrHfO3/BaSnO3, as in the case of the 2DEG of (AlGa)As/GaAs.

In combination with a new high-k perovskite dielectric oxide BaHf0.6Ti0.4O3 as a gate oxide, 2D charge density larger than 1014 cm-2 can be modulated by field effect. By alloying the high dielectric strength BaHfO3 with the high dielectric constant BaTiO3, we have created a new perovskite dielectric oxide BaHf0.6Ti0.4O3 which exhibits both a high-k dielectric constant and a high dielectric strength (low leakage current and high breakdown field).

When a lattice matched ferroelectric PbZr0.7Ti0.3O3 is used as a gate oxide, ferroelectric FET can be realized. The interface at PbZr0.7Ti0.3O3/BaSnO3 can work as a model system to study the switching properties of ferroelectric/semiconductor structure. We will discuss the implications of the ferroelectric and semiconducting material parameters on the switching performance.

Lastly, I will try to put the potentials of BaSnO3 systems into perspective for new science and technology.

CONTROLLING THE EPITAXIAL ORIENTATION OF WAFER-SCALE MOS$_2$ MONOLAYERS ON C-PLANE SAPPHIRE

Chen Chen (2D Crystal Consortium, Materials Innovation Platform, Pennsylvania State University), Rohini Sanikop (2D Crystal Consortium, Materials Innovation Platform, Pennsylvania State University), Andrew R. Graves (2D Crystal Consortium, Materials Innovation Platform, Pennsylvania State University), Joan M Redwing (2D Crystal Consortium, Materials Innovation Platform & Department of Materials Science and Engineering, Pennsylvania State University)

Monolayer molybdenum disulfide is a two-dimensional direct band gap semiconductor with promising electrical properties that are of interest for next-generation nanoelectronics. Epitaxial growth of MoS2 monolayers on c-plane sapphire substrates has emerged as a key synthesis method for single-crystal wafer-scale films. However, the in-plane epitaxial alignment of MoS2 relative to the underlying sapphire has been observed to vary depending on the specific growth technique employed. Epitaxial MoS2 films grown by MOCVD using Mo(CO)6 and H2S in a H2 carrier gas exhibit direct in-plane alignment such that (11"2" ¯0) MoS2 ∥ (11"2" ¯0) Sapphire.1 In contrast, MoS2 films grown using MoO3 and sulfur powder in an Ar carrier gas exhibit a 30° rotation such that (101¯0) MoS2 ∥ (11"2" ¯0) Sapphire.2 In both cases, 60° rotated twin domains are also present due to the non-centrosymmetric lattice of MoS2. While the specific epitaxial alignment is associated with the atomic arrangement and chemistry of the sapphire surface, its dependence on growth chemistry is not well understood.

The MoS2 monolayers were grown at 1000 °C using MoO2Cl2 and H2S with nitrogen as the carrier gas. The nucleation density of MoS2 on sapphire was found to be significantly reduced using MoO2Cl2 compared to Mo(CO)6 resulting in larger domain sizes prior to coalescence and an overall improvement in crystal quality as assessed by in-plane XRD diffraction. Interestingly, the in-plane epitaxial orientation of the MoS2 domains was found to vary depending on the S/Mo ratio employed during growth. Lower S/Mo ratios resulted in direct in-plane alignment (11"2" ¯0) MoS2 ∥ (11"2" ¯0) Sapphire with R0o/R60o rotational twin domains while the epitaxial orientation was observed to shift to (101¯0) MoS2 ∥ (11"2" ¯0) Sapphire with R±30o rotational twins at higher S/Mo ratios.

By controlling the miscut direction of the sapphire substrate, it was possible to break the degeneracy of the two antiparallel MoS2 twin domains and promote unidirectional single-domain alignment. The use of c-plane sapphire substrates with 0.2° miscut toward the M-axis resulted in unidirectional domains for MoS2 grown at lower S/Mo ratios while substrates with 1.0° miscut toward the a-axis promoted unidirectional domains for MoS2 grown at higher S/Mo ratios. The results demonstrate the need to carefully control both the growth chemistry and sapphire substrate miscut to yield high-quality MoS2 epitaxial monolayers.

MONITORING NUCLEATION PATHWAYS OF CALCIUM CARBONATE AND GIBBSITE VIA IN SITU NMR

Ying Chen (Pacific Northwest National Laboratory), Jin Biao (), Xin Zhang (, Jim De Yoreo ()

Due to its high sensitivity to local chemical environment and molecular motions, along with its quantitative and non-invasive nature, in situ solution- and solid-state NMR spectroscopy provides unique insights into speciation evolution during nucleation and crystal growth. For calcium carbonate, in situ 13C and 1H solution- and solid-state NMR reveals the transformation of Ca·HCO3 ion pairs into a Ca·HCO3 dense liquid phase (DLP), followed by the decomposition reaction of the DLP to hydrated ACC, releasing water, CO2, and bicarbonate to the bulk solution. For gibbsite, combined in situ and ex situ solid-state 27Al multiple quantum magic angle spinning (MQMAS) NMR demonstrates that a large, purely hexa-coordinated aluminum cluster forms directly from amorphous aluminum hydroxide gel and converts to gibbsite via the release of Al-O monomers, whereas tetra- and penta-coordinated clusters act as intermediates that cannot directly transform into the crystalline phase. The different effects of solution-state NMR, solid-state NMR, and TEM experimental setup on nucleation pathway are also discussed.

DESIGN OF MICROSTRUCTURE AND DEFECT IN BATIO3 THIN FILMS AND SUPERLATTICES FOR ENHANCED PERFORMANCE

Aiping Chen (Los Alamos National Laboratory)

In this talk, I will discuss the strategies of designing interface and domain structure in doped BaTiO3 thin films and superlattices to achieve enhanced relaxor ferroelectric behavior for energy storage applications. In the first part, I will discuss the design of (Ba0.7Ca0.3)TiO3 (BCT) and Ba(Ti0.8Zr0.2)O3 (BZT) superlattices via a high-throughput combinatorial approach. In the second part of the talk, I will discuss strategies to further optimize domain structures and suppress the leakage current in BZT-BCT films via a machine learning approach. The large polarization and the delayed polarization saturation lead to greatly enhanced energy density of 80 J/cm3 and transfer efficiency of 85% over a wide temperature range. Such a data-driven design recipe for a slush-like polar state is generally applicable to quickly optimize functionalities of ferroelectric materials.

CHARACTERIZATION OF SPOKE PATTERN OF STACKING FAULTS IN 4H-SIC WAFERS GROWN BY PHYSICAL VAPOR TRANSPORT METHOD

Zeyu Chen (Stony Brook University), Jianpei Zhang (Stony Brook University), Shanshan Hu (Stony Brook University), Kaixuan Zhang (Stony Brook University), Yuzhuo Li (Stony Brook University), Haochi Wang (Stony Brook University), Balaji Raghothamacha (Stony Brook University), Yafei Liu (Onsemi), Campbell Bouch (Onsemi), Ryan Philpott (Onsemi), Scott Turchetti (Onsemi), Pete Schunemann (Onsemi). Michael Dudley (Stony Brook University)

Silicon carbide (SiC) is a semiconductor with a wide bandgap and exceptional electronic and physical properties, including high saturation velocity, high breakdown field, and excellent thermal conductivity [1]. These attributes make SiC a highly promising material for demanding applications involving high voltage, high power, and high temperature environments. The development of large-scale, high-quality single crystal SiC is crucial for enhancing device performance and broadening its application scope. Among the available growth techniques, physical vapor transport (PVT) [2] is the most widely used method, as it allows the production of large SiC substrates with controllable growth rates. However, the presence of various crystallographic defects, such as threading screw/mixed dislocations (TSDs/TMDs) and micropipes (MPs) can significantly impact device performance, limiting the full potential of SiC-based technologies [3,4]. Therefore, the generation and impact of such defects during PVT growth should be thoroughly investigated to improve the growth processing and furnace design.

In this study, one 4H-SiC wafer was analyzed by synchrotron white beam X-ray topography (SWBXT)while mappings of TSDs/TMDs density for the sequence of wafers sliced from the same boule were conducted by high resolution X-ray topography (HRXRT) in 0008 reflection. Variation of TSD/TMD density in spoke shape can be observed from HRXRT and formation of mixed Frank and Shockley type stacking faults due to deflection of the TSDs/TMDs can be observed in the region between the spoke pattern via SWBXT in 1-100 and 1-101. Density maps of TSDs/TMDs from the seed side to the dome side, where higher density of TSDs/TMDs were observed in the earlier growth stage near the facet region and the TSD/TMD density decreases as the wafer is closer to the dome side. Here, the spoke feature near the center of the wafer will be specifically analyzed.

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CHARACTERIZATION OF HIGH ENERGY IMPLANTED 4H-SIC EPIWAFERS FOR SUPERJUNCTION DEVICES VIA X-RAY METHODS

Zeyu Chen (Stony Brook University), Shanshan Hu (Stony Brook University), Balaji Raghothamachar (Stony Brook University), Michael Dudley (Stony Brook University)

Silicon Carbide (SiC) is a wide bandgap semiconductor recognized for its strong potential in power electronics, thanks to its large bandgap, high breakdown voltage, and excellent thermal stability [1]. The growing demand for high-voltage 4H-SiC devices is driven by their applications in hybrid vehicles, shipboard power systems, electrical infrastructure, and high-speed rail systems. These devices are typically fabricated on 4H-SiC wafers with thick epitaxial layers to support higher breakdown voltages [2]. However, achieving uniform doping throughout these thick layers poses a significant manufacturing challenge. A promising solution involves the use of multi-step high-energy ion implantation by the Tandem Van de Graaff accelerator at Brookhaven National Laboratory(BNL) [3]. Lattice strain induced during the ion implantation process must be effectively recovered, and the dopant atoms activated through an annealing process. Synchrotron X-ray Plane Wave Topography (SXPWT) and Reciprocal Space Mapping (RSM) were employed to measure and map the strain resulting from high-energy implantation of aluminum and nitrogen into 4H-SiC across various implantation patterns and subsequent annealing treatments. It is observed that the strain levels correlate with the total fluence levels. PiN diodes fabricated on these implanted wafers were then annealed at temperatures ranging from 1700 to 2000 °C for 60 min. The result suggests that for the same annealing time, higher temperature leads to better lattice recovery. 4H-SiC epiwafers implanted at different temperatures (room temperature, 300 °C, and 600 °C) analyzed by RSM measurements showed tensile strain, which decreased with higher implantation temperatures. Post-implantation annealing at 1700 °C was performed to further recover the lattice, with RSM measurements revealing that wafers implanted at higher temperatures retained the lowest residual strain. Additionally, employing a Silicon Energy-Filtered Ion Implantation (EFII) technique for aluminum implantation in a single step to a depth of 15 μm was found to further minimize lattice strain compared to wafers implanted without EFII at the same doping concentration.

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OPTIMIZATION AND SCALE-UP SYNTHESIS, PURIFICATION, AND CRYSTAL GROWTH OF CSPBBR3

Duck Young Chung (Argonne National Laboratory)

The all-inorganic perovskite $CsPbBr_3$ has emerged as a promising semiconductor for room-temperature high-energy radiation detection, offering excellent charge transport properties and operation with energy resolutions approaching 1% for ^{137}Cs γ-ray (662 keV). However, synthesis, purification, and crystal growth remain significant challenges that directly impact detector performance, stability in long-term operation, and scalability of spectroscopic grade crystals.

A key obstacle in producing high quality $CsPbBr_3$ crystals is controlling stoichiometry and phase purity, as undesired phases ($CsPb_2Br_5$ and Cs_4PbBr_6) as well as extrinsic impurities can form during synthesis and crystal growth, introducing charge trapping centers. Additionally, structural phase transitions - from cubic to tetragonal at 133°C and tetragonal to orthorhombic at 88°C - can induce physical defects to the crystals, affecting long-term device performance. The presence of defects, grain and twin boundaries, and charge carrier trap states further limits detector sensitivity and stability of the devices.

To address these challenges, we have developed an optimized chemical synthesis and purification process, achieving >99.999% purity to minimize metallic and halide defects that introduce deep trap states. We have also refined the Bridgman-based melt growth technique to produce large, crack-free single crystals with minimal grain boundaries and improved crystal uniformity. This presentation will discuss strategies to mitigate defects, enhance phase stability, and improve $CsPbBr_3$ crystal quality for scalable production. Our findings highlight the crucial role of synthesis and crystal growth optimization in advancing $CsPbBr_3$ radiation detectors for applications in homeland security, non-proliferation, and medical imaging applications.

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ON THE SYNTHESIZABILITY OF HIGH ENTROPY ROCKSALT OXIDE PHASES

Cristian Ciobanu ()

In the quest for understanding and tailoring the formation and properties of entropically stabilised ceramics, rocksaltstructured (MgNiCoCuZn)O occupies a central place. To date, most of the reported high-entropy rocksalt oxides (HERSOs) are derivatives of the original (MgNiCoCuZn)O, and only a couple of other novel HERSOs have been synthesised. To pave the way for the discovery of new HERSOs, we seek rapid and effective methodologies for screening large compositional spaces such as those associate with high entropy oxides. In this letter, we analyse modifications of the Hume-Rothery (HR) rules that govern the formation of solid-solution metallic alloys. We propose that HERSOs can form based on maintaining an oxidation state of +2 for all cations and a low value for the coefficient of variation associated with the lattice constants of the unmixed constituent oxides in a (hypothetical or actual) rocksalt phase. As a result of applying Hume-Rotheryinspired rules, we provide an heuristic explanation for the synthesizability of three experimentally realised HERSOs, and list a significant number of other HERSO compositions that can potentially be realised via similar methodologies. The rules devised in this work for HERSOs should provide guidance for future synthesis efforts, and we expect that community use could lead to further refinements as well as to modifications for application-specific screening.

ML WITH EMBEDDED THEORETICAL AND EXPERIENTIAL KNOWLEDGE FOR INDUSTRIAL SCALE CRYSTAL GROWTH

Katie Colbaugh (Leucite), Petia Koutev (Leucite)

The demand for high-quality industrial crystals is increasing, necessitating more rigorous testing, precise design, advanced data analysis, and optimized production processes. Manufacturers face significant challenges, including a shrinking skilled workforce, low-cost competition, and persistent supply chain disruptions. Existing data-driven ML/AI methods are not effective for increasing production yield due to the long cycle times, high cost of experimentation, and complexity of the crystal growth processes. Recent advancements in material and process informatics associated with crystal growth ML models have displayed the need for advanced physics-informed models.

Here we have developed a patent-pending, deep-tech approach to efficiently combine industrial crystal growth domain experience, theoretical knowledge, and ML models. This benchmark study on industrial crystal growth systems validates the predictive capabilities of physics-informed models for use in crystal growth manufacturing. The hybrid ML models identify trends linking material properties to process parameters, rank parameters responsible for defect formation, predict crystal growth run success, and guide parameter adjustments to achieve higher yield. The software developed in this work enables data-driven decision-making, accessible to any level of employee, and provides industrial crystal growers with a platform to visualize data and perform analysis on growth runs in real time, informed by historical data.

DATA-DRIVEN IN SITU STUDIES OF COMPLEX OXIDE FILM GROWTH AND CHARGE TRANSFER

Ryan Comes (University of Delaware, Department of Materials Science and Engineering)

The challenges of synthesis by molecular beam epitaxy for quantum materials research demand both new approaches to growth and new data streams to optimize film quality. In this talk, we explore two interconnected advancements: the observation of charge transfer phenomena in complex oxide heterostructures and the application of big data analytics to enhance film growth monitoring. By integrating experimental interface studies with computational big data techniques, this work bridges fundamental materials physics with next-generation automation, accelerating discovery in quantum oxide systems.

I will begin by discussing our work leveraging machine learning and big data analytics to extract deeper insights from in situ reflection high-energy electron diffraction (RHEED) during film growth. By training a convolutional neural network on epitaxial SrTiO3 films, we predict film composition from RHEED images, enhancing precision and reproducibility in synthesis. This approach paves the way for AI-assisted control of thin film growth for improved synthesis of oxides that exhibit interfacial phenomena.

Additionally, using plasma-assisted molecular beam epitaxy (MBE), we grew (SrCoO3)n/(SrIrO3)n superlattices, revealing interfacial charge transfer that drives emergent electronic and magnetic behaviors. Synchrotron-based spectroscopy and in vacuo X-ray photoelectron spectroscopy confirmed Co and Ir valence changes, indicating charge transfer with signs of orbital polarization in both B site ions. The interfacial charge transfer stabilizes SrCoO3 in the perovskite phase rather than the vacancy-ordered Brownmillerite SrCoO2.5. These results are corroborated by density functional theory modeling of the materials to understand emergent electronic and magnetic phenomena. Ongoing work focuses on the understanding of emergent magnetic behavior in these heterostructures through polarized neutron reflectometry and other magnetic characterizations. These findings contribute to the design of novel quantum materials with strong spin-orbit coupling and topological magnetic states.

III-V/SI HETEROEPITAXY: UNDERSTANDING AND MASTERING GROWTH FUNDAMENTALS

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The co-integration of group III-V and group IV semiconductors via heterogeneous epitaxy is of major interest for applications in integrated photonics and solar energy. In the 1980s, pioneering work by H. Kroemer [1] identified the main challenges associated with III-V/Si epitaxial growth. However, recent experimental studies have revealed inconsistencies with this early understanding [2]. In this work, we combine advanced epitaxial growth techniques, in situ microscopy, and Density Functional Theory (DFT) calculations to investigate the role of surfaces or interfaces in the Volmer-Weber growth of III-V monodomain islands on Si. We predict and observe in situ the equilibrium shapes of these islands, and examine their influence on the formation and propagation of antiphase boundaries (APBs) [2–8]. Particular attention is given to the chemical mismatch at the III-V/Si interface, which significantly affects charge distribution between the two materials. We then provide experimental evidence that APBs originate from the coalescence of monodomain islands and highlight the critical role of substrate miscut in breaking surface symmetry [8–10]. Finally, we demonstrate how these insights enable control over the spatial distribution of antiphase domains, and we present the experimental realization of a quasi-periodic one-dimensional APB pattern in a GaAs layer grown on Si [10]. These findings are discussed considering their implications for future device development [11].

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GROWTH AND CHARACTERIZATION OF A- AND ß-PHASE MNXSEY BY CHEMICAL VAPOR DEPOSITION

Jennifer DeMell (Laboratory for Physical Sciences), Elias Kallon (University of Maryland), Jimmy Kotsakidis (Laboratory for Physical Sciences), Kevin Daniels (University of Maryland)

Theory predicts that MnxSey is strongly magnetic thin film with a high TC of nearly 250 K and stability in ambient conditions, unlike many other leading 2D ferromagnets.1 Despite the material's suitability as a large-scale, high TC magnetic thin film, much is still unknown and the crystallographic phases of thin-film MnxSey and their properties are still not well understood. In this work, we demonstrate the controllable growth of α- and ß-phase MnxSey in a three-chamber chemical vapor deposition system using Se and MnCl2 precursor powders in an argon- and hydrogen-rich atmosphere on a sapphire substrate. A thorough characterization of each phase is performed with Raman spectroscopy, atomic force microscopy, and scanning electron microscopy. We observe distinct Raman peaks at 129 cm-1 and 255 cm-1 for the α and ß phases using a 532 nm laser excitation source with a 10 mW spot power, which have been reported previously in the literature as the longitudinal acoustic αMnSe mode and A1g Mn-Se stretching mode, respectively.2 Finally, we discuss the primary parameters impacting crystal nucleation for each growth phase: chamber pressure, growth time, and, in particular, the effects of argon/hydrogen atmospheric partial pressure and precursor vapor pressures.

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THE ENGULFMENT OF BUBBLES DURING BULK CRYSTAL GROWTH

Jeffrey Derby (University of Minnesota), Swanand Pawar (University of Minnesota)

Bubbles of 5–100 microns in size are observed in many bulk crystals grown from the melt, such as sapphire and silicon. While the engulfment of solid particles during solidification has been well studied [1-2], bubble engulfment is comparatively poorly understood, though often quite consequential. For example, a single argon bubble engulfed during the Czochralski growth of single-crystal silicon can produce stresses high enough to generate dislocations, resulting in a catastrophic loss of structure. A better understanding of the fundamentals of bubble engulfment will thus increase process yields and reduce costs.

Bubble engulfment during solidification is determined by a balance of repulsive van der Waals forces between the bubble and the solidification interface versus drag forces arising from the flow of the melt around the bubble. When drag forces overcome repulsive forces, the bubble is engulfed, otherwise it is steadily pushed ahead of the advancing interface. Since drag increases with bubble size and velocity, there exists a critical growth velocity at which a bubble of a certain size is engulfed. However, drag forces are strongly dependent upon flows along the bubble surface, including thermocapillary flows, and shape of the solid-liquid interface as the bubble approaches. Thus, the critical velocity is affected by significant and nonlinear interactions involving heat transfer, fluid dynamics, and interfacial phenomena.

We apply computational analyses to understand bubble engulfment during bulk crystal growth from the melt. This research builds upon prior steady-state and dynamic models that have been developed to study the pushing or engulfment of a solid particle at a moving, solid-liquid interface [1-2]. We highlight the significant differences between bubble and solid particle engulfment. The relationship between critical growth velocity and bubble size is computed for argon bubbles during Czochralski silicon crystal growth, providing guidelines to avoid engulfment.

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OPTIMIZING ACRT TO REDUCE INCLUSIONS DURING VGF GROWTH OF CZT

Jeffrey Derby (University of Minnesota), Mia Divecha (University of Minnesota), Jedidiah McCoy (Washington State University)

Cadmium zinc telluride (CZT) is an important material for large-volume, gamma-ray spectrometers featuring high energy resolution and room-temperature operation. The vertical gradient freeze (VGF) process, a variant of the classical Bridgman technique, can achieve growth rates that are at least an order of magnitude faster than in the traveling heater method (THM). However, VGF growth results in material that is often of poor quality due to populations of large, second-phase, tellurium-rich particles.

We summarize the results of a synergistic modeling and experimental studies to assess the use of the accelerated crucible rotation technique (ACRT) to reduce tellurium inclusions during the growth of CZT via VGF [1-2]. Using a metric based on the classic Mullins and Sekerka criterion for morphological instability, we optimize and provide mechanistic explanations for a preferred ACRT schedule. Two, different ACRT rotation schedules and a no-rotation case are assessed in growth experiments. Growth under ACRT resulted in crystals with inclusion size and volume significantly decreased from levels found in material grown with no rotation. However, material grown using the computationally-optimized rotation schedule (Ekman ACRT) exhibited a median inclusion size that was smaller and with a sharper distribution than in material grown via a classical schedule (Mixing ACRT). Such results promise to improve material quality and process yields.

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COMPOSITIONAL EFFECTS ON THE ENGULFMENT OF PARTICLES DURING CRYSTAL GROWTH

Jeffrey Derby (University of Minnesota), Yutao Tao (University of Minnesota)

While particle engulfment has been studied in many systems [1], very little attention has been paid to the fundamental role of compositional effects. Specifically, if a solute changes the solidification melting temperature, the interaction of the particle with the segregated solute at the growth interface redistributes its concentration in the liquid, thereby affecting the shape of the solidification interface under the particle and the critical conditions for engulfment. In addition, if the particle has nucleated from a supersaturated melt, it continues to grow while it is approaching the melt-crystal interface, further affecting the concentration distribution and engulfment behavior.

We employ a rigorous, finite-element model to study the engulfment of a precipitated solid particle during solidification in a supersaturated melt, in which solute segregation, compositional effects on melting temperature, and reaction of the solute with the particle occur [2]. The case of a silicon carbide particle approaching a solid-liquid interface in a silicon melt supersaturated with carbon is specifically considered. Critical engulfment velocities are computed for particles with different surface reaction rates, as characterized by the Damköhler number, a dimensionless ratio of reaction to diffusion. Consistent with prior studies, an inert particle is predicted to be more likely to be engulfed when solute effects are present. However, a particle with fast surface reaction is less likely to be engulfed than in a system without solute effects, which is relevant for SiC particles during silicon crystal growth. Most interestingly, a particle for which the surface reaction is characterized by a Damköhler number of order unity is predicted to never be engulfed.

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STABILITY-BASED OPTIMIZATION OF ACRT FOR THE GROWTH OF CZT BY THM

Jeffrey Derby (University of Minnesota), Jeff Peterson (University of Minnesota), Zachary Cosenza (University of Minnesota)

A novel, multi-scale modeling approach is developed to study the effects of accelerated crucible rotation technique (ACRT) rotation schedules on the growth of cadmium zinc telluride (CZT) by the traveling heater method (THM). This system is particularly prone to morphological instability via a lee-wave flow that forms in the liquid zone, trapping tellurium rejected at the interface and producing constitutional supercooling. Increased mixing of the liquid zone is needed to overcome this undesirable feature so that growth rates may be increased [1].

Using data provided by high-fidelity growth simulations, a new model is developed to predict the amplitude of disturbances associated with cellular interface morphologies that develop over time and across the liquid-solid interface [2]. This disturbance amplitude measure is used to assess the ability of ACRT to stabilize the growth interface and thereby minimize inclusion formation processes. Notably, our analyses reveal that interfacial instability is not well correlated with melt undercooling, explaining why classical ACRT approaches to reduce undercooling simply via mixing may not stabilize growth. Computations show that interface stability is best achieved via rotation schedules that accentuate outward Ekman flows during spin-up and, during spin-down, eliminate Taylor-Görtler flows, and minimize inward Ekman flows.

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DRIVING GROWTH IN THE GERMANIUM MARKET: UMICORE'S STRATEGIC INNOVATIONS

Kristof Dessein (Umicore EOM), Robin Vanuytven (Umicore EOM), Laurie Mouchel (Umicore EOM), Jinyoun Cho (Umicore EOM), Rajiv Sharma (Umicore EOM), Alexandre Chapotot (Umicore EOM)

Dislocation free Ge substrates are today used in many applications, where they are essential to the functioning of the device. Umicore has a long history of refining Ge and transforming it into crystals and wafers. Today, Umicore is offering solutions ranging from infrared optics over 150mm Ge substrates for space solar cells to 200mm Ge wafers for photonic devices.

Today, those markets are rapidly growing. Two megatrends are at the origin of that. New Space is moving away from big GEO satellites to constellations, effectively tripling the demand of space power. Secondly, ongoing miniaturization in the field of micro-electronics eventually requires hetero integration. As Ge is compatible with both GaAs III-V and Si CMOS, it's regarded as the ideal substrate to bridge both worlds. This growth puts pressure on the Ge supply side. Indeed, Ge is a critical minor metal and stringent Chinese export restrictions limit the availability of Ge. This growth also puts pressure on the product offering, as with increased volume, customers expect a better deal, both in price and quality.

In this presentation, we show how Umicore is reacting to these new conditions. In the first part, it will be explained how we optimized our growth conditions for Ge crystals to increase puller output as to keep the cost of crystals under control.

Secondly, substantial research has been conducted to understand the physics behind crystal voids, largely unavoidable in dislocation-free crystals. Overgrowing these with III-V's results in micron-size hillock defects. Though they do not really impact the efficiency of solar cells, they pose a reliability threat and prevent full scale adhesion during wafer bonding, a crucial step in hetero integration.

Thirdly, Umicore has been working on re-usable Ge substrates. That research stems from the fact that for certain functional devices, only a couple of microns of Ge is needed. The remainder of the material is used for support purposes only, a function that can be taken up by other materials. A re-usable substrate consists of a Ge foil of tunable thickness, weakly attached to a Ge bulk substrate. After device processing, the foil can be mechanically detached, allowing for further re-use of the mother substrate. The weak layer underneath the foil is formed by electrochemical etching, followed by a subsequent annealing. That way, the re-usable substrate offers a pristine growth surface, while also decoupling material demand from Ge availability.

MONOLAYER MANGANESE AT GRAPHENE/6H-SIC INTERFACE: AN AIR-STABLE FERROMAGNETIC FILM

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Two-dimensional (2D) mentals have recently garnered considerable attention due to their novel physicochemical properties, unique behaviors at the monolayer limit, and promising applications in advanced electronics, optoelectronics, catalysis and energy storage1. However, the environmental sensitivity and limited lateral dimensions of 2D metals remain significant bottlenecks to their practical deployment under ambient conditions and their integration into a wide range of applications1. Recent advances in intercalating metals at the epitaxial graphene (EG)/silicon carbide (SiC) interface have inspired our approach, dubbed “confinement heteroepitaxy (CHet)”, to synthesize scalable, environmentally stable 2D metals that exhibit distinct properties from their bulk counterparts2,3. For instance, monolayer Ag confined between EG and SiC is a 2D semiconductor with a ~1 eV band gap3.

2D Mn between EG and SiC is predicted to be ferromagnetic, and a Dirac half metal enabling the quantum anomalous Hall effect4. Therefore, experimental realization of 2D Mn will be beneficial for exploring and understanding its structures, properties and potential applications in information storage and quantum devices. Here, we will discuss our advances toward realizing large-area, atomically thin manganese (Mn). X-ray photoelectron spectroscopy confirms the coexistence of Mn-Mn and Mn-Si bonding, indicating successful Mn intercalation in EG/SiC interface. High-resolution transition electron microscopy further confirms the Mn is monolayer. Due to the presence of Si dangling bonding in the interface of as-grown EG, Mn diffusion is hindered, leading to the formation of patch-like domains. However, when these dangling bonding are passivated by pre-intercalated hydrogen, the Mn atoms diffuse more uniformly, resulting in the formation of a continuous monolayer film. Scanning Tunneling Microscopy and DFT further reveal the presence of two distinct structural phases in monolayer Mn. Furthermore, Superconducting Quantum Interference Device magnetometry demonstrates

that monolayer Mn is ferromagnetic, indicating its potential for future applications in low-dimensional magnetism and quantum materials research.

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VALENCE FLEXIBILITY AND STRUCTURE–PROPERTY RELATIONSHIPS IN CHROMIUM-CONTAINING COMPLEX OXIDES

Yingge Du (Pacific Northwest National Laboratory)

The extraordinary redox versatility of chromium offers a unique platform for exploring and controlling structure–property relationships in complex oxides. In this talk, I will present our recent efforts on the epitaxial growth and characterization of Cr-based oxides, focusing on how Cr's variable valence states can be harnessed to engineer novel phases and functionalities.

Cr^{3+} is the most stable oxidation state in perovskite ABO_3 oxides, as exemplified by $LaCrO_3$. However, we demonstrate that higher valence states—Cr^{4+} and Cr^{5+}—can be stabilized through a combination of aliovalent doping, epitaxial strain, and controlled growth conditions. In $SrCrO_{2.8}$, we observe the emergence of vacancy-ordered superstructures, including rhombohedral phases and a brownmillerite-like structure induced by Fe doping. Using atomic-resolution STEM and electron energy loss spectroscopy (EELS), we uncover a striking layer-resolved modulation of Cr valence, revealing Cr's exceptional adaptability to changes in local oxygen coordination.

Building on these insights, we investigate high-entropy oxide systems such as $La_{1-x}Sr_x(5B)O_3$, which incorporate multiple 3d transition metal cations (Cr, Mn, Fe, Co, Ni). These systems further highlight Cr's flexibility, with undesirable Cr^{6+} forming readily under oxidative conditions. Interestingly, we find that chemical potential can be leveraged as a powerful thermodynamic handle to selectively stabilize metastable Cr-rich configurations and promote the formation of non-equilibrium phases within $La(5B)O_3$. This approach opens new pathways to tailor Cr coordination environments and drive emergent functionality in complex oxide systems. In addition to valence tuning, our work reveals strong nanoscale compositional fluctuations in high-entropy oxides, reflecting the complex interplay among competing cationic interactions. These results underscore the central role of Cr's redox behavior in enabling adaptive, responsive oxide chemistries.

Taken together, these findings provide new strategies for rationally designing metastable structures and tuning functional properties in transition metal oxides via targeted control of chemical potential, valence states, and structural motifs.

FABRICATION OF 80 µM-THICK GAAS SEMICONDUCTOR OPENING SWITCHES USING HALIDE VAPOR PHASE EPITAXY

Mario Dumont (National Renewable Energy Laboratory), Steven Hayden (Nation Renewable Energy Laboratory), James Schrock (Air Force Research Laboratory), Brad Hoff (Air Force Research Laboratory), Susan Heidger (Air Force Research Laboratory), Aaron Ptak (National Renewable Energy Laboratory), John Simon (National Renewable Energy Laboratory), Kevin Schulte (National Renewable Energy Laboratory)

We present the fabrication of 80-micron-thick GaAs PN junctions using Halide Vapor Phase Epitaxy (HVPE) for applications in high power RF pulse generation. Switches are instrumental components in RF pulse generators, and opening switches offer better performance than closing switches due to faster energy transfer. When used as opening switches, thick PN diodes with a large, low-doped depletion region exhibit a nanosecond-cutoff of high-density reverse current, called the Semiconductor Opening Switch (SOS) effect, which delivers a high power pulse to the load. The strength of the SOS effect increases with the depth of the junction. Silicon achieves depths of 100-300 microns through the onerous diffusion of dopants in a furnace for multiple weeks. GaAs devices offer the benefit of higher operating voltages and narrower pulses attributed to its higher maximum electric field and higher electron mobility. However, producing devices with 100-um-thick depletion regions in GaAs is not feasible by thermal diffusion or ion implantation of dopants, and would be cost-prohibitive by incumbent epitaxial growth techniques. HVPE can achieve growth rates of 500 microns/h and the low intrinsic carrier concentration needed for SOS devices, which makes it uniquely suited to epitaxially grow SOS structures.

In this talk, we present results on the development of GaAs SOS devices using a variable-pressure HVPE system. The growth conditions were studied to yield low surface roughness and low hillock density at a growth rate of 150 microns/h, and the origins of hillock defects were investigated by cross-section microscopy. We investigated the minimum controllable carrier concentrations in n- and p-type material and the grading of doping profiles in the 10^15 cm^-3 range over 25-50 microns. Additionally, this material demonstrated mobility values comparable to incumbent growth techniques. We grew 80-micron-thick devices with hole and electron active region carrier concentrations at or below 1x10^16. Devices from this material were fabricated and their potential as SOS switches was evaluated.

SPECTROSCOPIC SIGNATURES OF MICRO-SEGREGATION IN MELT-GROWN GALLIUM OXIDE

Benjamin Dutton (Washington State University), Drew Haven (Luxium Solutions LLC), David Joyce (Luxium Solutions LLC), Jani Jesenovec (BAE Systems), Matthew McCluskey (Washington State University), John McCloy (Washington State University)

One of the primary advantages of β-Ga2O3 over incumbent wide-bandgap semiconductors is the ability to grow directly from the melt. As β-Ga2O3 substrates continue to develop and increase in size, it is imperative to understand idiosyncrasies inherent to the various methods employed for β-Ga2O3 crystal growth. In this work, we describe how laser Raman systems can be used to map and spatially correlate Cr3+ photoluminescence, electronic-coupled Raman scattering from Ir4+ d-d internal transitions, and the Raman line attributed to hydrogenic shallow donors. Laser ablation inductively coupled plasma mass spectrometry directly measured spatially-dependent relative impurity concentrations, confirming spectroscopic signals resulted from heterogeneous solute concentrations in β-Ga2O3 crystals grown by Czochralski, floating zone, vertical gradient freeze, and edge-defined film-fed growth methods.

VALENCE BAND ENGINEERING OF GA_2O_3 FOR P-TYPE CONDUCTIVITY

Chioma Vivian Ezeh (City University of Hong Kong), Kingsley Egbo (City University of Hong Kong), Jamal-Deen Musah (City University of Hong Kong), Kin Man Yu (City University of Hong Kong)

Gallium oxide (Ga_2O_3) has emerged as a highly promising material for high-power and deep-ultraviolet (UV) optoelectronics due to its wide bandgap and unique electronic properties. However, its application potential is hindered by the absence of a reliable p-type counterpart, as Ga_2O_3 is effectively doped only n-type. This study explores the modification of Ga_2O_3 electronic bands through alloying with nickel oxide (NiO) to create p-type conducting Ga_2O_3-NiO (NixGa1−xO) thin films. Sputter deposition at room temperature yields stoichiometric and oxygen-rich films with distinct structural transitions: amorphous phases dominate at low Ni content ($x < 0.22$), while higher Ni content ($x \gtrsim 0.22$) results in polycrystalline rocksalt (RS) structures. Oxygen-rich RS alloys exhibit p-type conductivity, with resistivity values as low as ~10 Ω-cm for $x \approx 0.6$, decreasing further with increasing Ni content. Optical characterization reveals that the bandgap (Eg) decreases monotonically from 4.98 eV ($x = 0$) to 3.53 eV ($x = 1$), following the virtual crystal approximation with minimal bowing (0.36 eV). Films with $x \geq 0.46$ also exhibit strong sub-gap absorption below 3.5 eV, attributed to a high concentration of nickel vacancies (VNi), which reduces optical transmittance from ~70% ($x = 0.3$) to ~40% ($x = 1$). The valence band maximum (VBM) undergoes a significant upward shift, rising from ~8 eV below the vacuum level in amorphous films to ~6.2 eV in RS structures ($x \approx 0.2$). This shift enables the observed p-type conductivity by effectively transforming deep acceptor levels into shallow ones. These findings suggest that further enhancement of p-type conductivity is achievable through targeted acceptor doping. The tunability of the electronic and optical properties of Ga_2O_3-NiO alloys makes them strong candidates for advanced optoelectronic and photodetection applications.

THERMAL LASER EPITAXY FOR ULTRACLEAN HETEROSTRUCTURES

Brendan Faeth (epiray Inc)

As the scope of known material systems and quantum electronic phenomena continues to expand, so too are the demands for improved control, purity, and thermodynamic versatility in thin film synthesis becoming ever more stringent. In particular, the need for greater variety and control of constituent sources has begun to strain the capabilities of conventional deposition techniques. Here, we demonstrate a new thin-film deposition technique that is especially suited to the growth of complex oxide heterostructures with atomic precision. Thermal laser epitaxy (TLE) employs continuous wave lasers to simultaneously heat both substrates and freestanding elemental sources. The lasers' virtually arbitrary power density allows for the evaporation of practically all elements of the periodic table in the same setup while maintaining process gas environments up to pressures as high as 10-1 mbar. For substrates heated directly via CO2 laser, temperatures up to and beyond 2000 °C can be reliably reached on virtually all commercially available oxide substrates, unlocking previously inaccessible growth regimes in many complex oxide systems of interest. In combination, these advantages suggest the potential of TLE to greatly expand thermodynamic parameter space for ultraclean epitaxial thin film synthesis.

CHALLENGES AND OPPORTUNITIES IN TEXTURED PIEZOELECTRIC CERAMICS

Mark Fanton (Penn State University), Beecher Watson (Penn State University), Joshua Fox (Penn State University), Christopher Eadie (Penn State University)

Directional tailoring of performance for electronic materials has been largely limited to taking advantage of anisotropies in single crystal materials. This talk outlines the process technology and scale up considerations for tailoring directionally oriented ceramic microstructures, with a focus on achieving single crystal-like performance from highly oriented ceramic piezoelectric materials. The engineering challenges associated with scaling each step of the manufacturing process will be outlined. Special attention will be paid to development of a textured microstructure during templated grain growth of Mn-doped PMN-PZT piezo-ceramic. In particular microstructure development during heating to the sintering temperautre, and the presence or absence of dopants, results in texture fractions above 90%. Much is unknown regarding the template/matrix interactions during this part of the process, and those unknowns will be highlighted. In addition, opportunities to create shapes, microstructures and symmetries to yield devices or properties not readily achievable in either random ceramic or single crystal materials will be outlined as potential pathways for innovation beyond material chemistry. A new material design paradigm may be opening, where composition and processing routes are tailored for simultaneous optimization of microstructure and macrostructure to produce new emergent properties.

TOPOTACTIC OXIDATION OF RUDDLESDEN-POPPER NICKELATE THIN FILMS REVEALS FAMILY OF INTERCALATED LAYERED NICKELATES

Dan Ferenc Segedin (Harvard University, Physics Dept), Jinkwon Kim (Cornell University), Harisson LaBollita (Arizona State University), Nicole Taylor (Harvard University), Suk Hyun Sung (Rowland Institute), Ari B. Turkiewicz (Harvard University), Grace A. Pan (Harvard University), Abigail Y. Jiang (Harvard University), Tobias Schwaigert (Cornell University), Casey Kim (Cornell University), Alpha T. N'Diaye (Advanced Light Source LBNL), Ismail El Baggari (Rowland Institute), Hua Zhou (Advanced Photon Source Argonne), Charles M. Brooks (Harvard University), Antia S. Botana (Arizona State University), Darrell G. Schlom (Cornell University), Julia A. Mundy (Harvard University)

The Ruddlesden-Popper (RP) nickelates, Rn+1NinO3n+1 (R = trivalent rare-earth cation), exhibit rich correlated electron phenomena, including charge/spin density wave order and, more recently, high-temperature superconductivity [1-2]. These compounds comprise n perovskite-like RNiO3 layers separated by rock salt RO spacer layers; the dimensionality (n) tunes the nickel oxidation state from 2+ (n=1) to 3+ (n=∞). Beyond structural dimensionality, RP nickelates offer significant tunable soft-chemical, topotactic modifications of the oxygen content [3]. Topotactic reduction via oxygen deintercalation, for example, yields the square-planar nickelates, Rn+1NinO2n+2, which consist of n square-planar RNiO2 layers separated by RO2 spacer layers, with nickel oxidation states ranging from 1+ (n=∞) to 1.5+ (n=2). Due to their structural and electronic similarities to high-Tc cuprates, the square-planar nickelates have garnered intense interest following the discoveries of superconductivity in hole-doped RNiO2 (n = inf) and five-layer Nd6Ni5O12 (n = 5) [4-5].

In this work, we introduce a complementary approach – topotactic oxidation via oxygen intercalation of rock salt spacer layers – revealing a novel family of intercalated RP nickelates, Lan+1NinO3n+1+δ. We synthesize epitaxial Lan+1NinO3n+1 (n = 1 – 4) thin films on NdGaO3 (110) via ozone-assisted molecular beam epitaxy (MBE) then anneal the films at ~300 °C under 1 atmosphere ozone. We observe a substantial ~17% c-axis expansion in La2NiO4 (n=1) after oxidation, with decreasing expansion for higher n. Synchrotron x-ray diffraction and Coherent Bragg Rod Analysis (CoBRA) reveals that the c-axis expansion is driven by oxygen intercalation of the rock salt spacer layers. Our findings highlight topotactic oxidation as a promising avenue to tune and expand the functional landscape of RP nickelates.

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CONTINUOUS CRYSTALLIZATION IN BIOPHARMACEUTICAL MANUFACTURING: THERAPEUTIC FULL-LENGTH MONOCLONAL ANTIBODIES

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A rapidly growing category of proteins is monoclonal antibodies (mAbs), considered the highest-selling class of biopharmaceuticals. This is mostly due to their specific action and reduced immunogenicity [1]. The rising demand for monoclonal antibodies as powerful therapeutic agents is coupled with the high cost of traditional chromatography columns, which requires the exploration of more cost-effective and sustainable alternatives [2]. Therefore, crystallization emerges as a cost-efficient purification strategy by reducing operational costs and facility footprint. The batch-to-continuous transition of biopharmaceutical production has been continuously advancing and applied during the last decade to improve product quality attributes at a low manufacturing cost [3]. Several review articles have been published to highlight an overview of continuous crystallization processes in pharmaceutical manufacturing. However, these reviews were mainly focused on active pharmaceutical ingredients (APIs) rather than on biomacromolecules; and only a few studies have reported experimental methodologies to continuously crystallize model biomacromolecules (e.g. lysozyme, insulin).

This study highlights, to the best of our knowledge, the first integrated crystallization-based platform to crystallize full-length mAbs. An overview of the experimental apparatus for one of the studied mAbs is shown in Figure 1, which comprises series-connected MSMPRs and the crystalline mAb suspension is transferred through a pressure-driven system. The crystallizers are designed to ensure high mixing efficiency by an in-house optimized impeller design and custom-built baffles. Moreover, PAT implementation on the apparatus allows for real-time monitoring of different mAb crystallization processes, including in-line CSD, microscopy and turbidity profiles (Blaze probe) as well as real-time Raman spectroscopy (Raman probe). Off-line sampling consists of microscopy imaging and mAb concentration measurement (HPLC). Additional analytical techniques are used to assess the quality and efficacy of the continuous process. Ultimately, needle-shaped crystals are obtained and characterized through SAXS and Cryo-EM. Lastly, AI-based image analysis is implemented to obtain CSD over time and mAb crystallization kinetics are quantified by PBM and considering a steady-state MSMPR model.

PREDICTING THE SHAPE-SELECTIVE SYNTHESIS OF METAL NANOCRYSTALS: A MULTIFACETED APPROACH

Kristen Fichthorn (Penn State University)

Metal nanocrystals have the potential to revolutionize established technologies such as catalysis, environmental remediation, plasmonic, photonic, and electronic devices, sensing, and photovoltaics. Additionally, metal nanocrystals will figure prominently in upcoming technologies, such as triboelectric nanogenerators, electromagnetic interference shielding, and a host of upcoming “smart” technologies, such as electro- and photo-chromic devices, wearable devices, and e-skin. For most established applications, there is ample evidence that the efficacy of a nanocrystal is sensitive to its shape. Theory can be beneficial in unraveling the many complex factors that can contribute to shape selectivity in solution-phase syntheses. In this talk, I will discuss the profound and synergistic role of halides, present as solution-phase additives or in metal salts, and organic additives in promoting facet-selective nanocrystal growth, oriented attachment, and assembly.[1-4] I will finish by highlighting prospects for future studies.

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ATOMIC-SCALE CRYSTAL DEFECTS FOR QUANTUM INFORMATION SCIENCE AND CHARACTERIZATION OF MATERIALS

Gregory Fuchs (Cornell University)

I will discuss isolated defects in wide bandgap materials as useful objects for quantum information science and magnetic material characterization. Isolated point defects in crystals with a long-lived spin and associated spin-dependent optical transitions allow one to use fluorescence as a probe of a single spin qubit, even at room temperature. The most famous example is the nitrogen-vacancy (NV) center in diamond, however, other defects in diamond, silicon carbide, silicon, and other materials are promising for applications in quantum sensing and quantum networking. After introducing the idea of "quantum defects" I will discuss the characterization of magnetic materials with nanoscale spatial resolution by scanning a diamond probe containing a single NV center. The NV center can serve as an exquisitely sensitive magnetic field sensor – or by operating the the NV center as a qubits – it can probe the magnetic dynamics. I will then discuss our discovery of new quantum defects hosted in GaN. Along with discussing their optical and spin properties as well as the open questions with these defect centers, I'll mention their potential applications as sensors integrated with electronic and photonic technologies.

3D MODELING OF CZ SI GROWTH IN AN ASYMMETRIC FURNACE WITH APPLIED HORIZONTAL MAGNETIC FIELD

Alex Galyukov (STR US, Inc.), Aleksa Crnobrnja (STR Belgrade), Petar Jovanovic (STR Belgrade),
Andrey Smirnov (STR Belgrade)

We present a study on the growth of 300 mm Czochralski (Cz) silicon crystals for microelectronic applications. Modern nanometer-scale devices impose tight requirements on the crystalline structure, defect size and density (COPs, BMDs), as well as impurity and dopant concentrations and their uniformity across the melt/crystal interface. To meet these numerous criteria throughout the entire crystal growth process, advanced modeling is necessary.

Previously published models have shown a good agreement between calculated and experimental data for interface shape and oxygen concentration [1]. However, even more elaborate modeling capabilities are needed to further fine-tune the crystal characteristics and achieve the crystal quality satisfying tight industry standards. This includes accounting for 3D effects such as asymmetric gas flow and asymmetric heat generation in the heater, detailed distributions of horizontal magnetic fields [2], and even the design of asymmetric heat shields [3]. The latter enables more precise control of the gas shear stresses over the melt free surface, which is critical for accurate modeling of the melt flow and oxygen concentration.

In this work, we introduce a novel approach that combines 3D global heat transfer modeling with a well-validated local 3D modeling approach for accurate simulation of the melt flows, interface shape, and impurity transport [1]. We specifically simulate the growth of a 300 mm silicon ingot in the furnace with asymmetric heat shield [3] and applied horizontal magnetic field.

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CONTROLLED DOPING AND TRANSPORT PROPERTIES OF (ULTRA)WIDE-BAND-GAP SB-DOPED RUTILE-GEXSN1−XO2.

Dipannita Ghosh (Oregon State University), Sumit Goswami (University of Oklahoma), Mark E Bowden (Pacific Northwest National Laboratory (PNNL)), Tien-Anh Nguyen (Oregon State University), Yingge Du (Pacific Northwest National Laboratory (PNNL)), Hanjong Paik (University of Oklahoma), Sieun Chae (Oregon State University)

Wide and ultrawide band-gap oxide semiconductors are gaining attention as promising materials for high-power and high-frequency electronics and deep ultraviolet optoelectronics. Among them, recently discovered rutile GeO2-SnO2 alloy (r-GexSn1−xO2) stands out as a potential candidate owing to a tunable bandgap from 3.81 eV to 4.68 eV, high thermal conductivity, and n-type conductivity. However, for its adoption in electronic devices, the ability to modulate of carrier density via controlled doping is a critical need. In this paper, we demonstrate systematic control of the electron concentration of r-GexSn1−xO2 (x=0.33) via antimony (Sb) doping and analyze its transport mechanism. Sb-doped r-GexSn1−xO2 (x=0.33) thin films are fabricated on sapphire substrates by suboxide molecular beam epitaxy (S-MBE) where Sb concentration is controlled by the Sb effusion cell temperature and measured by X-ray photoelectron spectroscopy. Despite the addition of Sb, our sample remains highly crystalline without the presence of impurity phases. At room temperature, undoped r-GexSn1−xO2 thin films are highly insulating. On the other hand, Sb doping provides tunable carrier concentration (n) from n = 5.01 × 1018 to n =5.01 ×1019 cm-3 with the highest mobility of 32.5 cm2 V−1 s−1 at n = 2.51 × 1019 cm−3. Temperature dependent Hall measurement reveals that the transport mechanism of Sb-doped r-GexSn1−xO2 at high doping concentration is three-dimensional (3D) Mott Variable Range Hopping (VRH), which is further supported by temperature dependent magnetoresistance measurements. The findings of this study highlight the potential of Sb-doped r-GexSn1−xO2 as a promising wide-bandgap (Eg = 4.04 eV) semiconductor for further device exploration.

UNDERSTANDING THE TILT OF HEXAGONAL AND LOWER SYMMETRY LAYERS ON MISCIT SUBSTRATES

Mark Goorsky (UCLA), Michael Liao (UCLA), Leon Sit (UCLA)

Heteroepitaxial growth on a miscut substrate introduces a tilt in the lattice planes of the epilayer compared to the same family of planes in the miscut substrate. The so-called Nagai model (H. Nagai, J. Appl. Phys., 45, 3789 (1974)) was developed to describe this observed tilt in lattice mismatched cubic materials systems. Here, we build upon our earlier work that demonstrated how the Nagai model incorrectly describes how interfacial distortions form at the interface in cubic systems and we extend our refined model to hexagonal and lower symmetry epitaxial layers as well-as to implant strain-induced systems.

Our model is based on the simple notion that the miscut surface is not a low index planar surface but rather that diffraction from the nearest low index planes in fact correspond to asymmetric reflections. Here, we extend our model to examples in hexagonal (III-nitrides and silicon carbide) and monoclinic (□-Ga2O3) systems. As in the cubic structures, the stress applied to an epitaxial layer in, for example, the GaN-AlN system or an ion-implanted structure, such as with SiC on a miscut substrate, is not along a low index (e.g. (0001)) plane. Under the framework of reciprocal space, the {000l} reflections would be symmetric reflections for on-axis substrates but are asymmetric reflections for miscut substrates. The tilt that is experimentally observed between the low index substrate planes and the epitaxial layer planes ((0001) for example with a miscut substrate) matches that which is predicted by treating the low index reflections as asymmetric reflections. A modified epitaxial tilt equation which takes onto account the miscut surface plane, the strain in the epitaxial layer and the material's Poisson ratio is provided. Examples from our laboratory as well as the literature will demonstrate that this model accurately predicts the measured tilt between epitaxial and substrate layers based on the lattice parameter mismatch as well as the Poisson ratio of the layer and can be applied to any crystal system.

ALN LAYER HETEROEPITAXY: NANO TO MICRO GROWTH USING X-RAY SCATTERING

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AlN templates on sapphire substrates are widely employed for subsequent epitaxial deposition of AlN-based device structures. Recent developments have led to high quality layers using both organometallic and molecular beam epitaxy growth techniques. The x-ray rocking curve peak widths are shown to be less than twenty arcsec but in many cases, a second lower intensity broader peak is superimposed on the sharp intense peak. This presence of a combined broad, low intensity peak and a sharp, high intensity peak has been observed in many other material systems as well. However, explanations for this behavior has been lacking.

We address this issue through a detailed x-ray analysis using synchrotron radiation and samples grown by molecular beam epitaxy. The initial nitridation of the sapphire substrate surface produced a 1.6 nm AlN layer. Synchrotron X-ray measurements and transmission electron microscopy revealed only (0001) AlN planes and a narrow (0002) rocking curve width of less than 30”. The (0001) orientation was maintained during subsequent AlN growth up to thicknesses on the order of microns. X-ray rocking curves for all thicknesses of AlN exhibited the combined sharp and broad peak components. Two-peak-component rocking curves have been reported by other studies in which it was often assumed that a defective initial layer was covered by a higher quality layer but the components’ characteristics had not previously been determined. The fact that such a combined peak exists even for nm-thick layers suggests another origin for this phenomenon. By observing the behavior of each rocking curve component at different orders of (000ℓ) symmetric reflections, it is ascertained that one component is attributed to lattice tilt (< 30” for 1.6 nm to 230 nm AlN films) or mosaic and the other is due to lateral coherence. We also demonstrate that the lateral coherence length depends only indirectly on thickness. The true dependence is on time at the growth temperature such that a thinner layer which is subsequently annealed such that the sum of the growth and annealing time is the same time as growth alone for a thicker sample will have a similar coherence length.

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CONTINUED PROGRESS IN HIGH-QUALITY III-V/SI EPITAXIAL INTEGRATION FOR OPTOELECTRONICS APPLICATIONS

Tyler Grassman ()

TBA

AUTOMATING CONTROL OF THE MOLTEN ZONE: DYNAMICS AND MATERIALS CONSIDERATIONS

Benjamin Gray (Air Force Research Laboratory, Materials and Manufacturing Directorate), Ryan Nelson (Core4ce), Joe Peoples (Riverside Research Institute), Alan Martinez (Air Force Research Laboratory, Materials and Manufacturing Directorate)

Laser Heated Pedestal Growth (LHPG) is a crucible-free miniature molten zone technique that has emerged as a crucial tool for the fabrication of high-quality single crystal fibers (SCFs). These fibers hold potential in several advanced applications, including photonic devices and sensors for extreme environments, owing to their exceptional electro-optical and magneto-optical properties, thermal stability, and mechanical durability. However, the LHPG technique presents significant material processing challenges, primarily due to the complex dynamics of the molten zone, where achieving precise control over fiber diameter, surface morphology, and optical properties is paramount.

This talk will discuss recent advancements in the automated control of the LHPG process, focusing on the development of a comprehensive framework for understanding and manipulating the dynamic behavior of the molten zone. A model-based control strategy, leveraging real-time monitoring via machine vision tools, will be presented. This approach enables dynamic stabilization of the molten zone and effective mitigation of disturbances, leading to improved fiber quality and enhanced process stability. The control system relies on a geometric description of the molten zone dynamics, using real-time monitoring with machine vision to achieve a stable, automated SCF growth process.

Furthermore, the talk will address the influence of material-specific properties on melt dynamics, an area often overlooked in generalized automation schemes. In particular, the challenge of controlling the large temperature gradients induced by laser heating, which significantly influence fiber characteristics, will be discussed. Preliminary results will be presented on the growth of oxide fibers with varying thermal properties, highlighting the challenges and potential solutions for achieving optimal growth conditions. These materials often present unique challenges due to their inherently high melting points. This characteristic can lead to steep temperature gradients during melt growth techniques, resulting in strained crystals with suboptimal mechanical and optical properties.

CRYSTALLIZATION AND PROPERTIES OF HBN GROWN AT HIGH NITROGEN PRESSURE

Izabella Grzegory (Institute of High Pressure Physics of the Polish Acadmy of Sciences)

In this talk the use of high N2 pressure for synthesis and crystal growth of hBN will be highlighted. For both fundamental studies and the pursuit of new applications, it is critical to produce high-quality crystalline hBN. Due to a melting temperature that exceeds 3000 °C, hBN, unlike silicon and GaAs, cannot be grown from its stoichiometric melt. Due to this limitation, two leading methods have emerged for the crystallization of hBN. One of them, involves very high pressures of 5 GPa or more, and Ba or Mg based solutions. In contrast to GaN and InN, hBN does not require a high N2 pressure to suppress its decomposition at high temperatures. So the alternative –is based on growth on the surfaces of molten transition metal alloys containing boron, and involves a flow of nitrogen gas at atmospheric pressure. For both approaches, crystals are limited in their lateral size and thickness.

In this work, single crystals of hBN have been grown on the surface of Ni and Ni-Cr alloys under pressure of N2 gas of 1000-1500 bar. Due to increased solubility of N it was possible to grow hBN crystals significantly thicker than by similar approach but at atmospheric pressure. The crystals were transparent, colorless and of high structural quality confirmed by Raman spectroscopy, PL measurements and application of thin hBN flakes exfoliated from the grown crystals in graphene containing heterostructures.

The results of the crystallization experiments are discussed in the context of the thermodynamic properties of III-N compounds and the effect of the solvent on the thermal stability of BN with respect to its components. A general tendency in the Ni-B system at low boron concentration and at (1000–2000)K, is that the activity of boron is much less than its corresponding concentration, indicating large deviation of the solution from ideality where no solute-solvent interaction is assumed. It induces a strong shift of the BN equilibrium curve towards higher N2 pressures. For 10at.% dilution of B in Ni, the shift is as high as 5-6 orders of magnitude and therefore the concentration of boron can be optimized to meet thermodynamic equilibrium for BN formation at 1 bar or even higher N2 pressure. The discussion will be extended towards systems even more suitable for hBN growth using high N2 pressure to increase N solubility but also to be closer to thermodynamic equilibrium.

New emerging high pressure approaches: zone melting and ammonothermal will be also introduced.

SEARCHING FOR IDEAL TOPOLOGICAL CRYSTALLINE INSULATORS AND TOPOLOGICAL SUPERCONDUCTORS IN PB-SN-IN-TE SYSTEM

Genda Gu (Brookhaven national laboratory)

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 topological superconductor, we have grown a large number of the single crystals of 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.

APPLICATION OF LABORATORY MICRO X-RAY FLUORESCENCE DEVICES FOR X-RAY TOPOGRAPHY

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It is demonstrated that high-resolution energy-dispersive X-ray fluorescence mapping devices based on a micro focused beam are not restricted to high-speed analyses of element distributions or for the detection of different grains, twins and subgrains in crystalline materials, but they can be also used for the detection of dislocations in high quality single crystals [1]. Si single crystals with low dislocation densities were selected as model materials to visualize the position of dislocations by the spatially resolved measurement of Bragg peak intensity fluctuations. These originate from the most distorted planes caused by the stress fields of dislocations. The results obtained by this approach were compared with the laboratory-based Lang X-ray topographs. It is evident that the presented methodology yields comparable qualitative results and it is of particular interest in the field of crystal growth, where fast chemical and microstructural characterization feedback loops are indispensable for short and efficient development times. The beam divergence was reduced via an Aperture Management System (AMS) to facilitate the visualization of dislocations for virtually as-grown, non-polished and non-planar samples with a very pronounced surface profile (Fig. 1). In addition to Si, we will present new experimental results on various other single-crystalline materials such as diamond, mullite (2:1 composition), periclase (MgO) and γ-LiAlO2.

Fig. 1: (a) Photograph of an investigated Si crystal with a similar viewing direction like the X-ray beam (b) superimposed greyscale-coded 2D intensity plot of peak flanks and peak maxima of the 337 and 448 reflections with a slight increase of contrast (Rh source with AMS) of the sample shown in (a).

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DETERMINATION OF NONLINEAR OPTICAL PROPERTIES OF SEMICONDUCTOR CRYSTALS

Shekhar Guha (Air Force Research Laboratory), Joel Murray (Air Force Research Laboratory), Kevin Cissner (Air Force Research Laboratory)

Key nonlinear optical properties of many crystals useful for optoelectronic applications still remain to be accurately determined. We have measured the two- and three-photon absorption coefficients, nonlinear refractive index and free carrier absorption and refraction cross-sections of several semiconductors, including ZnSe, CdS and CdSe.

FERROELECTRIC TRANSITION IN SN2P2SXSE(6-X) ALLOYS

Timothy Gustafson (Core4ce LLC in support of Air Force Research Laboratory Materials and Manufacturing), Shiv Halasyamani (University of Houston), Mariacristina Rumi (Air Force Research Laboratory Materials and Manufacturing)

Sn2P2S6 (SPS) has been a material of interest for effects observed like the Pockels effect and piezoelectric effect due to its high spontaneous polarization. A primary advantage for SPS is transparency further into the infrared than oxides like lithium or potassium niobate which typically have at least one absorption band near 3 μm due to OH-. Chalcogenides sidestep this problem while also pushing the infrared absorption edge to longer wavelengths. Changing to a selenide composition over sulfur would further enhance the longer wavelength transparency. However, Sn2P2Se6 (SPSe) is centrosymmetric (space group P21/c) at room temperature and must be cooled to around 200 K to become ferroelectric. At room temperature, SPS is in non-centrosymmetric space group Pc. However, SPS undergoes a phase transition, at about 67 °C, to centrosymmetric space group P21/c becoming paraelectric. The optimal alloy would maximize selenium content with minimizing required cooling for the ferroelectric phase. In this study, we look at several different Sn2P2SXSe6-X alloys and their phase transitions directly through non-ambient x ray diffraction (XRD). Typically, XRD has not been of sufficient resolution to capture this phase transition so supplementary techniques have been employed such as second harmonic generation or dielectric coefficient measurements. A few groups have observed this transition in SPS directly with XRD. However, this represents the first set of XRD across the range of SPS to SPSe alloys detailing their phase transitions.

INTRINSIC POINT DEFECTS IN CS4PBCL6: AN EPR STUDY

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Cs_4PbCl_6 is a material of interest primarily for luminescence and scintillation applications. It is the Pb-deficient and Cs-excess polymorph of the all-inorganic perovskite $CsPbCl_3$. Both materials have excellent transparency into the infrared, are easily grown through solution or bridgeman, and are more resistant to atmospheric water than their bromide analogs. While important to their optical and electronic properties, point defects remain to be identified and characterized. The alkali halide binary salts provide examples of many fundamental point defect types. The conventional wisdom is many of these will manifest in the metal halide perovskites and related compositions. These expectations have been tempered through computational efforts to anticipate stable defect types. However, few experimental studies exist to that end. Also, which of the defects observed in binary salts will be observed in the ternaries remains largely unknown. In this study, we use electron paramagnetic resonance (EPR) to identify intrinsic point defects in single crystal Cs_4PbCl_6. Comments will be given on multiple EPR spectra observed. The bulk of the discussion will be around a spectrum caused by Pb^+. A model will be proposed for this defect as well.

TRANSFER OF MONOLAYER AND QUASI-FREESTANDING BILAYER EPITAXIAL GRAPHENE FROM SIC(0001)

Jenifer Hajzus (US Naval Research Laboratory), Daniel Pennachio (US Naval Research Laboratory), Shawn Mack (US Naval Research Laboratory), Rachael Myers-Ward (US Naval Research Laboratory)

Epitaxial graphene (EG) on SiC can be grown with high quality at the wafer scale, but certain applications require transfer of graphene from the SiC substrate. This work utilizes a dry transfer technique in which a metal stressor film is used to exfoliate EG from SiC and transfer to target substrates [1]. We investigate the transfer of monolayer epitaxial graphene (MEG) and hydrogen-intercalated, quasi-freestanding bilayer graphene (QFBEG) grown by sublimation of Si from 6H-SiC(0001) in a CVD reactor in Ar ambient. To exfoliate and transfer the graphene, a magnetron sputtered Ni stressor layer is used, where the Ar pressure during sputtering can be varied to impact the stress, density, and roughness of the Ni film. With appropriate sputtering conditions, the entire Ni/graphene film exfoliates from the SiC substrate using thermal release tape. Raman spectroscopy mapping shows that predominately monolayer graphene is transferred from MEG, while predominately bilayer graphene is transferred from QFBEG. After MEG exfoliation, the $6\sqrt{3}$ buffer layer that forms during growth on SiC(0001) remains on the SiC substrate. Consequently, for regions of exposed $6\sqrt{3}$ buffer layer in the as-grown MEG on SiC, there are corresponding gaps in the transferred graphene film where the areas of exposed buffer layer do not transfer. The buffer layer is not present in QFBEG due to the hydrogen-intercalation process, which severs the covalent bonds between the $6\sqrt{3}$ buffer layer and SiC and converts the buffer layer to an additional graphene layer. It is found that the same Ni sputtering conditions that led to uniform exfoliation and transfer of MEG result in micron-scale tears in the Ni/QFBEG film. By modifying the stress and thickness of the Ni film, these tears can be reduced or eliminated.

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MULTIMODAL DEFECT ANALYSIS FOR CRYSTALLINE MATERIALS USING PERSPECTIVE TRANSFORMATION

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We have developed a novel multimodal non-destructive method combining birefringence imaging using polarized light microscopy, X-ray topography (XRT), and other defect recognition techniques for the precise analysis of threading mixed dislocations (TMDs) in silicon carbide (SiC). SiC is widely used in power devices due to its excellent physical properties, but defects such as threading mixed dislocations significantly degrade device performance and reliability. Accurate identification and characterization of these defects, particularly their Burgers vectors, are essential for enhancing device reliability.

In this study, birefringence imaging was first employed to identify the edge components of TMD Burgers vectors based on stress-induced optical contrasts. Subsequently, X-ray topography was utilized to identify the screw components through characteristic contrast patterns. Additional defect recognition techniques were integrated to enhance analysis accuracy and comprehensiveness. The results obtained from this multimodal analysis were validated against transmission electron microscopy (TEM) and large-angle convergent beam electron diffraction (LACBED), showing excellent consistency.

This combined multimodal approach significantly improves defect characterization in SiC wafers, enabling efficient, non-destructive screening of harmful defects prior to device fabrication, ultimately enhancing the reliability and productivity of SiC power devices. Furthermore, this methodology demonstrates potential applicability to other wide-bandgap semiconductor materials such as GaN, underscoring its versatility and importance in semiconductor device research and quality control.

BULK GROWTH OF OFFCUT (100) Β-GA2O3 BY EFG: ESTABLISHING A DOMESTIC SOURCE OF GALLIUM OXIDE SUBSTRATES

Drew Haven (Luxium Solutions, LLC), David Joyce (Luxium Solutions, LLC), John Frank (Luxium Solutions, LLC), Robert Lavelle (Pennsylvania State University, Applied Research Laboratory), David Snyder (Pennsylvania State University, Applied Research Laboratory), William J. Everson (Pennsylvania State University, Applied Research Laboratory), Luke A. M. Lyle (Pennsylvania State University, Applied Research Laboratory), Daniel J. Erdely (Pennsylvania State University, Applied Research Laboratory), Scott W. Pistner (Pennsylvania State University, Applied Research Laboratory), Katherine Burzynski, AFRL)

Among ultra-wide bandgap (UWBG) materials, beta phase gallium oxide (β-Ga2O3) has shown increasing promise in recent years as an excellent material for high voltage power switching and high frequency transistors. This is due in large part to its ultra-wide bandgap (~4.8 eV), high electric breakdown field (8 MV/cm), and excellent Baliga's figure of merit. Additionally, β-Ga2O3 is unique among wide bandgap (WBG) and ultra-wide bandgap (UWBG) materials in that it can be directly grown from a melt, which offers significant cost and manufacturing advantages. However, in order to scale to industrial sizes and volumes, significant materials challenges must be overcome. This includes the propensity of β-Ga2O3 to decompose above its melt temperature, low thermal conductivity, two easily activated cleavage planes, and gallium attack of the iridium crucible, among others.

Edge-defined Film-fed Growth (EFG) presents itself as an advantageous growth method in the face of these challenges. In particular, the crucible can be grown empty, limiting the effects of material decomposition; dopants are not segregated back into the melt pool, keeping dopant concentrations consistent through growth; and growth scaling occurs largely in two dimensions, limiting the thermal challenges associated with scaling boule size. At Luxium Solutions, EFG growth processes for both insulating (Fe-doped) and conductive (Sn-doped) Ga2O3 crystals are under development. Conductive, n-type crystals are of particular interest for vertical, high-power devices, so emphasis has been placed on achieving the desired doping range with good compositional uniformity.

This presentation discusses the history of EFG growth at Luxium Solutions, and how the unique growth challenges have been overcome and have helped to shape the direction of the bulk growth program. It will also highlight significant progress in substrate fabrication methodologies. Together, this has enabled β-Ga2O3 substrates of very high crystal quality and ultra-low surface roughness, and demonstrates a path toward high quality, domestically produced, β-Ga2O3 substrates.

MOCVD TECHNOLOGY FOR 2D MATERIALS SYNTHESIS EXTENDING TO 300 MM SCALE

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Two-dimensional (2D) layered materials, with their unique properties at monolayer thickness, have the potential to address the scaling and performance limitations of current semiconductor technology and to enable novel "beyond Moore" applications. To realize these applications, substantial progress is needed in the synthesis and integration of 2D materials. Especially, achieving wafer-scale growth uniformity and reproducibility is crucial for the reliable and consistent performance of 2D materials devices at the circuit level. Here, we report on the latest advancements in the synthesis of transition metal dichalcogenides, graphene and hexagonal boron nitride (hBN) on substrates up to 300 mm using a Close Coupled Showerhead® (CCS) MOCVD system. In the first part of the talk, we will focus on the MOCVD technology and demonstrate in-situ techniques, including pyrometry and reflectometry for 2D growth optimization and statistical process control. For process optimization and quantitative uniformity assessment, we introduced metrology standards to evaluate the preparation of epitaxial substrates prior to 2D growth, as well as 2D materials growth on both amorphous and epitaxial surfaces (Fig. 1). The second part of the talk will focus on the controlled synthesis of multilayer hBN, which is explored as an active material in memristor applications and sought for dielectric integration, retaining a clean interface with other materials. To efficiently assess hBN films on wafer-scale, we developed a method for evaluating layer thickness using spectroscopic ellipsometry (Fig.1b,c), accounting for stress-induced changes in the optical properties of the epitaxial hBN film on foreign substrates. hBN is synthesized by CVD route using borazine as a single precursor. Presence of AlN revealed by XPS analysis points to active nitrogen species from borazine pyrolysis playing important role during the initial stages of growth. Overall, the presented developments in MOCVD technology and processes pave the way for the reliable integration of 2D materials into next generation (opto)electronic devices.

SUPPLY CHAIN DEVELOPMENT OF 150 MM THICK-SIC EPIWAFERS AND IMPROVED TRANSISTOR PERFORMANCE THROUGH ADVANCED GATE OXIDES

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Transistor gate oxides affect device performance and durability through several mechanisms. Most importantly, the process by which the oxide is deposited or grown drives the density of interfacial trap state density between the oxide and semiconductor channel interface. Switching and on-state losses are reduced when trap state density is minimized. Additionally, the oxidation process can influence mobility and lifetime of the charge carriers in the channel. Mainstream Engineering and the Pennsylvania State University's Applied Research Laboratory have developed a novel high growth rate SiC epitaxy process and combined this process with an in-situ method to grow novel sacrificial epilayers to form a gate oxide layer with extremely low interfacial defect density. Scalable pre-oxidation and oxidation processes have been developed that further improve defect density. The combination of materials and processes developed have resulted in an interfacial carrier density as low as 7 x 10^10 cm-2eV-1. Our novel chemistry and epitaxial process enables the growth of thick (100's micrometer) SiC epilayers on 150 mm wafers. It also enables heteroepitaxial growth with polytype control to form thin sacrificial epilayers specifically tailored to grow a gate oxide that improves overall device performance. This conference proceeding will discuss the challenges and benefits of our vapor phase epitaxial processes, the influence of pre-oxidation and thermal oxidation conditions on defect density, device test structure performance, pathways for further improvement, production of 200 micrometer epitaxial films on 150 mm wafers, and the development of extremely high kV/kW SiC transistors.

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MICROSTRUCTURAL STUDY ON INITIAL SELECTIVE-AREA MOVPE GROWTH OF INP FILMS IN LATERAL ASPECT RATIO TRAPPING METHOD

Hiroya Homma (NTT Device Technology Laboratories), Hiroki Sugiyama (NTT Device Technology Laboratories), Tatsurou Hiraki (NTT Device Technology Laboratories), Tomonari Sato (NTT Device Technology Laboratories), Shinji Matsuo (NTT Device Technology Laboratories)

Monolithic integration of III-V semiconductors on Si platform by selective-area metal-organic vapor-phase epitaxy (MOVPE) based on vertical and lateral aspect ratio trapping (ART) methods has attracted much attention for low-cost III-V/Si integration on large-diameter wafers [1, 2]. By using the vertical ART method, electrically driven GaAs-based laser diodes (LDs) have been fabricated on Si wafers [1]. However, fabrication of InP-based LDs by these methods and their current-injection operations in telecommunication wavelengths have not yet been reported. One reason is the difficulty in minimizing defect densities in the Si/III-V interface region. Although the defect generation process needs to be understood to further improve crystal quality, few analyses have been reported so far on the initial growth of III-V material films in the lateral ART (LART) method. In this paper, we report a detailed microstructural analysis of the initial growth stage in LART method. Formation mechanisms of stacking faults (SFs) and incoherent twin boundaries (TBs) in InP films are revealed.

The fabrication process of silicon-on-insulator (001) substrates for the LART method and MOVPE growth conditions are described in our previous report [3]. Scanning electron microscope (SEM) observation revealed that low-temperature-grown GaAs and InP buffer layers were uniformly deposited on Si {111} seed surfaces. At the initial stage of 570°C growth, two types of InP microcrystals (MCs) A and B with specific facets appeared. Type A normally inherited the crystal orientation of the Si substrate and consisted of {111} and {110} front and {100} side facets. Type B corresponded to rotational twin whose facets reflect the rotation around <111> crystal direction. As InP growth proceeded, the coalescence of the type-A MCs tended to cause SFs propagating in the [110] direction. In addition, the coalescence of type-A and -B MCs formed incoherent TBs. These plane defects significantly affect the qualities of InP films.

In conclusion, the formation processes of SFs and incoherent TBs in InP films fabricated by the LART method were clarified by intensively investigating the initial growth process. To avoid these defects being generated, coalescence and twinning of MCs must be precisely controlled at the initial stage of film growth.

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COMPLEX OXIDES DESIGNED BY FREESTANDING MEMBRANES

Seung Sae Hong (University of California, Davis)

Freestanding oxide membranes synthesized via thin-film epitaxy represent a new class of low-dimensional oxide materials, expanding the landscape of complex oxides. While epitaxial thin-film growth on single-crystalline substrates enables atomic-level material design, the freestanding nature of these membranes—free from bulk substrate constraints—opens new avenues for tailoring material structures and properties. This talk will highlight a few examples of oxide membranes we are beginning to explore, including topotactic oxide $SrCoO_x$ and ferroelectric oxide $BaTiO_3$. Through electron microscopy and optical spectroscopy, we have observed how the absence of epitaxial constraints significantly alters their structures and properties. The presentation will also explore potential strategies for harnessing novel functionalities in oxide membranes.

STACKING FAULT ANALYSIS FOR THE EARLY-STAGES OF PVT GROWTH OF 4H-SIC CRYSTALS

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With wide band gap, high thermal conductivity, and high breakdown field, silicon carbide, typically 4H-SiC, has steadily become the material of choice for next generation high-power electronic devices. However, the presence of defects especially dislocations and stacking faults (SFs), such as threading screw dislocations (TSDs), threading edge dislocations (TEDs), threading mixed dislocations (TMDs), basal plane dislocations (BPDs), Frank dislocations, Shockley SFs and Frank SFs, are hindering the widespread application of 4H-SiC device due to their harmful effects on the reliability of high-performance SiC power devices. In particular, SFs are particularly deleterious as they degrade the blocking and on-state conduction performance and/or reliability of devices.

A recent approach to lowering defect densities is to closely examine the early-stages of crystal growth when many defects are nucleated. Recently, we have reported on defect behavior during the early growth stage. Continuing these early-stage studies, we seek to better understand the effects of various growth parameters on resulting defect structures, especially stacking fault formations. Multiple short duration growths have been carried out under varying conditions of nucleation temperature, thermal gradients, and N incorporation. In this study, four types of stacking faults are observed distributed across the growth surface: Type A, Shockley stacking faults expansion in the facet region; Type B, stacking faults bounded by 2 opposite sign Frank type dislocations; Type C, stacking faults bounded by a pair of same sign Frank-type dislocations. As higher partial pressures of N2 are deployed, the occurrence of the Type B stacking fault is found to be suppressed; Type D, stacking faults regions shown as “carrot” defects on the as-grown surface of crystal. The formation mechanisms of these stacking fault formation will be suggested. The implications of these observations to achieve better control of the PVT growth process and resultant defect reduction will be discussed.

STATUS AND NEW FEATURES OF THE TOPOGRAPHY BEAMLINE 1-BM AFTER THE ADVANCED PHOTON SOURCE UPGRADE

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The beamline 1-BM at the Advanced Photon Source (APS), a bending-magnet beamline with a large X-ray beam size of ~90 mm by 3 mm, has comprehensive and unique synchrotron topography and rocking curve imaging capabilities for characterization of single crystals (particularly wide-bandgap semiconductors). This beamline is equipped with a white-beam topography stage with fully automated angular and scanning motors for fast imaging of up to 8-inch wafers. It also has a double-crystal diffraction set-up, of which the second stage can be used for monochromatic-beam topography in either the stepped rotation mode or the single exposure mode. The first stage has different beam conditioners in the grazing-incidence geometry that can expand the vertical beam size from 3 mm to ~100 mm for double-crystal rocking curve imaging when it is combined with the second stage. After nearly two years of “dark time”, during which the APS was upgraded to a modern 4th-generation light source, 1-BM has resumed its normal operation for general users since January 2025. The upgraded APS has led to new features at 1-BM. For example, the much smaller X-ray source remarkably improves the topography image resolution and quality. The much higher flux/brightness of the new source significantly improves the imaging speed, and the reduced exposure time noticeably mitigates the mechanical drifting/instabilities. In addition to the hardware, the beamline supporting software tools LauePt and HXRD for simulating Laue patterns and rocking curves, respectively have also been upgraded. In this presentation, we will introduce the status of 1-BM and all these new features.

SOLVENT INCLUSION AND MACROSTEP BEHAVIOR REVEALED BY IMPURITY DISTRIBUTION IN SOLUTION GROWTH OF P-TYPE 4H-SIC

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In the solution growth of 4H-SiC, high-quality crystals with low threading dislocation density can be obtained. However, "solvent inclusion" occurs, where the solvent is incorporated into the growing crystal, significantly degrading its quality. Until now, evaluations have mainly been conducted through observations of the crystal surface. With the recent increase in crystal diameter and length, it has become necessary to assess solvent inclusion within the crystal as well. In this study, solvent inclusions incorporated within the crystal were analyzed through cross-sectional observations of the crystal.

A p-type 4H-SiC crystal doped with Al was grown for 30 hours using a seed crystal with an off-angle of 1°. The grown crystal was cut parallel to the step-flow direction, and both sides were polished to prepare thin sections with a thickness of 500 μm. The thin sections were illuminated from the back, and the transmitted images were observed using an optical microscope. Additionally, the impurity concentration distribution in the crystal was measured using SIMS.

Through transmission observations, solvent inclusions were observed as point-like images that did not transmit light. The transmitted image also revealed that the crystal consists of bright and dark layers, with solvent inclusions forming exclusively in the bright layers. Observations near the crystal surface and impurity analysis using SIMS revealed that the bright layers correspond to the propagation trajectory of macrosteps, where the concentration of Al, an impurity, is low.

When comparing regions where solvent inclusion has formed with those where it has not, differences in the thickness and inclination of the bright layers can be observed. In the regions with solvent inclusion, the bright layers are thicker and have a greater inclination. The thickness of the bright layers is considered to reflect the height of the macrosteps at the time of growth, while their inclination is thought to represent the propagation speed of the macrosteps. Therefore, in regions with solvent inclusion, the macrosteps were higher and propagated more slowly during growth. Conversely, in regions without solvent inclusion, the macrosteps were lower and propagated more quickly. From these findings, cross-sectional transmission observations can be used to estimate the height and propagation speed of macrosteps during growth. It was also determined that solvent inclusion tends to form in regions with higher macrosteps.

STATE OF BARIUM CHALCOGENIDE CRYSTAL GROWTH FOR NWIR TO MWIR – LWIR CONVERSION

Jani Jesenovec (BAE Systems), Kevin Zawilski (BAE Systems)

In recent years there has been an increasing amount of study in the family of barium chalcogenide single crystals [BaGa4Se7 (BGSe), BaGa4S7 (BGS), BaGa2GeSe6 (BGGSe), BaGaGeS6 (BGGS), Ba2Ga8GeS16 (B2GGS)], which are capable of NLO frequency conversion from as low as 1 µm to 18 µm for high power laser applications. This family of crystals is notable for a rare combination of wide band gap (in the visible, as low as 400 – 500 nm) and long phonon cut-off wavelength (18 µm), and ability to grow single crystal boules from the melt. The wide bandgap of these crystals correlates to a large laser damage threshold, suited for high power applications. Further, this family of crystals demonstrates high conversion efficiencies compared to oxide NLO converters, coupled with very broad transparency windows. BGSe specifically demonstrates an extremely flat tuning curve, allowing supercontinuum generation of light from 4 µm – 13 µm all at one pump wavelength about 2 µm. Persistent photodarkening has been observed in BGSe when lasing, but the phenomenon does not seem to be detrimental to NLO applications compared to similar crystals such as AgGaSe2 (AGSe) and AgGaS2 (AGS). Most of the barium compounds have improved thermos-mechanical properties compared to their AGS and AGSe analogs, which make them attractive as NLO devices in next generation systems.

BGSe synthesis and growth at BAE Systems, Inc. has improved in recent years, reducing impurity and bulk inclusion defects, and yielding large single crystal boules. Off-stoichiometric melt behavior has been curtailed and available aperture of crystals has increased, allowing production of 1 cm3 devices. In literature, researchers have stated that active mixing was required for high quality synthesis, however, did not provide specific parameters. We found that it was necessary to optimize dwell times and temperatures during synthesis, and it was found that active mixing was not required. Parameters which have been optimized for BGSe may also be applicable to the rest of the family of barium chalcogenides, due to similar issues during synthesis and growth.

These improvements allow commercial production of BGSe devices with at least 10 x 10 mm2 aperture. Future scale-up efforts aim to produce BGSe apertures up to 25 x 25 mm2 for large beam diameter applications, as well as improve growth of the other crystals in the family of barium chalcogenides.

SCALABLE AND FAST EPITAXY OF HIGH QUALITY, SINGLE CRYSTAL ZNSE SUBSTRATES

Jesse Johnson (Mainstream Engineering Corporation), Brian Tucker (Mainstream Engineering Corporation, Rockledge, FL), Daniel Erdely (Pennsylvania State University Applied Research Laboratory, State College, PA), Randall Cavalero (Pennsylvania State University Applied Research Laboratory, State College, PA), William Everson (Pennsylvania State University Applied Research Laboratory, State College, PA), David Snyder (Pennsylvania State University Applied Research Laboratory), Justin Hill (Mainstream Engineering Corporation)

Commercially available single crystal ZnSe lacks the true single crystallinity and quality required for the most demanding optoelectronic infrared applications in optical communications, sensors, and defense technologies. The ZnSe optical material manufacturing industry has been nearly completely offshored to Asia for standard optics. Reshoring this manufacturing in general, but specifically for reliable supply of pristine single crystal materials is essential for maintaining U.S. competitiveness and security in optoelectronics technology and sensitive domestic applications. To enable the development of ZnSe-based optoelectronic devices, bulk growth of high quality, single crystal ZnSe to thicknesses > 1 mm are needed on both native and non-native substrates. Mainstream Engineering and the Pennsylvania State University's Applied Research Laboratory have developed a novel high growth rate vapor phase homoepitaxial and heteroepitaxial ZnSe growth process that has demonstrated significant improvements compared to commercially available ZnSe substrates. Our process is highly controllable with growth rates from 100 – 700 microns/hour. At these high growth rates, we demonstrated 50 mm diameter wafer scale heteroepitaxial growth of ZnSe approaching 1 mm thickness with a 2x improvement in crystal quality over commercial single crystal material. Additionally, we demonstrated homoepitaxial growth on commercial 10x10 mm ZnSe substrates to a thickness of ~2 mm with a 3x improvement in crystal quality compared to the commercial single crystal substrates. These results have spurred renewed and consequential interest in this class of materials for high power optics, lasing, and communications. Future work will focus on scale-up and eventual commercialization of our high growth rate, single crystal epitaxial process.

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SYNTHESIS OF SMB6 THIN FILMS ON SILICON BY CHEMICAL VAPOR DEPOSITION

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In 2010, Dzero et. al predicted that SmB6¬, a known Kondo insulator, could exhibit a topological insulating phase. While electrical transport shows many signs of topological surface states, unrefuted verification has proven difficult due to issues involving polarized surfaces and the small Kondo gap of only ~20meV that cannot be resolved by most ARPES measurements.

Additionally, inconsistent low temperature properties have highlighted the role impurities play in the various aspects of SmB6. It has been proposed that inconsistent evidence showing bulk metallic behavior at low temperature could be due to samarium vacancies, a common issue in float zone samples, act as “Kondo Holes” that lead to local metallic behavior resembling the room temperature Fermi surface. Bulk conductance has also also been correlated with dislocations that can occur during growth.Evidence of bulk conduction has been reported in some sputtered films, but not all. These films are typically nanocrystalline, and the effects grain boundaries may have on the hybridization gap is still lacking. Because thin films are a necessary for most practical test devices, this motivates continued research on the effects impurities have on thin film growth and exploring additional methods for growth to compare results with.

This research focuses on the scalable synthesis of SmB6¬ thin films by chemical vapor deposition (CVD) using powder precursors. Most research has been done on bulk crystals grown though Al based flux or float zone methods. CVD nanostructures and sputtered Thin films of 50-500nm have also been grown. The films in this work are grown on metal catalyzed silicon, where a gold-silicon eutectic is used to promote nucleation, similar to VLS, however the absence of gold after growth and presence of partially continuous films suggest a VS mechanism.

XRD and Raman suggest better crystallinity, with average grain size on the order of a few microns, compared to other thin films. However, surface roughness and uniformity remain issues. Resistivity vs temperature measurements show a low temperature to high temperature ratio (R_3K/R_300K) of ~70 between that of reported bulk (> 10^3).

DEVELOPMENT OF GAAS(Y)P(1-Y)/SI VIRTUAL SUBSTRATES FOR GA(X)IN(1-X)P-BASED OPTOELECTRONICS

Lauren Kaliszewski (Ohio State University), Tyler Grassman (Ohio State University)

Monolithic, heteroepitaxial integration of III-V (opto)electronic devices, such as the (AlzGa1-z)1-xInxP quantum well LED structures of interest here, requires production of high-quality virtual substrates. Previous work from our group has led to the development of n-GaP/Si virtual substrates, grown on 2° offcut Si(001), that are free of antiphase domains/boundaries and stacking faults. These optimized templates enable ultra-low threading dislocation density in GaP (TDD < 105 cm-2 at 50 nm), as well as device-quality (≤ 3×106 cm-2) GaAs0.75P0.25 using a GaAsyP1-y step-graded buffer (SGB). However, (AlzGa1-z)1-xInxP alloys tend to favor higher degrees of vicinality (typically ≥ 6°). Initial efforts toward the production of 6° offcut GaP/Si templates following our standard 2° optimized process yielded notably roughened surface morphologies and excessive TDD, thus requiring process optimization tailored for 6° offcut. A correlative analysis for surface roughness and TDD of early-stage growth was completed across multiple variables for the atomic layer epitaxy (ALE) nucleation procedure, wherein significant differences were found between the 2° and 6° optimal processes. The new process enables production of 6° offcut n-GaP/Si templates with only slightly higher TDD (2×105 cm-2 at 50 nm) than the 2° version.

Additionally, our standard GaAsyP1-y SGB, which possesses an average peak-to-valley crosshatch roughness of ~19.3 nm when grown on the 6° templates, was found to yield a high degree of nanoscale faceting and surface roughness during AlxIn1-xP growth. Work toward optimization of the SGB, on both 2° and 6° templates, revealed a trend between V/III growth ratio with both surface roughness and TDD. Increasing the V/III growth ratio by 1.6× was found to significantly reduce the surface faceting, decrease the crosshatch corrugation (from 19.3 nm to only 8.5 nm), and limit introduction of new dislocations. These improvements to the 6o GaAsyP1-y/Si virtual substrate have allowed for the creation of Ga0.71In0.29P-based quantum well LED-type structures, on Si, with a TDD ≤ 5.5×106 cm-2 and an emission of 2.16 eV at 20K. Because the Ga0.71In0.29P is significantly ordered (η = 0.35, yielding 54 meV bandgap reduction), we anticipate that use of a surfactant (e.g. Sb) during growth will enable green light emission (~2.2 eV). Work toward this end, and demonstrating full LED devices is currently in progress, and will be presented at the conference.

DEVELOPMENT OF OPTICAL GUIDING SCINTILLATORS USING TL DOPED CS3CU2I5 FOR HIGH RESOLUTION AND SENSITIVITY X-RAY IMAGING

Kei Kamada (Tohoku Univ.), Masao Yoshino (Tohoku University), Yoshiyuki Usuki (C&A corporation), Akira Yoshikawa (Tohoku University)

In this study, optical-guiding crystal scintillator (OCS) fibers sing Tl doped Cs3Cu2I5 were developed. It consists of single crystal scintillator cores and glass clads . The refractive index of the halide single crystals are higher than the glass in this system. Generated scintillation light above the critical angle is totally reflected at the interface with the glass and optically waveguided like an optical fiber. Owing to light guiding system, the OCS plate can show high sensitivity and high spatial resolution for radioactive particles. This study demonstrated that the diameter of the OCS core could be reduced to 1 μm. Spatial resolution equivalent to the core diameter is expected. The presentation will include details on fabrication methods, crystal quality, luminescence properties, different combinations of scintillator and glass materials, radiation response, and imaging properties.

OPTICAL PROPERTIES OF BR-DOPED N-TYPE SNS SINGLE CRYSTALS: CHARACTERIZATION VIA PR AND PL MEASUREMENTS

Sakiko Kawanishi (Kyoto University), Issei Suzuki (Tohoku University), Takahisa Omata (Tohoku University), Yoshikazu Terai (Kyushu Institute of Technology)

Recently, anisotropic 2D materials (A2DMs) with low in-plane symmetry have attracted much attention due to their potential polarization-driven optical applications. Main group metal chalcogenides are one of the A2DMs and exhibit unique optical properties that depend on polarization, offering new degrees of freedom that were not available before. Tin sulfide (SnS), which has been attracting attention as solar cell and thermoelectric materials, is one of such materials; however, there are many unveiled issues regarding the polarization dependence of its optical properties. In this study, we aimed to clarify the polarization dependence of the optical properties of SnS. Photoreflectance (PR) and photoluminescence (PL) measurements were performed for high-quality Br-doped n-type SnS single crystals grown by solution growth. Two polarization-dependent PR signals were detected in the temperature range from 9 to 300 K, which correspond to direct transitions. The direct transitions were analyzed as 1.682 and 1.385 eV at 9 K, which polarized along the c- and b-axes in the in-plane, respectively. In PL measurements, polarization-dependent emissions by the direct transitions were also confirmed at 1.6 and 1.3 eV at 300 K. In addition, an emission at 1.081 eV with strong polarization properties in the b-axis was detected at 9 K. The temperature and excitation power dependences suggest that the emission at 1.081 eV originates from the transition at the indirect band gap via donor level. The band transitions of SnS revealed by the temperature dependencies of PR and PL measurements will also be discussed at the conference.

VISUALIZATION OF CHANGES IN PH AND ION CONCENTRATION DISTRIBUTION DURING CRYSTAL GROWTH/DISSOLUTION PROCESSES

Jun Kawano (Faculty of Science, Hokkaido University)

To understand the crystal growth mechanism in aqueous solutions, analyzing the local conditions at the crystal-solution interface is essential. We have successfully visualized changes in the pH and calcium ion concentration distribution around crystals dissolving or growing in aqueous solutions by using fluorescent probes, whose fluorescence intensity changes depending on the pH and calcium ion concentration. This method allows us to understand the formation and dissolution processes by directly observing the behavior of specific ions at the crystal-solution interface. Here we report the results of visualizing the (1) dissolution, (2) formation, and (3) phase transformation processes of carbonate and phosphate crystals under an optical microscope. In the present study, HPTS and Rhod-FF (or Rhod-5N) were used for the pH and Ca concentration indicators, respectively, for simultaneous imaging of these parameters.

(1) Dissolution of calcium carbonate: Soon after a crystal was exposed to the solution, the distributions of pH and Ca ion concentration changed concentrically. The tendency of Ca ion concentration increasing around a dissolving crystal was well explained with the diffusion equation with the previously reported value of diffusion coefficient, while observed pH was significantly smaller than the value estimated by the measured Ca concentration. This means that excess HCO3- ions were released during the dissolution of calcium carbonate. (2) Formation of calcium carbonate in the gel matrix: During the synthesis by the counter diffusion method, different polymorphs (calcite and aragonite) formed in environments with different trends in pH change. Furthermore, pH just around the formed calcite was about 0.1 lower than the surrounding pH, while such local heterogeneity was not observed around aragonite. These differences may have influenced the formation of different polymorphs. (3) Phase transformation of calcium phosphates: The solvent-mediated phase transformation of metastable octacalcium phosphate (OCP) into stable hydroxyapatite (HAP) occurs when these phases coexist in aqueous solutions. The results of visualizing this process showed that there were conditions where Ca ion concentration and pH between these two phases had opposite slopes, and that the flow of ions was not simply from the metastable to the stable phases.

The behavior of ions revealed by this method is expected to provide new insights into our understanding of crystal growth.

MULTISCALE MODELING OF SIC VAPOR PHASE GROWTH ON OFF-AXIS 4H-SIC SUBSTRATES: IMPACT OF TEMPERATURE AND SURFACE STEPS

Kevin Kayang (Stony Brook University), Aakash Kumar (Stony Brook University), Balaji Raghothamachar (Stony Brook University), Michael Dudley (Stony Brook University), Dilip Gersappe (Stony Brook University)

Monocrystalline 4H-SiC is a promising semiconductor material due to its wide bandgap, superior thermal conductivity, and exceptional high-temperature stability. These characteristics make it well-suited for power electronics operating in extreme environments. Achieving high-quality 4H-SiC films through the physical vapor transport (PVT) process at ~2400 °C is crucial for effective device performance. However, precise growth control is challenging due to elevated operating temperatures and limited real-time monitoring, often resulting in structural defects such as micropipes and dislocations.

This work combines density functional theory (DFT) calculations to evaluate the thermal stability of the surface steps within a range of high temperatures, and subsequently molecular dynamics (MD) simulations to examine the deposition and growth of silicon carbide (SiC) on 4H-SiC (0001) substrates with 4° off-cut angles. The substrate model incorporates surface steps by tilting the [0001] axis toward the $[112\bar{0}]$ axis by the off-cut angle. The study aims to reveal the atomic-scale mechanisms governing the SiC nucleation, defect formation, and the impact of temperature and substrate inclination on film stress and surface morphology.

Simulation results show nucleation begins once an amorphous layer forms on the substrate, followed by atomic rearrangement into the 4H-SiC crystal structure. The findings suggest that surface steps play a crucial role in enhancing the structural integrity and mechanical properties of the grown 4H-SiC film. Careful control of substrate angle and temperature is essential for reducing defect density, managing residual stress, and improving the overall film quality.

CHARACTERIZATION OF SURFACE FEATURES AT A THREE-PHASE BOUNDARY FROM GROWTH OF HEAVILY DOPED DISLOCATION-FREE SINGLE CRYSTAL SILICON

Joel Kearns (NASA Headquarters)

Single crystal dislocation-free silicon, heavily doped with electronic impurities such as arsenic or antimony, is used as starting material to make the lowest power-consumption electronics for cars, laptops and cell phones. The crystals are grown by Czochralski pulling technique, which is a normal freezing process. The dopant concentration in the liquid at the solid-liquid interface during crystal growth is elevated, due to dopant partitioning during solidification. This can lead to constitutional supercooling, where the planar solid-liquid interface shape deforms, generating channels of impurity enriched-melt bounded by solid silicon.

Constitutional supercooling can occur if the ratio of temperature gradient to solidification rate exceeds a material- and dopant concentration-specific parameter. Dislocations can nucleate near the locations of the channels, but the cause of dislocation nucleation is not understood. Once dislocations are present, the crystal is not usable for devices.

Constitutional supercooling can take place at or near the three-phase boundary, as the crystal diameter is increased from the small seed and neck to the full wafer sized crystal body. Corrugated features on the surface of an initially dislocation-free silicon crystal were examined by optical microscopy, scanning electron microscopy, energy dispersive x-ray spectroscopy and electron backscatter diffraction. The measured characteristics are compared to criteria for constitutional supercooling and accepted models for dislocation nucleation.

GROWTH TWINS IN GALLIUM DOPED, DISLOCATED SINGLE CRYSTAL SILICON FROM NEOGROWTH CRYSTALLIZATION METHOD

Joel Kearns (NASA Headquarters)

A new bulk crystal growing technique called “NeoGrowth” has been developed that produces large single crystal, but not dislocation-free, silicon ingots. The resulting (100) orientation cylindrical ingots are sectioned into square cross section bricks to provide full square cross-section, <100> orientation solar cells. Because of the small segregation coefficient of gallium in silicon, there could be constitutional supercooling ahead of the solid-liquid interface during solidification. During process development, the gallium-doped NeoGrowth ingots sometimes exhibited growth twins. The process developers described the cause of twinning as particles impacting the growth interface, or local high thermal undercooling.

Several NeoGrowth silicon ingots were characterized. It was found that the twins occur on the large, dislocated habit lines (from the {111} facets) and on other locations in the ingots. There was evidence of high carbon concentrations in most samples, and in some cases entrapped inclusions that led to unusual surface features (raised ridges, mounds and nodules). The twin nucleation locations on one specimen habit line showed dimpled structural features similar to the twin nucleation region of a dislocated, heavily arsenic doped Czochralski-grown silicon crystal. The dimples in the NeoGrowth specimen may indicate sub-surface voids or inclusions. The largest crystals exhibited surface deposition patterns evoking dendrites.

Results of calculations of the gallium-doped process indicate that constitutional supercooling is not present at the crystal-melt interface for this growth condition. Twinning at locations other than the habit lines may be due to dislocation bunching, with a high dislocation density leading to new distinct grains. The surfaces of the 450mm diameter NeoGrowth crystals are decorated by small random debris in the pattern of dendrites, and some crystals have porous surfaces. Surface porosity may indicate that the polycrystalline silicon feed was not completely melted before it was incorporated into the ingot, so new orientation grains (such as twins) may result.

COERCIVE FIELD CONTROL IN EPITAXIAL FERROELECTRIC HF0.5ZR0.5O2 THIN FILMS BY NANOSTRUCTURE ENGINEERING

Ji Soo Kim (University of Cambridge), Nives Strkalj (University of Cambridge/Institut za fiziku), Alexandre Silva (University of Minho), Veniero Lenzi (University of Minho/University of Aveiro), Luis Marques (University of Minho), Megan O. Hill, University of Cambridge/Lund University), Ziyi Yuan, University of Cambridge), Yi-Xuan Liu, University of Cambridge), Maximilian Becker, University of Cambridge/Hahn Schickard), Simon M. Fairclough, University of Cambridge), Caterina Ducati, University of Cambridge), Yizhi Zhang, University of Purdue), Jianan Shen, University of Purdue), Zedong Hu, University of Purdue), Hongyi Dou, University of Purdue), Haiyan Wang, University of Purdue), Jose P.B. Silva, University of Minho), Judith L. Driscoll, University of Cambridge)

The discovery of ferroelectric hafnium oxide has spurred great interest in the semiconductor industry, enabled by its complementary metal-oxide-semiconductor compatibility and scalability. However, many questions remain on the origin of the ferroelectric phases and the tunability of ferroelectric properties.

In this work, we explore the influence of laser fluence on coercive field (Ec) in 10-nm-thick epitaxial rhombohedrally distorted orthorhombic (r-d o) Hf0.5Zr0.5O2 (HZO) films grown by pulsed laser deposition on La0.7Sr0.3MnO3-buffered (001) SrTiO3 substrates. When laser fluence is decreased from 1.3 Jcm−2 to 0.5 Jcm−2, the Ec decreases from ~3.3 MV/cm to ~2.7 MV/cm. Lower laser fluence produces pure (111) oriented grains while higher laser fluence produces an additional (11-1) orientation, leading to low angle tilt grain boundaries and associated dislocations which can act as domain pinning sites. The stabilization of the (11-1) orientation and the grain tilting at higher deposition energetics are consistent with density functional theory calculations. To achieve a low Ec in HZO, important for energy efficient ferroelectric memory applications, low energetic growth conditions are required, producing the most highly perfect films.

ELECTRICAL AND OPTICAL CHARACTERISTICS OF RU-DOPED INP GROWN BY MOCVD FOR BURIED HETEROSTRUCTURE QUANTUM CASCADE LASERS

Honghyuk Kim (Department of Photonics and Nanoelectronics, Hanyang University), JoonHyun Kang (Nanophotonics Research Center, Korea Institute of Science and Technology), Il Ki Han (Nanophotonics Research Center, Korea Institute of Science and Technology)

Quantum cascade lasers (QCLs) are unipolar semiconductor lasers based on intersubband transitions in engineered quantum well structures, enabling emission from the mid-infrared to terahertz range. Their wavelength tunability and high output power make them ideal for applications such as gas sensing, spectroscopy, and free-space communication. Buried heterostructures (BHs) are essential in QCLs to ensure strong optical and electrical confinement and efficient heat dissipation, especially under continuous-wave (CW) operation. Semi-insulating indium phosphide (InP) serves as an effective lateral cladding material due to its high resistivity and lattice compatibility. Fe-doped InP has traditionally been used for semi-insulating layers in BHs, but limitations in doping control, strong memory effects in MOCVD processes, and scalability issues have posed challenges. In contrast, Ru-doped InP offers enhanced thermal stability, improved electrical compensation, and reduced memory effects. As a result, major laser diode manufacturers are beginning to transition toward Ru-doped InP for BH device fabrication, underscoring its promise for next-generation optoelectronic applications. Despite growing interest, there are no prior studies on the use of Ru-doped InP as a semi-insulating cladding material in BH-QCLs, nor on its optical properties in the mid- to long-wavelength infrared (MWIR/LWIR) range. Here, we report the electrical and optical properties of MOCVD-grown Ru-doped InP, including its complex refractive index in the MWIR/LWIR range. Our preliminary results indicate that InP:Ru exhibits low optical absorption, comparable to that of InP:Fe, in the MWIR/LWIR spectral range. Additionally, we found that increasing the growth temperature up to 700 °C leads to a significant decrease in electrical resistivity, highlighting the critical role of growth temperature. Although the measured resistivity values ($\sim 10^6\ \Omega\cdot\text{cm}$) are slightly lower than those typically observed in Fe-doped InP within n-InP/SI-InP/n-InP mesa structures, our findings demonstrate that such resistivities are sufficient to enable room-temperature continuous-wave (CW) operation of BH-QCLs.

SYNTHESIS OF MULTISCALE HIGH-PERFORMANCE BIOLOGICAL COMPOSITES

David Kisailus (University of California, Irvine)

TBA

B-GA$_2$O$_3$ CRYSTAL GROWTH WITH COLD CONTAINER CRUCIBLES: THE OXIDE CRYSTAL GROWTH FROM COLD CRUCIBLE (OCCC) METHOD IN LARGE SCALE

Masanori Kitahara (FOX corporation), Taketoshi Tomida (FOX corporation), Vladimir Kochurikhin (C&A Corporation), Gushchina Liudmila (C&A Corporation), Kei Kamada (Institute for Materials Research, Tohoku University, Japan), Yasuhiro Shoji (FOX corporation), Koichi Kakimoto (Institute for Materials Research, Tohoku University), Akira Yoshikawa (Institute for Materials Research, Tohoku University)

β-Ga$_2$O$_3$ is an emerging material as a wide band-gap semiconductor for high-power and low-loss power devices because it can be produced as large size single crystals by melt-growth techniques. However, due to high costs and defect density, it is still in the research stage. Common melt growth techniques for β-Ga$_2$O$_3$ single crystal include the edge-defined film-fed growth (EFG) method, the Bridgman method, and the Czochralski (CZ) method, all of which typically require the use of precious-metal crucibles.

An alternative approach for producing β-Ga$_2$O$_3$ single crystals without using precious metal crucibles is the oxide crystal growth from cold crucible (OCCC) method. The process employs high-frequency induction heating, similar to conventional high-frequency melting methods. However, the key difference lies in the frequency used: OCCC employs heating at frequencies typically an order of magnitude higher than conventional methods. This is due to the relationship between high-frequency heating and the penetration depth of the electromagnetic field into the material, as described by the following equation:

$$\delta = 5.03\sqrt{(\rho/\mu f)}$$

Where: ρ: electrical resistivity of the material (Ω·m), μ: magnetic permeability (H/m), f: frequency (Hz)

δ represents the skin depth, and an ideal penetration depth for induction heating is $d/\delta > 3.5$ (d: diameter of heated object). Oxide melts commonly have two orders higher electrical resistivities resulting in higher frequency requirements.

Recent studies have demonstrated the effectiveness of this method, particularly in the growth of β-Ga$_2$O$_3$ crystals. To achieve bigger crystal growth for mass production substrates, we have tried to grow the crystal in a larger diameter basket.

In this experiment, crystals have been successfully grown by this process. The growth rate of the crystal was 5-15 mm/hour. The material was charged into a water-cooled basket with a diameter of 150 mm. The starting material was high-purity β-Ga$_2$O$_3$ with a purity higher than 99.99%. The materials were set as powders and sintered material shapes. The frequency of the heating was adjusted to around 300kHz- 5MHz.

Some crystals were successfully grown in this process, with a maximum size of more than 2 inches. The grown crystals and their properties are explained in the presentation.

GROWTH OF SINGLE CRYSTAL FIBERS OF LUTETIUM OXIDES BY LASER HEATED PEDESTAL GROWTH

Joseph Kolis (Clemson University), Allen Benton (Clemson University), Rylan Terry (Clemson University), Brian Topper (Clemson University)

Single crystal fibers represent a hybrid form of matter combining the optical and thermal qualities of single crystals with the wave guiding advantages of fibers, making them very attractive as potential lasers hosts. Advances in Laser Heated Pedestal Growth (LHPG) in the early 2000's resulted in a new generation of single crystal fiber optic laser systems, mostly based on doped YAG. Recently the desire for higher power and better beam quality led to exploration of alternate single crystal fiber materials. This talk will highlight advances in the growth of new single crystal fiber materials, mostly based on lutetium ion hosts and Yb doped analogs in particular. Particular focus will be paid to doped Lu_2O_3 and $Lu_3Al_5O_{12}$ (LuAG)

The Yb doped lutetium based materials are attractive because the high thermal conductivity of lutetium based single crystals is not significantly reduced by doping with Yb in any concentration. The growth of single crystal Lu_2O_3 fibers with a wide range of Yb^{3+} ion doping will be discussed along with that of Yb:LuAG growth. The particular demands of the high temperature growth of Lu_2O_3 will be considered. Thermal conductivity of the doped materials and Raman scattering will be presented, along with spectroscopic measurements and preliminary amplification studies.

An important aspect of this work involves development of a single crystal cladding of the doped cores. The growth of single crystal cladding layers on single cores presents an unusual challenge. Early results of single crystal cladding using high temperature hydrothermal growth of undoped cladding onto the faceted cores will be discussed as a unique solution to this problem.

NEXT GENERATION OF EXPERIENCE-BASED FEEDFORWARD CONTROL OF CZOCHRALSKI GROWTH PROCESS USING DATA PROCESSING.

Jan Kovar (CRYTUR, spol. s r.o.), Martin Klejch (CRYTUR, spol. s r.o.), Jan Polak (CRYTUR, spol. s r.o.), Jindrich Houzvicka (CRYTUR, spol. s r.o.)

For the well-known Czochralski growth process there is nonexisting steady state operating point [1]. As solution, many types of feedforward control methods were proposed [1,2]. These methods need detailed model of growth process. For mass production it is advisable to use experience based model. For this type it is necessary to log crucial parameters of growth process. That means, to record parameters of growth process every few seconds.

The goal in first step was predict time dependent function of heater power. This approach is limited to one growing setup. Accuracy of prediction decreases with any change in hot zone. Any changes between two consecutive growth cycles requires a new training model.

LOW-BACKGROUND CARRIER DENSITY INTENTIONALLY AND UNINTENTIONALLY DOPED (010) Β-GA2O3 DRIFT LAYERS AND SCHOTTKY DIODES

Sriram Krishnamoorthy (University of California Santa Barbara), Carl Peterson (Materials, UCSB)

We report on the growth and characterization of 6.5 μm thick MOCVD grown (010) β-Ga2O3 drift layers with intentional doping (ID) and unintentional doping (UID) electron concentrations ≤ 1016 cm-3 and the performance of Schottky diodes on these epilayers. Growth was performed on an Agnitron Agilis 100 cold-wall MOCVD reactor with a remote injection vertical showerhead. TMGa was used as the Ga precursor, pure O2 as the Oxygen source, Silane (SiH4) as the Si dopant gas, and Argon as the carrier gas. To optimize the growth conditions for high quality thick drift layers, we began with a TMGa flow Vs. growth rate (GR) series which showed a linear dependence between the two variables . GR was able to be varied from 0.55 to 4.5 μm/hr. corresponding to TMGa molar flows ranging from 20 to 340 μmol/min. at 60 Torr. Next, we found that decreasing the growth pressure from 60 to 15 Torr at a constant TMGa flow (340 μmol/min.) increased the GR from 4.5 to 7.2 μm/hr., signifying that GR is limited by gas phase pre-reactions. Decreasing the growth pressure also improved the electron mobility and RMS surface roughness of the films. The UID carrier concentration varied mainly between 1015 – 1016 cm-3 with 4-corner Hall mobilities up to 169 cm2/Vs. A growth temperature sweep showed that at 900 °C there was lower mobility and some compensation effect of carriers, whereas at 1000 °C the films showed higher mobilities and minimal compensation. Overall, optimal conditions for thick TMGa growths were found to occur at a VI/III ratio of around 500, growth temperature of 1000 °C, GR of 4 μm/hr., and a growth pressure of 15 Torr. To characterize the baseline performance of the MOCVD films, Schottky diodes were fabricated on two 6.5 μm thick films grown with the aforementioned optimal condition, one ID film with an ND-NA of 1 x 1016 cm-3 and one UID film with 3 x 1015 cm-3 . Circular planar Schottky diodes were formed using Ni/Au Schottky pads with Ti/Au used as the backside ohmic metal; no field management was used for these devices. High Voltage CV on 1 mm2 Schottky pads showed a relatively flat doping curve for the ID sample . Another key observation for these films was that breakdown occurred at the location of hillock defects on the sample surface.

III-V INTEGRATION IN SILICON PHOTONICS: CHALLENGES AND OPPORTUNITIES

Bernardette Kunert (imec, Belgium)

TBA

SEGREGATION TRENDS IN COMPOSITIONALLY COMPLEX RARE EARTH ALUMINUM GARNETS GROWN BY THE CZOCHRALSKI METHOD

Rebecca Lalk (University of Tennessee Knoxville), Yauhen Tratsiak (University of Tennessee Knoxville), Luis Stand (University of Tennessee Knoxville), Mariya Zhuravleva (University of Tennessee Knoxville), Charles L. Melcher (University of Tennessee Knoxville)

The compositional space of high entropy oxides describes materials that involve equimolar mixing of three or more elements on one sublattice. These materials are under investigation due to potential phase stabilization or interesting functional properties for catalysts, energy storage, and optical materials, among others. However, any optical application, like LEDs or scintillators, the concentrations of optically active elements can heavily influence their performance. Therefore, understanding elemental segregation of principal elements during single crystal growth is important for investigating large-scale crystals for commercial applications. Specifically, compositionally complex rare earth aluminum garnets of the form A3B5O12 could be interesting optical materials since their compositionally simpler counterparts, like Y3Al5O12 and Lu3Al5O12, already have widespread use as matrices for lasing media, lighting technology, and scintillators. In this work, elemental segregation is investigated in two compositionally complex rare earth aluminum garnets: (Lu,Y,Gd)3Al5O12:Ce and (Lu,Y,Tb,Gd)3Al5O12:Ce. Czochralski growth and macroscopic mechanical defects are discussed. Elemental concentration is investigated using samples from various locations along the <1 1 1> growth axis of each crystal boule using a combination of SEM/EDS, ICP-OES, and EPMA. These data are fit to the Shiel equation that describes axial elemental segregation in Czochralski crystals as a function of solidification fraction and the effective segregation coefficient of an element, keff. From this data as well as data from other crystals published in literature, a trend between keff and the difference between ionic radius (r) and average ionic radius (AIR) of the dodecahedral site is established. This keff-(r-AIR) trend allows the prediction of elemental segregation compositionally complex rare earth aluminum garnets. This trend can help guide the design of compositionally complex rare earth aluminum garnets for optical applications where understanding the concentration gradients of optically active species is of high concern.

GROWTH AND CHARACTERIZATION OF THICK EPITAXIAL 4H-SIC WAFERS FOR HIGH-VOLTAGE DEVICES

Yuzhuo Li (Stony Brook University), Jianpei Zhang (Stony Brook University), Haochi Wang (Stony Brook University), Shanshan Hu (Stony Brook University), Zeyu Chen (Stony Brook University), Kaixuan Zhang (Stony Brook University), Balaji Raghothamachar (Stony Brook University), Michael Dudley (Stony Brook University)

Silicon carbide (4H-SiC) is vital for power device technologies due to its wide bandgap, superior thermal conductivity, and high critical electric field strength. Thick epitaxial layers (≥60 μm) are essential for planar FETs and superjunction devices operating in the 6.5 to 10 kV range, as they ensure uniform electric field distribution and prevent electrical breakdown. Lower defect densities (dislocations, inclusions, micropipes) are critical for device reliability.

In this study, high-quality epitaxial layers of 60 μm and 110 μm thickness were grown on 6-inch diameter 4H-SiC substrates using a multi-wafer warm-wall epi reactor by Coherent Inc. . Synchrotron X-ray topography, employing grazing-incidence and transmission geometries, systematically characterized defects. Results demonstrated exceptional crystal quality with significant defect reduction compared to typical published values. Basal plane dislocations from substrates did not propagate into epitaxial layers, reflecting improved growth conditions. The density of 3C inclusions was notably low (~30 per 60 μm layer, ~60 per 110 μm layer), significantly lower than typical inclusion densities. Micropipes were rarely observed, a significant advancement over typical literature values. Threading dislocation densities measured between 1000–2000 cm^{-2} were substantially below common published densities exceeding 4000 cm^{-2}.

These findings confirm superior crystalline quality and defect characteristics, providing substantial advantages for developing high-performance, high-reliability power electronic devices. This study also contributes valuable insights for epitaxial growth optimization and effective defect-control strategies in the SiC industry.

A SELF-POWERED ACOUSTIC TRANSMITTER FOR LONG-TERM FISH MONITORING

Huidong Li (Pacific Northwest National Laboratory), Jun Lu (Pacific Northwest National Laboratory), Hyunjun Jung (Pacific Northwest National Laboratory), Zhaocheng Lu (Pacific Northwest National Laboratory), Bingbin Wu (Pacific Northwest National Laboratory), Stephanie Larson (Pacific Northwest National Laboratory), Daniel Deng (Pacific Northwest National Laboratory)

The limited service life of active fish tags and the subsequent need for battery replacements pose significant challenges for fish tracking applications, as recapturing tagged fish in the wild is often improbable. To address this issue, we recently developed an implantable self-powered acoustic tag (SPT) that uses a PZT-5A Macro Fiber Composite (MFC) beam to harnesses mechanical energy from the bending movements of a fish's body as its sole power source. We implanted prototypes of a battery-free version of the SPT into juvenile white sturgeons (Acipenser transmontanus) to evaluate their energy harvesting (EH) performance through device transmissions. The fish showed successful recovery from the implantation surgery and were able to swim freely in a tank. However, the transmissions lasted only a few weeks because of piezoelectric performance degradation of the PZT-5A ceramic caused by the cyclic mechanical loading. To evaluate the degradation of the piezoelectric material in the MFC for this application, we performed accelerated fatigue testing of MFCs made using different types of piezoelectric materials to evaluate their fatigue resistance. The bending conditions applied in these tests were established based on an analysis of video footage of juvenile white sturgeons in a laboratory setting. In this presentation, we compare the power outputs of these MFCs as functions of the bending cycles as well as the acoustic transmission results of the SPT prototypes using these materials in live juvenile white sturgeons. We also report a more advanced version of the SPT recently developed. It features a rechargeable battery, environmental sensors, and improved circuitry for more efficient energy transfer. In contrast to the battery-free version of the SPT, which transmits only when the host fish is in motion and depends significantly on the fish's continuous movements for operation, this new variant of the SPT offers continuous functionality independent of the fish’s movement.

SELECTIVE AREA GROWTH OF CUBIC GAN ON PATTERNED SILICON FORMED BY INTERFACIAL PHASE TRANSITION DURING OMVPE GROWTH

David Lister (Simon Fraser University), Sara Fortin (Simon Fraser University), Bilal Janjua (Hyperlume), Moshen Asad (Hyperlume), Karen Kavanagh (Simon Fraser University), Simon Watkins (Simon Fraser University)

Cubic GaN (c-GaN) is a promising material for optoelectronics due to the natural growth direction being non-polar, reducing the quantum confined Stark effect in quantum wells. The challenge for this material is growing it with high enough phase purity and low enough defects to build devices. We grow c-GaN inside V-grooves and pyramids formed by Si(111) facets formed by a KOH etch on a patterned Si(100) substrate. After an AlN buffer layer, hexagonal GaN (h-GaN) growth on the Si(111) facets until opposing crystals meet, a highly defective grain boundary is formed where spontaneously c-GaN will form and continue growing. We analyze both the c-GaN and h-GaN grown on patterned Si using x-ray diffraction, notably the c-GaN rocking curve width is 2100 arcseconds despite many independent c-GaN crystals being sampled by the x-ray beam. Using TEM, we confirm the material phases and study the defects at the interface. Using dark-field TEM, we see stacking faults on both hexagonal to cubic interfacial planes during the first 50 nm of growth, after which the defect density drops significantly. To understand the mechanisms in greater detail we look at the structural conditions necessary for this interfacial phase transition to be possible, the thermodynamic conditions to drive it forward and kinetic models to understand the rate of formation. We find the polarity of the c-GaN faces leads to groove geometries being preferred over pyramids due to polarity mismatch between h-GaN grown on adjacent Si(111) facets. We developed a model to understand how the relative interface and bulk energies affect the process and find that interface energies determine whether the interfacial phase transition can occur and that there is a geometry-dependent critical ratio of interfacial energies required. Finally, we use a geometric argument to predict the length that the hexagonal crystals are in contact prior to the nucleation of the cubic phase material.

CRYSTAL ORIENTATION QUANTIFICATION IN LESS THAN 10 SECONDS

Destiny Lopez (Malvern Panalytical), Dirk Kok (Malvern Panalytical)

We present here work on the orientation determination of bulk crystals for several different steps of wafer manufacturing (seeding, cutting, grinding, end control, etc.).
X-ray diffraction is one of the standard analytical methods that are routinely utilized for both materials research and quality control. It is non-destructive and offers high precision and accuracy in lattice orientation measurements. The classic orientation method via rocking curves at different azimuthal angles is widely spread and yields results in 10-20 minutes for small off-orientations. For routine processes, this measurement time can adversely affect throughputs, and a faster solution is needed. Here we present a method two orders of magnitude faster, which determines an offcut magnitude in 10 seconds with precision of 0.003° 1σ. This is a strong improvement in methods compared to current industrial standards and enables control of each individual wafer at a throughput of up to 1 million wafers per automated wafer tool per year at single point per wafer. We will demonstrate the capabilities of this method with various examples. For the in-depth analysis of a single sample, we offer mapping stages. Due to the high accuracy and short measurement time of the azimuthal scan, this method is very useful to manage the HVPE-specific problem of quantification of lattice plane bending. This offcut mapping can be combined with a rocking curve mapping, which was demonstrated on quartz wafers.
Finding the orientation of a crystal on the diffractometer is only the first step. The sample then has to be transferred to the next processing step without losing the orientation. With our orientation transfer technology , we can enable, for example, accurate cutting and grinding. With our stacking frame, up to twelve ingots of, for example, SiC, can be attached to a saw beam for parallel cutting.

Figure 1. Figure 1 a): Graphical representation of measured quantities of our azimuthal scan method. B) Surface tilt corrected measurement of lattice tilt (100mm HVPE GaN).

LIFTING THE FOG – LESSONS LEARNED IN THE SYNTHESIS FOR FERROELECTRIC COMPLEX OXIDES THIN FILMS

Lane Martin (Rice University)

Despite our best intentions and efforts, our ability to manipulate and control complex materials – such as binary, ternary, and higher order complex oxides – remains rudimentary as compared to the precise control of materials demonstrated in other fields (e.g., the ppb-level control of defects in traditional semiconductor materials). In complex oxide thin films, although modern approaches to epitaxial thin-film growth have enabled unprecedented control of single/multi-layer systems, emergent physical phenomena, and marked advances in our fundamental understanding of these materials, controlling material chemistry, and in turn, defects at even the 0.1-1% level is challenging. In turn, defects, be they intrinsic or extrinsic in nature, play a critical role in the evolution of material properties and phenomena. In this talk, we will investigate a series of “lessons learned” about your our limitations in producing complex-oxide materials with the level of control we desire to have, what those limitations mean for the study, understanding, and utilization of these materials for devices, and, in turn, the opportunities for the community to embrace these defects and utilize their presence as a new design parameter. We will call upon examples of processing-defect-property relationships in a range of epitaxial thin-film ferroelectric materials including Ba1-xSrxTiO3, PbZr1-xTixO3, (1-x)PbMg1/3Nb2/3O3-(x)PbTiO3, BiFeO3, HfO2, some novel new materials, and others. We will highlight the role of the synthesis process in determining the film chemistry, defect structures, how epitaxy can influence the evolution of the same, and, ultimately, what all of these things do to the properties. Along the way, we will discuss different ways of probing these factors, explore ways of developing deterministic control of these factors, and examine ways the community can work to avoid common pitfalls.

CHARACTERIZATION OF 100 MM ALN SINGLE CRYSTAL SUBSTRATES PREPARED USING PHYSICAL VAPOR TRANSPORT METHOD

Shogen Matsumoto (Crystal IS, Inc. and Asahi Kasei Corporation), Robert T. Bondokov (Crystal IS, Inc.), Kasey Hogan (Crystal IS, Inc.), Griffin Q. Norbury (Crystal IS, Inc.), Connor G. Carr (Crystal IS, Inc.), James Grandusky (Crystal IS, Inc.)

Aluminum nitride (AlN) is a promising ultrawide bandgap (UWBG) material for deep UV (DUV) LED devices and power electronic devices due to its excellent thermal properties (> 290 W m−1 K−1), optical properties (6.2 eV), and its low mismatch to other III-Nitrides like gallium nitride (GaN). Crystal IS supplies large quantities of 2-inch AlN single-crystal substrates which have sufficient crystalline quality for device fabrications to date. However, 100 mm AlN substrates with equal or better quality are needed to meet the potential demand for device development. We have previously demonstrated the world's first 100 mm AlN growth. The current efforts are focused on improving the crystal quality. In this work, we report on the preparation of 100 mm AlN single crystals as well as the characterization results with regard to optical and thermal properties.

AlN single crystals are grown by physical vapor transport (PVT) method. Several generations crystals were grown to expand the diameter from 2-inch to larger than 100 mm. The boules are processed in several steps; ground and sliced into wafers, then polished to obtain epi-ready surfaces. The single-crystal area of the 100 mm AlN substrates defined by using high-resolution cross-polar imaging (HR-CPI) technique and double-axis X-ray diffraction (XRD) rocking curves exceeds 99%. The FWHM values of the rocking curves are in the range of 29 – 70 arcseconds. The etch pit density (EPD) evaluated using KOH-NaOH eutectic melt is in the range of 1×10^4 – 1×10^5 cm−2. The impurities of AlN substrates are investigated by secondary-ion mass spectrometry (SIMS). The concentrations of carbon and oxygen are below 1×10^17 cm−3, and there was no other dominant contamination. The thermal conductivity of 100 mm AlN substrates measured using flash technique shows values as high as 295 W m−1 K−1 at a room temperature. The data reported here indicates that our 100 mm AlN substrates can be used for next-generation power electronics and related applications.

GROWTH AND SCINTILLATION PROPERTIES OF CE DOPED LICAALF$_6$/LIF EUTECTICS FOR THERMAL NEUTRON DETECTION APPLICATIONS

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Neutron detectors are used in a wide range of applications such as homeland security, non-destructive testing, and nuclear decommissioning. Especially, in a nuclear decommission field in Japan, there is an urgent need to sort and store debris from the Fukushima Daiichi Nuclear Power Plant. During the handling of reactor debris, it is necessary to detect thermal neutrons in areas where very high γ-ray dose rates exceed 10 Gy/h. Currently, solid scintillators containing 6Li are widely used for thermal neutron detection. A research group from JAEA and Tohoku University has developed a thermal neutron and γ-ray discrimination detector using Ce-doped 6LiCaAlF6 (Ce:LiCAF) single crystal [1,2]. Due to its fast decay time (8–40 ns) and the use of a 100 μm-thick crystal to suppress γ-ray sensitivity, it can detect thermal neutrons under high γ-ray dose rates. However, to enhance thermal neutron sensitivity, it is required to increase the 6Li concentration. Recently, our group has been developing 6Li-containing eutectic scintillators, instead of single crystal, for enhancing the 6Li concentration. Up to now, fluorides such as 6LiF/CaF2 [3] or 6LiF/6LiYF4 [4], chlorides such as 6LiCl/BaCl2 [5] or 6LiCl/Li2SrCl4 [6], and bromides such as 6LiBr/CeBr3 [7] or 6LiBr/LaBr3 [8] have been reported.

In this study, Ce:LiCAF/LiF eutectics was developed. Here, Ce:LiCAF works as a scintillator phase and both Ce:LiCAF and LiF phases work as neutron capture phases by 6Li(n,α) reaction. The eutectics was grown by the vertical Bridgeman-Stockburger method using graphite crucibles. The eutectic structure was actually observed through backscattered electron imaging and confirmed by powder XRD. Emission wavelengths attributable to Ce:LiCAF at 320 nm and 340 nm were observed under X-ray irradiation. In this presentation, details of eutectic growth and structure, scintillation properties, the pulse shape discrimination (PSD) performance between thermal neutrons and γ- rays will be reported.

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MICROSTRUCTURE ANALYSIS OF QUANTUM CASCADE LASERS GROWN BY OMVPE ON LATTICE-MISMATCHED SUBSTRATES

Luke Mawst (University of Wisconsin-Madison), Nikhil Pokharel (University of Wisconsin-Madison), Cheng Liu (University of Wisconsin-Madison), Shining Xu (University of Wisconsin-Madison), Jeremy Kirch (University of Wisconsin-Madison), Benjamin Kniper (DRS Daylight Solutions), Dan Botez, (University of Wisconsin-Madison)

The growth of InGaAs/AlInAs mid-infrared quantum cascade lasers (QCLs) on non-native, lattice-mismatched substrates, such as GaAs and Silicon, would enable a mechanically stable (and low-cost) substrate as well as allow for the integration with existing photonic integrated circuit platforms. QCLs, being unipolar devices based on intersubband transitions with short carrier lifetimes, show great promise to being relatively insensitive to the defect-driven nonradiative processes that have plagued the performance and reliability of conventional diode-laser sources fabricated on mismatched substrates. In fact, device performance on par with that grown on native InP substrates has been demonstrated by both MBE and OMVPE. While high performances can be achieved, there is still a lack of understanding as to how crystal dislocations affect the QCL growth, and the role of defects on electron tunneling and scattering mechanisms, which in turn impact device operational characteristics. Here, we have performed microstructure analysis of QCLs grown by OMVPE on GaAs substrates, using in-plane and cross-sectional electron channeling contrast imaging (ECCI) and atom probe tomography (APT). The structure consists of a OMVPE-grown ~ 8.5 μm-emitting 35-stage lattice-matched InGaAs/AlInAs/InP active region QCL on an InP buffer layer on top of a GaAs substrate, where the buffer layer utilizes InxGa1-xAs strained QW-based dislocation filters (DFs). Cross-sectional ECCI provides a quantitative measure of the dislocation densities within the individual layers comprising the device structure. This analysis reveals that while the DFs reduce threading dislocations by a factor of three, the dislocation density in the active region remains at 1.52 × 108 cm-2. APT measurements of the active region provides quantitative information on in-plane rms roughness, correlation length, and interfacial compositional grading, all of which are important parameters needed for the accurate design of QCLs. Despite the relatively high residual threading dislocation in the active region, we find interfacial roughness and compositional grading lengths which are comparable to values reported previously for QCLs grown on native InP substrates.

B-GA2O3 DOPING AND DEFECTS

John McCloy (Washington State University), Ben Dutton (Washington State University), Nathan Sakaguchi (Washington State University), Marc Weber (Washington State University), Matt McCluskey (Washington State University)

Gallium oxide continues to retain interest for many researchers due to its combination of ultrawide bandgap and relatively facile bulk crystal synthesis. In this presentation, we contextualize our recent work on doping and bandgap tailoring studies in Czochralski-grown Ga2O3. Additionally, we compare recent investigation of optical float zone crystals. Finally, we discuss laser and electron damage studies and quantification of vacancy concentrations in Ga2O3 using positron annihilation spectroscopy.

TRANSFORMATION OF CACO3 TO CRYSTALLINE SPHERES AT THE MINERAL-ORGANIC BOUNDARY

John Mergo (Arizona State University), Moneesh Upmanyu (Northeastern University), John Seto (Arizona State University)

Hierarchical mineralized structures are found throughout biology and biological materials. The ability for biological systems to harness structures and materials of disparate sizes enables their generation of these complex structures. Mineral-organic interfaces introduce a way for an organism to produce custom growth conditions for biogenic crystal formation. In the recent work of Kahr et al., extensive experimentation with amorphous calcareous bodies observed in a variety of organisms was at one time considered a pioneering chapter in inorganic chemical morphogenesis before falling out of focus after the birth of X-ray crystallography and the development of classical nucleation theory – a chapter worth reopening. Here we demonstrate that the synthesis of amorphous calcium carbonate in the presence of gum arabic creates a model system that allows for the exploration of the effects of long-range electrostatic ordering in biological and hybrid materials. Solid microspheres readily form in this system, which we characterize via scanning electron microscopy. We show that these spheres are composed of calcium carbonate via dispersive X-ray analysis. Furthermore, X-ray microtomography results show that the microspheres are hollow. Ongoing work with simulation of the mineral-organic interface focuses on the effects of the nearby interface on constituent particles, creating an opportunity for complexity in crystal formation through a combination of electrostatic and kinetic effects.

IMPROVED PIEZOELECTRIC PERFORMANCE OF SINGLE CRYSTAL AND TEXTURED MATERIALS USING PULSE POLING

Michael Mervosh (Penn State University), Clive Randall (Penn State University)

There has been much interest in recent years to improve upon Direct Current Poling (DCP) for piezoelectric materials. While a majority of the research in this area has been focused on Alternating Current Poling (ACP), pulse poling has shown the potential to outpace both DCP and ACP. Pulse poling subjects samples to short pulses of field (10µs in length) in rapid succession. Previous pulse poling work found that pulses of low electric field facilitated domain nucleation while those of high electric field promoted domain growth. This allows for highly tailorable domain engineering, such as a 2-stage nucleation followed by growth pulse procedure. When tested on both hard and soft single crystal samples (Mn: PIN-PMN-PT and Sm: PIN-PMN-PT respectively), pulse poling has been able to increase the d33 and εr of the system by 80% and 70% respectively relative to DCP. The coupling coefficients of these crystals have also seen increases as high as 70%. In the case of textured ceramics (Mn: PMN-PZT-PT), pulse poling generates similar d33 and εr values compared to DCP but also results in a 20% increase in Qm. The pulsed textured samples notably show a reduction in high field hysteretic losses compared to DCP.

To further improve the properties of the material, the samples were then subjected to pulse poling at higher temperatures; 80°C for the single crystals and 120°C for the textured. When pulsed at these temperatures, the measured properties of the hard piezoelectric samples (crystal and textured) increased after poling contrary to previous piezoelectric aging rates. These properties rose for several weeks (over a month in the case of the single crystals) and increased by as much as 60%. The origin of this aging is still unknown, though some measurements suggest it is derived from a field induced phase change. Given that this has only been observed in the hard piezoelectric samples, it is likely that defect dipoles play a significant role and are developing through a relaxation process that follows a stretched exponential. This positive aging process was tracked with d33, εr, Qm, Pr, and Rayleigh characteristics to quantify the changes of the intrinsic and extrinsic domain dynamic contributions.

We will summarize these contributions and demonstrate the considerable potential that pulse poling has to act as a viable alternative to both DCP and ACP in advancing the electromechanical performance of textured and single crystal materials.

EPITAXIAL GROUP IV MID-INFRARED MATERIALS AND DEVICES

Oussama Moutanabbir ()

Mid-infrared (MIR) optoelectronic devices are of utmost importance to a plethora of applications such as night vision, thermal sensing, autonomous vehicles, free-space communication, and spectroscopy. To this end, leveraging the ubiquitous silicon-based processing has emerged as a powerful strategy that can be accomplished through the use of group IV germanium-tin (Ge1−xSnx) alloys. Indeed, due to their compatibility with silicon and their tunable bandgap energy covering the entire MWIR range, Ge1−xSnx semiconductors are frontrunner platforms for compact and scalable MIR technologies. However, the Ge1−xSnx large lattice parameter has been a major hurdle limiting the quality of Ge1−xSnx epitaxy on silicon wafers. These limitations are further exacerbated as Ge1−xSnx layers and heterostructures with Sn contents at least one order of magnitude higher than the solubility are needed for device structures relevant to MWIR applications. In this regime, the as-grown layers are typically under a significant compressive strain, which impacts the bandgap directness and increases its energy at the Γ point, thus hindering the device performance and limiting the covered range of the MIR spectrum. This compressive strain build-up not only affects the band structure but also limits the incorporation of Sn atoms in the growing layer, making the control of Sn content a daunting task.

In this presentation, we will show and discuss how sub-20 nm Ge nanowires provide effective compliant substrates to grow Ge1−xSnx alloys with a composition uniformity over several micrometers with a very limited build-up of the compressive strain. Ge/ Ge1−xSnx structures with Sn content spanning the 6 to 18 at.% range are achieved. We will also demonstrate the integration of the obtained materials in optoelectronic device processing leading to tunable detectors, phototransistors, and lasers [1-4]. For instance, photodetectors based on these materials were found to exhibit a high signal-to-noise ratio at room temperature and provide a tunable cutoff wavelength covering the 2.0 μm to 3.9 μm range. Additionally, the processed detectors were also integrated into uncooled imagers enabling the acquisition of high-quality images under both broadband and laser illuminations without the use of the lock-in amplifier technique. Progress towards achieving nanoscale GeSn lasers will also be discussed [4]. Finally, the potential introduction of GeSn in spin qubits and quantum memories will be highlighted [5-7].

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COMPOSITIONAL CHANGES IN RU-MO-W SINGLE-CRYSTAL WIRES GROWN BY THE DEWETTING MICRO-PULLING-DOWN METHOD

Rikito Murakami (Institute for Materials Research, Tohoku University), Kotaro Yonemura (Graduated School of Engineering, Tohoku University), Naveenkarthik Murugesan (Graduated School of Engineering, Tohoku University), Shiika Itoi (C&A Corporation), Kei Kamada (New Industry Creation Hatchery Center, Tohoku University), Akira Yoshikawa (Institute for Materials Research, Tohoku University)

[Background]

We have recently developed a Ru-Mo-W alloy single-crystal wire (Ruscaloy®) expected for commercial use to improve vacuum deposition efficiency in organic electroluminescence thin films. This wire endured over 3000 h of current heating at 1600°C under high vacuum—three times longer than conventional Ta wire—enables easy room-temperature deformation, and showed higher energy efficiency than conventional materials in organic EL film deposition [1].

The dewetting micro-pulling-down (µ-PD) method used to grow Ruscaloy involves melting feedstock in a ceramic crucible and solidifying it unidirectionally. Empirically, it was found that the alloy composition changes due to segregation or shifts in the system environment. Previous work revealed that Mo and W concentrations in Ru60Mo15W25 single-crystals change over the growth period. Hence, we grew Ru60Mo15W25 single-crystals at different pulling rates to examine how growth rate and growth time affect alloy composition.

[Experimental Methods]

Ru, W, and Mo (purity ≥ 99.9%) were arc-melted to form a Ru60Mo15W25 ingot. Single-crystal wires (φ0.8 mm) were grown via the dewetting µ-PD method at pulling rates of 10, 30, 100, and 160 mm/min, then heat-treated at 1800°C for 3 h in high-purity Ar. We used SEM and EBSD for microstructural observations, and ICP-MS and WDX for compositional analysis. The yttria stabilized zirconia (YSZ) crucibles were also crushed and examined by SEM/WDX.

[Results]

Wires of 6.8, 6.2, 8.0, and 11.3 m were obtained at pulling rates of 10, 30, 100, and 160 mm/min. Growth times were 11.4, 3.8, 1.4, and 1.7 h, respectively. In all wires, Mo and W concentrations decreased with time, contradicting phase diagram-based segregation predictions, and pulling rate did not significantly affect these changes. The YSZ crucible surface discolored to yellowish-green, indicating oxide formation from reactions with Mo/W. We established guidelines to control pulling rate and growth time to limit compositional fluctuation in Ru60Mo15W25 single-crystals.

Reference

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EVALUATION OF ALLOY MELT–CRUCIBLE REACTIONS IN RU-MO-W SINGLE CRYSTAL WIRE GROWTH BY THE DEWETTING MICRO-PULLING-DOWN METHOD

Rikito Murakami (Institute for Materials Research, Tohoku University), Kotaro Yonemura (Graduated School of Engineering, Tohoku University), Naveenkarthik Murugesan (Graduated School of Engineering, Tohoku University), Shiika Itoi (C&A Corporation), Kei Kamada (New Industry Creation Hatchery Center, Tohoku University), Akira Yoshikawa (Institute for Materials Research, Tohoku University)

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We have recently developed a Ru-Mo-W alloy single-crystal wire (Ruscaloy®) expected for commercial use to improve vacuum deposition efficiency in organic electroluminescence thin films. This wire endured over 3000 h of current heating at 1600°C under high vacuum—three times longer than conventional Ta wire—enables easy room-temperature deformation, and showed higher energy efficiency than conventional materials in organic EL film deposition [1].

In the dewetting micro-priming down (μ-PD) method used to grow Ruscaloy, the raw material is melted in a ceramic crucible and solidified in one direction. According to the Ru-Mo-W ternary equilibrium phase diagram, in the Ru solid-solution region, Mo and W concentrations should increase with increasing crystallization yield. However, in practice, these alloy elements often decrease along the longitudinal direction in the grown long wire. Thus, it has been suggested that Mo and W are excluded from the molten alloy via reactions with the yttria-stabilized zirconia (YSZ) crucible during growth. In this study, we focused on the feature of this process wherein the effective segregation coefficient approaches 1 at high pulling rates. By intermittently pulling the crystal at a high rate over fixed time intervals, we could effectively "sample" the melt composition in the crucible, thereby aiming to quantify the reaction rate between Mo, W, and the YSZ crucible.

[Experimental Methods] Ru, W, and Mo (purity ≥ 99.9%) were arc-melted to form a Ru60Mo15W25 ingot. Using a YSZ crucible with a φ0.8 mm hole, the crystal was pulled at 100 mm/min every two hours. After growth, the single crystal wire was cut and heat-treated, and their compositions were analyzed using WDX. The used YSZ crucible was crushed and examined by XRD.

[Results]

Crystal growth was carried out for a total of 24 hours, and the Mo and W concentrations decreased over this period. For the first four hours, their concentrations declined linearly, and after that, the slope decreased, indicating a reduction in concentration drop rate. This result suggests that there is initially a reaction rate–limited stage at the crucible interface, followed by a diffusion-limited stage within the reaction layer. Consequently, it became possible to determine the net effective segregation coefficient by excluding the influence of these reactions.

[1] R. Murakami, A. Yoshikawa et al., Int. J. Refract. Met. Hard Mater. 114 (2023) 106235.

ADVANCED CRYSTAL GROWTH TECHNIQUES FOR II-VI SEMICONDUCTORS

Magesh Murugesan (Washington State University), Jing Shang (Washington State University), John McCloy (Washington State University)

II-VI semiconductors, including CdTe, CdSe, CdSeTe, ZnTe, and CdZnTe are vital for solar cells, radiation detectors, and optoelectronics. Advance crystal growth technique such as Vertical Gradient Freeze (VGF) and High-Pressure Bridgman (HPB) are widely used to grow crystals alongside method like the Accelerated Crucible Rotation Technique (ACRT) and various crucible design. This study investigates the influence of supporting systems, such as Zircar and SiC, on thermal management, growth rate variation, temperature gradient, off stoichiometric growth, and defect mitigation such as tellurium inclusion control and secondary nucleation suppression. Optimized growth conditions lead to superior crystallinity and enhance electronic properties, paving the way for next generation semiconductor detector.

MOCVD GROWTH AND IN SITU PROCESSING OF GALLIUM OXIDE THIN FILMS AND HETEROSTRUCTURES

Hari Nair (Cornell University)

β-Ga2O3 with an ultra-wide bandgap of 4.8 eV has emerged as a promising material for next generation power electronics and radio frequency (RF) devices. In this talk, I will outline our work on metal-organic chemical vapor deposition (MOCVD) synthesis, in situ processing, and characterization of β-Ga2O3 epitaxial thin films and heterostructures for next generation power and RF devices.

In the first half of the talk, I will describe our work on MOCVD synthesis of β-(AlxGa1-x)2O3/Ga2O3 based modulation-doped heterostructures using triethylaluminum (TEAl) and triethylgallium (TEGa) as precursors for Al and Ga, respectively. At low growth temperatures, TEAl and TEGa undergo pyrolysis via β-hydrogen elimination mitigating carbon contamination in the epilayers. This enabled us to synthesize β-(AlxGa1-x)2O3/Ga2O3 heterostructures at low substrate temperatures, key for forming sharp interfaces, abrupt doping profiles and minimal carbon contamination. Electrical characterization of these two-dimensional electron gas (2DEG) revealed record high room temperature electron mobility of 187 cm2/Vs, the highest to-date for MOCVD grown β-(AlxGa1-x)2O3/Ga2O3 2DEGs. Moreover, at cryogenic temperatures, some of these 2DEGs display Shubnikov-de Haas oscillations.

In the second half of the talk, I will describe our efforts in developing an process for in situ etching of gallium oxide using tert-butyl chloride (TBCl) in an MOCVD reactor. In situ etching followed by regrowth opens up the possibility of forming contact layers for gallium oxide based electronic devices where the critical highly doped contact to channel interface is not exposed to atmospheric contamination. This enable pushing the performance envelope of gallium oxide-based RF and power devices. I will discuss the etch mechanism of gallium oxide using TBCl and electrical characterization of in situ etched and regrown ohmic contacts.

Finally, I will discuss our ongoing work on growth and characterization of delta-doped gallium oxide channels for RF devices with sheet carrier densities exceeding 1.5 x 1013 cm-2.

PRECIPITATION-DIFFUSION COUPLING ENABLES RECOVERY OF CRITICAL MATERIALS FROM PERMANENT MAGNET AND BATTERY FEEDSTOCKS

Elias Nakouzi (Pacific Northwest National Laboratory), Qingpu Wang (Pacific Northwest National Laboratory), Pacific Northwest National Laboratory (Andrew Ritchhart), Sebastian Mergelsberg (Pacific Northwest National Laboratory), Pacific Northwest National Laboratory ()

Crystallization is widely used at industry scale for chemical separations, but the products often require additional processing steps due to co-crystallization of various components. We anticipate that coupling ion transport, nucleation, and growth offers a new paradigm for efficiently and selectively separating critical elements from liquid feedstocks, beyond crystallization from batch solutions. Inspired by the classic Liesegang experiment, this approach selectively and sequentially extracts competing metal ions according to a delicate interplay between their diffusion and precipitation kinetics. We present a proof-of-concept for recovering pure neodymium from recycled permanent magnets and pure manganese from battery electrodes. Our overarching vision is to achieve the energy- and atom-efficient separation of rare earth elements, transition metals, and other critical elements from unconventional domestic feedstocks using non-thermal, reactive separations without costly membranes, ligands, toxic solvents, or other specialty chemicals.

PURIFICATION AND GROWTH OF TL-BASED CRYSTALS

Yaroslav Ogorodnik (Radiation Monitoring Devies, Inc.), Edgar van Loef (Radiation Monitoring Devies, Inc.), Joshua Tower (Radiation Monitoring Devies, Inc.), Lakshmi Soundara Pandian (Radiation Monitoring Devies, Inc.), Jarek Glodo (Radiation Monitoring Devies, Inc.)

Thallium-based compounds are of significant interest for radiation detection, serving as both high-performance scintillators and wide-bandgap semiconductors. Materials utilizing Tl include scintillators such as Ce-doped Tl2LaCl5, pure TlCaCl3, and Be,I-doped TlCl, as well as semiconductors such as TlBr. However, achieving optimal scintillation and semiconductor properties requires minimizing impurity levels, as trace contaminants degrade charge transport, light yield, and energy resolution. In this work, we investigate the purification of Tl-based precursor materials using zone refining, optimizing processing parameters to reduce metallic and oxygen-based impurities. We analyze impurity segregation behavior, revealing preferential removal trends and their impact on the electronic and scintillation properties of grown crystals. High-purity precursors are subsequently used for single-crystal growth via the Bridgman method, and the resulting materials are characterized in terms of their quality, electronic transport, optical properties, and scintillation performance. Comparisons between purified and unpurified crystals highlight the critical role of precursor refinement in enhancing detector performance. This work establishes a link between precursor purification and improved radiation detection capabilities, guiding future advancements in Tl-based crystal growth.

RAMAN SCATTERING MICROSCOPY CHARACTERIZATION OF EXTENDED DEFECTS IN SIC CRYSTALS

Noboru Ohtani (Kwansei Gakuin University, School of Engineering)

In the last decade, significant progress in the quality improvement of silicon carbide (SiC) single crystals has been made, and 150- and 200-mm diameter 4H-SiC epitaxial wafers with a low defect density have been brought to market, and using these wafers, high performance SiC power devices are fabricated. However, widespread commercialization of the devices is still hindered by technological issues related to extended defects in SiC crystals, and thus it is abundantly clear that further successful development of SiC semiconductor technology relies on understanding the nature and formation mechanisms of extended defects in SiC crystals and, based on them, improving the technology of manufacturing SiC crystals.

In this presentation, I will talk about Raman scattering microscopy characterization of extended defects in 4H-SiC bulk crystals and homoepitaxial thin films, particularly focusing on the local carrier concentration variations due to the defects in SiC crystals. Raman scattering microscopy is a powerful tool to detect and characterize extended defects in SiC crystals, which enables structural and electric characterization of the defects with both high spatial resolution and high sensitivity. I have applied Raman scattering microscopy characterization to several types of extended defects in SiC crystals and successfully demonstrated its ability to extract unique information on extended defects in 4H-SiC crystals, not attainable with other characterization techniques.

ACCELERATED THROUGHPUT PERFORMANCE OF HYDRIDE VAPOR PHASE EPITAXY FOR GAAS-BASED SOLAR CELLS

Ryuji Oshima (National Institute of Advanced Industrial Science and Technology), Yudai Shimizu (Taiyo Nippon Sanso Corporation), Yasushi Shoji (National Institute of Advanced Industrial Science and Technology), Akinori Ubukata (Taiyo Nippon Sanso Corporation), Kikuo Makita (National Institute of Advanced Industrial Science and Technology), Hiroki Tokunaga (Taiyo Nippon Sanso Corporation), Takeyoshi Sugaya (National Institute of Advanced Industrial Science and Technology)

High-efficiency III-V photovoltaic (PV) devices have already been demonstrated as power sources for satellites and are expected to be deployed in a wide range of new applications, including unmanned aerial vehicles, solar electric vehicles, thermophotovoltaic power generation, and laser power converters. However, one of the obstacles to the practical application of such PVs is the high manufacturing cost. In terms of crystal growth, hydride vapor phase epitaxy (HVPE) is a fast growth technique that uses inexpensive group III precursors and is a potential method to reduce the cost of III-V devices. We previously demonstrated high-speed growth of GaAs solar cells at 200 um/h with 24.0% in conversion efficiency by a 2-inch HVPE system [1],[2]. Based on these developments, we recently expanded to 6-inch HVPE to improve throughput performance. This system employs a showerhead for supplying source gases and a high-speed substrate rotation of 500 rpm, achieving an in-plane non-uniformity of approximately 10%. In addition, we have demonstrated high growth rates of up to 270 um/h for GaAs and 20 um/h for GaInP, as well as abrupt GaInP/GaAs heterointerfaces via an internal run/vent switching component in the reactor. In the defect analysis using deep-level transient spectroscopy (DLTS), although the EL2 trap density tends to increase with increasing growth rate, n-type GaAs grown under V/III = 3.5 at 200 um/h has an EL2 trap density of 1.0 x 10^14 cm^-3, which does not appear to affect the performance of the resulting solar cell. As a result, a conversion efficiency of 20.0% was achieved in a GaAs front homojunction solar cell. In the future, the introduction of AlCl3 source gas [3] and the adoption of a rear heterojunction cell structure [2] are expected to improve device performance. These developments could be a breakthrough towards the mass production of low-cost III-V solar cells. [1] R. Oshima et al., Jpn. J. Appl. Phys. 57, 08RD06 (2018). [2] R. Oshima et al., Crystals, 13, 370 (2023). [3] Y. Shoji et al., Solar RRL 8, 2300845 (2024).

ADVANCES IN MOCVD GROWTH OF HIGH-SCANDIUM CONTENT ALSCN FOR FERROELECTRIC AND ELECTRONIC APPLICATIONS

Andrei Osinsky (Agnitron Inc.), Will Brand (Agnitron Inc.), Ben Brand (Agnitron, Inc), Vitalii Soukhoveev (Agnitron Inc.), Fikadu Alema (Agnitron Inc.)

Aluminum Scandium Nitride (AlScN) is a promising material for GaN-based HEMTs and ferroelectric devices due to its enhanced polarization and piezoelectric properties. At ~12% Sc content, AlScN becomes lattice-matched to GaN and exhibits higher spontaneous polarization than AlN, enabling increased 2DEG densities without critical thickness limitations. Above ~20% Sc, AlScN demonstrates ferroelectric switching, expanding its potential to non-volatile memory and logic applications.

We report on the MOCVD growth of AlScN using a custom reactor with a high-temperature Sc precursor delivery system, enabling stable growth with precise composition control. Crystalline films with up to 40% Sc retain the wurtzite structure, while incorporation up to 47% Sc was achieved, resulting in amorphous films. Growth of epitaxial AlScN films was demonstrated on various substrates, including Silicon, Platinum, and GaN, broadening the integration possibilities across different device platforms.

On SiC substrates, AlScN/AlN/GaN heterostructures exhibited 2DEG densities up to 2×10^{13} cm^{-2} and electron mobilities near 900 cm^2/V·s. Uniformity across 2” wafers showed <1% thickness variation, >95% Sc composition uniformity, and <0.3 nm RMS roughness.

We will present detailed characterization of the structural, electrical, optical, and ferroelectric properties of MOCVD-grown AlScN films, and compare their polarization behavior and ferroelectric switching with films produced by magnetron sputtering. These results establish MOCVD as a scalable approach for high-quality ferroelectric III-nitride materials across multiple substrates and clearly demonstrate the technique’s strong potential for integration with CMOS technology.

ORBITAL FOUNDRIES FOR NEXT-GENERATION SEMICONDUCTORS

Divya Panchanathan (Axiom Space)

The growing commercial space economy is lowering launch costs and enabling the construction of large-scale orbital infrastructure, paving the way for industrialization in space. The unique conditions of LEO – such as the absence of convection and the availability of high vacuum – can enable the growth of large defect-free crystals of Wide Bandgap semiconductors, photonics, and quantum materials which cannot be produced at commercial scale on the ground today. This will unlock new levels of performance and efficiency in critical applications like electric vehicles, renewable energy, and advanced computing.

This talk will explore how commercial space stations, space logistics providers and large-scale orbital infrastructure are together unlocking the production of next-generation semiconductors in space. It will also highlight commercial case studies demonstrating the feasibility and potential of this transformative technology.

ULTRAWIDE BANDGAP ALN/ALGAN EPITAXY

Shubhra Pasayat (University of Wisconsin-Madison)

UWBG Al(Ga)N semiconductors hold promise for power electronic devices and deep UV emitters. Doping control is crucial for Al-rich AlGaN (>85%) due to its low conductivity from high Si dopant activation energy and other factors. Si-doping in Al-rich AlGaN is well-documented for most MOCVD reactors, but close-coupled showerhead (CCS) vertical reactors lack sufficient studies. State of the art carrier concentrations were achieved for n-AlN and n-AlGaN with compositions exceeding 0.95, details of which will be presented on sapphire substrate.

Concurrently, the transport properties of the UWBG AlGaN channel HEMTs suffer due to multiple scattering phenomena that limit their performance. The design of epitaxial layers can also influence transport properties by introducing compressive strain, degrading morphology, and reducing crystalline quality, as AlGaN channel HEMTs are typically deposited on bulk AlN or AlN-on-sapphire templates. I will discuss the transport properties of UWBG Al0.84Ga0.16N/AlN/Al0.65Ga0.35N channel HEMTs and various scattering mechanisms at play. A fabricated HEMT device with optimized epitaxial design showed state-of-the-art contact resistivity (ρ_C=8.35×10^-6 Ω.cm2), low leakage current (<10^-6 A/mm), high ION/IOFF ratio (>10^5), a breakdown voltage of 2.55 kV and a Baliga's figure of merit (BFOM) of 260 MW/cm2.

PRESSURE-INDUCED NUCLEATION IN AMORPHIZING CARBON MONOXIDE-OXYGEN MIXTURES

Reetam Paul (Lawrence Livermore National Laboratory), Nikhil Rampal (Lawrence Livermore National Laboratory), Rhys Bunting (Lawrence Livermore National Laboratory), Margaret Berrens (Lawrence Livermore National Laboratory), Maximilian Boehme (Lawrence Livermore National Laboratory), Jonathan Crowhurst (Lawrence Livermore National Laboratory), Stanimir Bonev (Lawrence Livermore National Laboratory)

We explore the formation and growth of polymeric crystals and amorphous structures in carbon monoxide-oxygen mixtures, when compressed to pressures above 20 GPa along low-temperature isotherms. Machine-learning molecular dynamics simulations are used to understand this evolution from energetics, kinetics, as well as a strain energy point-of-views.

IN SITU GRAPHENE CVD FOR SIC EPILAYER TRANSFER

Daniel Pennachio (US Naval Research Laboratory), Jenifer Hajzus (US Naval Research Laboratory),
Rachael Myers-Ward (US Naval Research Laboratory)

Transferred 2D two-dimensional (2D) material, such as graphene, is commonly used for a release layer in remote epitaxy (RE), but the transfer step can degrade the film and increase process complexity [1]. To avoid this, we examine in situ graphene growth on SiC substrates before subsequent SiC epitaxy in the same chemical vapor deposition (CVD) RE process. RE SiC and subsequent SiC epilayer transfer is desired since isolated SiC membranes are excellent for quantum photonics and SiC substrate reuse can provide significant cost savings. Despite these benefits, the high-temperature hydrogen-containing CVD environment can damage graphene, making RE difficult under standard SiC growth conditions.

This study established growth windows for in situ graphene via propane-based hot wall CVD. This propane-based graphene growth enables an efficient transition to subsequent SiC deposition using established SiC growth conditions since it shares a similar hydrogen ambient to standard SiC CVD. Growing at 1620 °C in 20 slm H2 with 20 sccm propane flow produced predominantly monolayer (ML) graphene films on on-axis 6H-SiC(0001) substrates with minimal defects found in Raman spectral maps. Films grown on 4° off-axis 4H-SiC(0001) substrates were multilayer (6 ML) graphitic carbon despite experiencing the same conditions as the on-axis substrates. This optimized graphene growth condition was used for subsequent RE attempts to study the effect of SiC precursor dose, C/Si ratio, and growth rate on epilayer crystallinity and graphene barrier damage. SiC crystalline quality appeared correlated to growth rate, with lower growth rates producing smoother films with fewer polytype inclusions. Single-crystalline, polytype-pure SiC epilayers was achieved on 4° off-axis CVD graphene/4H-SiC(0001). Effects of initial SiC growth parameters on the graphitic carbon release layer were explored via cross-sectional transmission electron microscopy (TEM) and attempts at epilayer transfer. Some growth interfaces exhibited non-uniform multilayer graphitic carbon, motivating further study of this growth system to improve boundary uniformity and SiC epilayer quality.

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ACENTRIC BARIUM CHALCOGENIDES FOR MID-IR FREQUENCY CONVERSION

Valentin Petrov (Max Born Institute for Nonlinear Optics and Ultrafast Spectroscopy)

The number of non-oxide nonlinear crystals for frequency conversion in the mid-IR (3-30 μm) part of the spectrum is limited and only few of them are commercially available. In the last decade there have been substantial efforts and progress in the development of new Ba chalcogenide compounds with improved properties compared to the classical I-III-VI2 chalcopyrites AgGaS2 (AGS) and AgGaSe2 (AGSe) with tetragonal symmetry which represent the benchmarks for frequency down-conversion of solid-state laser systems operating near 1 μm (Nd- or Yb-lasers) and near 1.5 μm (Er-lasers).

In this presentation I will review the main properties, including transmission, dispersion, birefringence, nonlinear coefficients, thermo-optic coefficients, etc., of five such non-centrosymmetric Ba crystals that have been characterized recently using large size single crystalline samples of high optical quality. These chalcogenide crystals have been grown by the vertical Bridgman-Stockbarger method. They include the orthorhombic (mm2) BaGa4S7 (BGS), the monoclinic (m) BaGa4Se7 (BGSe), the trigonal (3) BaGa2GeS6 (BGGS) and BaGa2GeSe6 (BGGSe), and the hexagonal (6mm) Ba2Ga8GeS16 (B2GGS). In almost all their characteristics, including thermo-mechanical properties such as expansion, conductivity and hardness, as well as their anisotropy, these new nonlinear materials seem to be superior compared to the corresponding sulphide (AGS) and selenide (AGSe) chalcopyrites. Based on the larger bandgaps, the same is expected for their damage resistivity in different temporal regimes. In addition, these new materials do not require post-growth annealing procedures and are chemically stable. The low-symmetry of the trigonal and monoclinic compounds, however, complicates the characterization and the orientation of the samples.

All of the Ba chalcogenide crystals possess the phase-matching capability to cover parts of the mid-IR spectral range by down-conversion of 1.064 μm laser radiation, show clear transparency and are free of two-photon absorption (TPA) at this pump wavelength. The selenides transmit up to ~18 μm, with clear transparency at 10.6 μm. The main applications of these nonlinear crystals will be in frequency down-conversion of advanced all-solid-state laser sources operating in the near-IR between 1 and 3 μm but also for harmonics generation of CO2 gas lasers (selenides only). The sulphides might prove unique for pumping near 1 μm.

AMMONOTHERMAL GROWTH OF RHOMBOHEDRAL BORON NITRIDE

Siddha Pimputkar (Lehigh University), Jacob Dooley (Lehigh University), Nathan Stoddard (Lehigh University), Kai Landskron (Lehigh University)

Boron nitride (BN) has advantageous physical and electrical properties for (opto-)electronic applications, yet growing large area, bulk single crystals has proven challenging. These materials are desired for the use as substrates and as device layers to take full advantage of the material properties.

Melt-based crystal growth methods are ill-suited for the growth of BN due to their inability to melt BN given its sublimation temperature of ~ 3000 °C. Gas phase approaches for the growth of BN have been demonstrated, though they are still dependent on the availability of existing seed crystals to grow upon, encouraging the pursuit of a true bulk crystal growth synthesis pathway.

Solution-based crystal growth approaches offer the most accessible path towards bulk BN growth. This talk will investigate the application of the ammonothermal method to the growth of BN. The ammonothermal method relies on the temperature-dependent dissolution of species, in this case BN, in a supercritical ammonia solution containing mineralizers to enhance solubility. Typical growth conditions occur at temperatures around 500-600 °C and pressures 150-250 MPa.

Building on prior studies evaluating the temperature-dependent solubility of BN in a sodium-containing supercritical ammonia solution,[1] this contribution will discuss the application of a temperature gradient across a baffled autoclave in this system for the first time. Both rhombohedral and hexagonal BN (rBN, and hBN, respectively) crystals were grown on the autoclave walls and on seed crystals of cubic BN (cBN) in the lower temperature, lower solubility zone of the autoclave.

The structure of the grown BN crystals is characterized via Raman spectroscopy, X-ray diffraction, transmission electron microscopy, selected area electron diffraction, and electron energy loss spectroscopy. An epitaxial relationship is identified for the preferential growth of rBN on the (111) cBN surface offering a pathway for bulk rBN growth.

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V:YAG AND CR:YAG SATURABLE ABSORBERS FOR SOLID STATE LASERS

Jan Polak (Crytur, spol. s r. o.), Jan Havlicek (Crytur, spol. s r. o.), Jindrich Houzvicka (houzvicka@crytur.cz)

Q-switching is a method to produce a pulsed output laser beam. Light pulses can reach very high peak power, significantly higher than in the same laser arrangement at continuous wave mode. Q-switching is achieved by inserting active or passive type of variable attenuator into the optical resonator of the laser. [1]

The passive Q-switch saturable absorbers has some advantages in comparison with the active one: they are compact, inexpensive and easy to operate. A saturable absorber is an optical component that exhibits a certain level of absorption loss, which decreases at high optical intensities. This nonlinear absorption can occur in a medium containing absorbing dopant ions, where intense light depletes the ground state of these ions. The primary applications of saturable absorbers include passive mode locking and Q-switching of lasers, which are techniques for generating short optical pulses. Additionally, saturable absorbers are valuable for nonlinear filtering outside of laser resonators, such as for cleaning up pulse shapes and in optical signal processing. For passive Q-switching of solid-state lasers in the 1-µm spectral region, Cr:YAG crystals are most popular. For 1.3 µm lasers, V:YAG can be used. [2]

This contribution will introduce the crystal growth by Czochralski method; followed by a discussion of their application properties and characterisation methods.

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ROOM-TEMPERATURE INFRARED EXTINCTION IN HIGHLY DOPED CDTE:CR CRYSTALS WITH QUASI-2D DOPANT-RELATED PRECIPITATES

Andrii Popovych (Ivan Franko Drohobych State Pedagogical University), Volodymyr Popovych (Ivan Franko Drohobych State Pedagogical University; Lviv Politechnic National University), Piotr Potera (University of Rzeszów), Ihor Stolyarchuk (Ivan Franko Drohobych State Pedagogical University)

Two-dimensional van der Waals magnetic materials show tremendous potential in spintronic device applications. The Cr3Te4 compound is among those with the Curie temperature above RT, and magnetic ordering is retained down to the monolayer. Compatibility of 2D magnets with semiconductors is one of the challenges in the practical realization of the spintronic components. In the present work, we study RT optical extinction of the heavily doped CdTe:Cr single crystals with a dense array of crystallography-oriented quasi-2D Cr3Te4 lamellas embedded in the host semiconductor matrix due to the dopant precipitation upon crystal growth. The spreading of the exponential absorption edge (Urbach edge) in such material is related to the fluctuating electric field created by the doping-induced point-charged defects randomly distributed in the CdTe lattice. The mean strength of the field and effective concentrations of the point-charged defects were determined within Bonch-Bruevich’s model of heavily doped semiconductors by analyzing the absorption edge. The extinction spectra of CdTe:Cr crystals in the near-IR were approximated as a sum of the selective absorption peak arising from the intra-shell transition within the 3d4 configuration of substitutional Cr2+ ions, and a power-law dependency describing the light scattering by the Cr-related nanoprecipitates. The concentrations of divalent Cr ions, calculated from the peak intensity, were about 1/3 of the total dopant content in the CdTe host matrix determined through secondary ion mass-spectroscopy measurements. The optical transparency of the investigated crystals is correlated with the density and size of the Cr3Te4 lamellas, suggesting that the extinction of the heavily doped CdTe:Cr crystals in the mid- and far-IR regions of the spectra is determined by the scattering on such quasi-2D dimensional defects. We believe that the controlled (driven by the growth conditions) precipitation of 2D magnetic doping-related phases is an effective approach to integrate them into semiconductor-based materials in a self-arranged way.

OXIDE FILMS FOR OPTICAL APPLICATIONS GROWN ON GLASS SUBSTRATES

Wilfrid Prellier (CNRS)

Transition metal oxides with perovskite structures form a fascinating and technologically important class of materials. These compounds exhibit various types of orderings, including ferromagnetic, orbital, and charge ordering, which can interact and coexist in complex and dynamic ways. What makes these systems particularly intriguing is their ability to have these orderings controlled through external stimuli, such as electric, magnetic, or stress fields, resulting in multifunctional properties like piezoelectricity and magnetoelasticity.

In this presentation, we will explore the growth of vanadium oxide thin films, prepared by pulsed laser deposition, and grown on unconventional substrates, like glass templates. We will show how the electronic and optical properties can be influenced with the growth temperature and the thickness of the films. Finally, we will also highlight the potential applications of these films in fields such as optics [1-4].

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OPTICAL SYSTEM FOR GROWING OPTICAL ISOLATOR SINGLE CRYSTALS BY THE LASER DIODE FLOATING ZONE METHOD

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The laser diode floating zone method is a crucible-free technique to grow single crystals of high purity from the molten phase. Instead of incandescent light bulbs or induction coils, diode lasers are used to provide the energy that is required to heat and consequently melt the feed rod material from which the single crystal is grown. Using a laser in combination with a process-adapted beam shaping system provides several fundamental advantages over the conventional lamp-based optical floating zone method. For example, the intensity distribution can be adjusted to achieve a defined energy input into the feed rod, resulting in a homogeneous heating of the rod which is essential for the stability of the growth process. Another advantage is the long-term stability of the laser sources which is more than one order of magnitude higher than for conventional lamps. In addition, due to the high focusability of laser radiation, power densities can be achieved that are high enough to enable the growth of monocrystalline materials with melting temperatures above 2000 °C.

For growing optical isolator crystals, we designed, set up and characterized an optical system. It consists of four identical beam shaping optics which collimate the ingoing radiation emerging from a 600 µm fiber and create a specifically homogenized intensity profile at the position of the feed rod. The characterization of the system includes the measurement of the beam profile and efficiency of the optics, as well as a high-power endurance test. After the tests, the system was integrated into an optical floating zone furnace and commissioned together with four fiber-coupled 3-kW diode laser modules. Currently, the system is applied to grow single crystals of a novel material based on Tb2O3 (terbium oxide). Pure Tb2O3 exhibits a Verdet constant that is more than 3 times higher than the Verdet constant of TGG (terbium gallium garnet), which makes it an ideal material for optical isolators to be used in miniaturized laser sources.

BEYOND CLASSICAL NUCLEATION THEORY: MOLECULAR INSIGHTS INTO NON-CLASSICAL PATHWAYS OF SPARINGLY SOLUBLE SALTS

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Nucleation is the initial step in phase formation and is traditionally described by classical nucleation theory (CNT). However, emerging evidence challenges its universality, revealing the prevalence of non-classical pathways. Using classical molecular dynamics (MD) simulations within a constant chemical potential regime, we investigate the nucleation of a sparingly soluble salt—a process that is challenging to resolve at the atomistic scale. This approach ensures stable supersaturation around the growing nucleus, enabling detailed analysis of nucleation behavior. At high supersaturation indices (SI), we observe non-classical pathways characterized by multi-ion clustering and intermediate metastable states, which deviate significantly from CNT predictions. Leveraging these structural insights, we develop a Generative Neural Network (GNN) Model to predict nucleation structures based on existing literature pair distribution data. This model provides a powerful predictive capability to uncover nucleation structures that are inaccessible to current experimental techniques. These findings offer critical insights into nucleation mechanisms, emphasizing the need to revisit classical assumptions. Furthermore, our study establishes a framework for exploring similar phenomena in other systems, advancing the understanding of phase transformations in complex environments.

MODELING THE GROWTH OF M-PLANE {1-100} GAN USING KINETIC MONTE CARLO SIMULATIONS: ROLE OF NITROGEN DESORPTION

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Film growth on non-polar Gallium Nitride (GaN) surfaces has been of interest due to the potential of higher efficiency in optoelectronic devices. Experimentally, it is observed that at high temperature, the growth of m-GaN in molecular beam epitaxy under N-rich conditions leads to good crystal quality. This is in sharp contrast to GaN growth on the polar c-plane where nitrogen rich conditions lead to rough crystal surfaces during growth.[1][2]
Quantum mechanical calculations on m-plane GaN suggest that, Ga-adsorption is stable, but N-adsorption leads to extraction of surface N-atoms, leading to N 2 formation on the surface.[3,4]
We incorprate these ideas in lattice-based kinetic Monte Carlo (kMC) simulations of homo-epitaxial MBE growth of m-plane GaN thin films. We consider both on-axis and vicinal surfaces, controlled by various growth parameters experimentally observed. A key feature of our kMC simulations is the desorption of surface nitrogen. Our results indicate that m-GaN growth at higher temperature produces smoother surfaces at more N-rich conditions. By carrying out simulations under varying experimental conditions we construct a phase diagram showing various growth modes with the growth parameters, Ga-flux, Ga/N flux ratio and temperature.

EPITAXY OF 2D VAN DER WAALS CRYSTALS - FROM FUNDAMENTALS TO APPLICATIONS

Joan Redwing (Pennsylvania State University)

TBA

COMPUTATIONAL DESIGN OF THE SiC CRYSTAL GROWTH PROCESS IN PVT FURNACES

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The physical vapor transport (PVT) method is key for producing large and high-quality SiC single crystals. Despite its widespread use, challenges remain, particularly with respect to controlling the temperature distribution and mass transport, which determine the growth rate and crystal defect densities. Direct observations of the growth phenomena are difficult since the process operates at temperatures between 2000 and 2500 °C in a closed reactor. Therefore, numerical modeling is an essential tool for understanding and optimizing SiC bulk crystal growth.

We present our current activities towards implementing a digital twin of the PVT furnace and the related crystal growth process. For this purpose, we combine data-driven and physics-based simulation methods on different length scales. On the macro-scale, we train machine learning algorithms to replace multi-physics simulations based on the finite element method (FEM) providing temperature field and diffusive fluxes. The surrogate model accelerates the FEM model by several orders of magnitude which is a key requirement to calibrate the model to experimental data based on Markov Chain Monte Carlo techniques and Bayesian inference. The calibration provides access to the material data of the furnace components at the high service temperatures and the possibility to monitor their degradation. Furthermore, the calibrated model allows optimizing the furnace geometry according to set design criteria.

On the atomic scale, the thermodynamics of the SiC polytypes and their interactions with gas particles will be presented. It is shown how doping can change the relative energetic alignment of polytypes. We study the interaction of gas molecules with the SiC surface and explore kinetic growth processes from molecular dynamics simulations and related techniques. We discuss the potential of the results to derive laws that can be used on the macroscale for modeling surface-vapor interactions that provide the boundary conditions for mass transport modeling, including the prediction of SiC crystal deposition and etching in the furnace. We close with an outlook on future activities of computational design of crystal growth.

V-GROOVE NANOPATTERNING FOR ORIENTATION-PATTERNED GAP

Theresa Saenz (National Renewable Energy Laboratory), Anica Neumann (National Renewable Energy Laboratory), John Mangum (National Renewable Energy Laboratory), Edgard Winter da Costa (National Renewable Energy Laboratory), Bill McMahon (National Renewable Energy Laboratory)

Orientation-patterned (OP) III-V semiconductors are nonlinear optical materials used in applications requiring longer wavelengths than what is accessible for periodically poled lithium niobate. OP III-Vs are currently produced by seeding a patterned array of antiphase domains (APDs) through a molecular beam epitaxy (MBE) and photolithography process and then propagating the APDs into a thick film via halide vapor phase epitaxy [1]. The MBE and photolithography process is costly and has low yield, limiting the usefulness of OP-III-Vs [2]. In this work, we demonstrate an alternative method for seeding the APD pattern in GaP through the use of V-groove Si nanopatterns and metalorganic vapor phase epitaxy growth. Antiphase boundaries are induced in the GaP wherever there is a 90˚ turn in the underlying {111}-faceted V-groove trenches due to the decrease in symmetry of GaP compared to Si. This method is promising as a more robust and simpler alternative to the current MBE-based approach.

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VAE-BASED RE-OPTIMIZATION FOR CRYSTAL GROWTH SYSTEMS UNDER STRUCTURAL CHANGES

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In the field of crystal growth, high-quality crystals are achieved by optimizing process conditions through experiments, simulations, and machine learning. However, various factors—such as reducing power consumption or reducing furnace stress—may require changes a furnace's structure (including its internal layout and component materials). Such changes can alter the growth environment and degrade crystal quality, requiring a full re-optimization that is both time-consuming and costly. In this study, we propose a method to re-optimize post-change conditions by leveraging the pre-change optimal growth environment. We also applied this method to optimize SiC crystal growth using the TSSG method. In this method, the temperature and flow distribution within the solution is crucial for achieving high-quality crystals.

Our objective function minimizes the difference between the features of the temperature and flow distributions under the previous optimal conditions and those in the modified furnace. We quantified these features using a Variational Auto-Encoder (VAE), which converts high-dimensional images into low-dimensional latent variables so that similar images yield similar representations. The mean squared error between these representations serves as our similarity measure. Additionally, we developed neural networks to predict the temperature and flow distributions and the crystal growth rate from process parameters. These models were trained on data from roughly 1,000 CFD simulations conducted under various conditions. During optimization, the predicted distributions were compared with the target using the VAE, while a genetic algorithm searched for the best process conditions. We also aimed to maximize and equalize the growth rate and minimize temperature differences in the melt.

We tested this method on 200 mm diameter crystal growth experiments. Under original conditions, a smooth surface was achieved; however, when the furnace structure (specifically, the insulation layout) was modified without re-optimization, many polycrystalline deposits formed at the center. In contrast, experiments under the optimized conditions produced smooth surfaces like those before the modification.

In conclusion, by leveraging existing optimal conditions across different systems, our method can greatly reduce the time and expense of re-optimization. Moreover, it applies not only to SiC crystal growth by the TSSG method but also to a wide range of crystal growth processes.

SUBOXIDES MBE ROCKS!

Darrell Schlom (Cornell University)

TBA

SIC PVT CRYSTAL GROWTH AND MANUFACTURING: TECHNOLOGY & MARKET CHALLENGES

Peter Schunemann (onsemi)

Advances in Silicon Carbide (SiC) Physical Vapor Transport (PVT) growth technology are vital to meet size, quality, & cost demands of the expanding power electronics market. The current market downturn (2024-2025) has constrained resources for SiC substrate suppliers across the industry, requiring cost-cutting & innovation at every stage of the process to remain competitive. Synthesis of high-purity, stoichiometric, homogeneous SiC source material with uniform size and morphology is vital to success, During the growth process, the source material sublimes incongruently at temperatures near 2500ºC to produce Si, Si2C, and SiC2 species with a net Si/C ratio that varies throughout the process. These vapor species transport and deposit on the cooler 4H SiC seed crystal near 2000ºC. This process takes place in the hot zone of the PVT furnace (which may be inductively or resistively heated) which consists of an isostatic graphite crucible with inserts, baffles (to optimize thermal profile), and in some cases porous graphite to control the flow of species to the growth surface. Crystalline defects (basal plane and threading dislocations, micropipes, low angle grain boundaries, unwanted polytypes) must be minimized in the seed wafers used for growth, and the propagation of these defects (as well as the nucleation of new ones) in the growing crystals must be minimized through tailoring of the growth process parameters. Modeling of the PVT growth process using STR's Virtual Reactor, COMSOL, ANSYS, or custom in-house software is vital for designing the hot zone, understanding the process chemistry, and controlling the evolution of the interface shape to minimize defects and stress in the final crystal. Statistical analysis of large process parameter data sets is invaluable for identifying and eliminating process deviations that negatively impact single crystal yield. Finally, the as-grown boules are annealed, carefully cooled, ground, sliced, and polished to produce substrate wafers (and/or seed wafers) which are fully characterized and delivered to our foundry for epitaxial growth, device fabrication, testing, packaging, and integration into power modules. Feedback from vertical integration is vital for continued process improvement. Current SiC manufacturing is predominantly based on 150-mm diameter substrates, but transition to 200 mm is rapidly progressing, and even 300 mm development is not far off, and will likely be required to minimize device costs.

LARGE-AREA DEPOSITION OF EPITAXIAL SILICON FOR TERRESTRIAL AND SPACE APPLICATIONS USING A NOVEL IN-LINE ATMOSPHERIC PRESSURE CVD PROCESS

Rick Schwerdtfeger ()

TBA

IN SITU OBSERVATIONS OF BIOGENIC MINERALIZATION WITH MICROFLUIDICS

Jong Seto (Arizona State University)

Numerous investigations have focused on the roles of organic moieties on CaCO3 nucleation and crystal growth processes especially in the sea urchin spicule, molluscan shell mineralization model systems. We demonstrate that with precise spatial and temporal control in a microfluidics platform that these mineral-organic interactions have another pathway for affecting mineralization. By focusing on prenucleation events, we observe that many of these moieties can interact with amorphous mineral precursors directly. We validate these interactions with a multimodal approach to demonstrate the versatility of these mineral-organic interactions in driving biological mineralization.

ELECTRO-OPTICAL PROPERTIES OF CD-SE-TE CRYSTALS WITH 30% SE AND GROUP V DOPANTS

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This study examines the impact of 30% Se and Group V dopants (P, As, Sb, Bi) on the electro-optical properties of Cd-Se-Te single crystals grown by the High-Pressure Bridgman (HPB) method. Comprehensive characterization was performed using X-ray diffraction (XRD), inductively coupled plasma mass spectrometry (ICP-MS), ultraviolet-visible spectroscopy (UV-Vis), current-voltage (IV) measurements, Hall effect measurements, and positron annihilation spectroscopy (PAS) to analyze structural, chemical, optical, and electrical properties. Post-growth Cd annealing effects on carrier concentration and mobility were also investigated. These findings provide critical insights for the advancement and optimization of Cd-Se-Te materials in optoelectronic and photovoltaic applications.

STRUCTURE AND STOICHIOMETRIC CONTROL OF EPITAXIAL TUNGSTEN OXIDE THIN FILMS VIA SURFACE-OXIDATION-ASSISTED MOLECULAR BEAM EPITAXY AND PULSED LASER DEPOSITION

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Precisely controlling the epitaxial growth, oxidation states, and defect structures in complex oxide thin films such as tungsten oxide remains an essential challenge due to their sensitivity to structural and compositional variations. Here, we present the epitaxial growth of tungsten oxide thin films using two different approaches: WO3 by surface-oxidation-assisted molecular beam epitaxy (MBE), which enables precise control of stoichiometry and reproducibility; and Magnéli-structured WOx by pulsed laser deposition (PLD), which facilitates atomic-scale defect modulation through strain engineering.

In the MBE process, we introduce an in-situ surface oxidation strategy where high-purity, refractory tungsten metal is oxidized at the source surface during electron-beam heating under controlled oxygen environments. By generating a stable and tunable flux of volatile oxide species, this technique enables precise control over the growth process and overcomes traditional challenges associated with traditional way of evaporating WO3 powder using MBE, including incongruent evaporation and instability. By systematically varying oxygen pressure and electron-beam power, we regulate the growth rate and achieve uniform, epitaxial WO3 thin films.

Furthermore, we synthesized a series of high-quality, epitaxial, Magnéli-structured WOx (<x<) films that exhibit tunable, one-dimensional aligned, atomic-scale defect by controlling the lattice strain and oxygen stoichiometry. Scanning transmission electron microscopy (STEM) confirmed the presence of W18O49-like phases with highly oriented hexagonal defect tunnels. In addition, combined X-ray photoelectron spectroscopy (XPS), X-ray absorption spectroscopy (XAS), and density functional theory (DFT) calculations demonstrated the significant influences of oxygen vacancies and lattice distortions on the electronic structure and properties of the tungsten oxide films.

Our study demonstrates that epitaxial control via MBE and PLD enables precise tailoring of both the growth and properties of tungsten oxide thin films, offering versatile approaches to modulate the fundamental characteristics of complex oxide materials.

SELECTIVE AREA HETEROEPITAXY OF III-V QUANTUM DOT LASERS ON SILICON PHOTONICS

Bei Shi (Aeluma, Inc.), Alec Skipper (Institute for Energy Efficiency, University of California, Santa Barbara), Rosalyn Koscica (Materials Department, University of California, Santa Barbara), Gerald Leake (Research Foundation of SUNY), Joshua Herman (Research Foundation of SUNY), James Turvey (Research Foundation of SUNY), David Harame (Research Foundation of SUNY), John Bowers (Institute for Energy Efficiency, University of California), Jonathan Klamkin (Aeluma, Inc)

Silicon photonics plays a pivotal role as a key enabler for a range of cutting-edge applications, including energy-efficient artificial intelligence (AI), quantum information processing, high-performance computing, and remote sensing. A central challenge under intensive investigation is the monolithic integration of on-chip semiconductor optical amplifiers (SOAs) and lasers on scalable, foundry-compatible silicon photonics platforms.

In this talk, I will present our latest progress on the monolithic integration of quantum dot lasers (QDLs) on 300 mm silicon photonics wafers via a heteroepitaxial approach. This material platform is enabled by a combination of fully selective-area heteroepitaxy of low-defect-density gallium arsenide (GaAs) buffers on recessed silicon (Si) trenches—within pre-fabricated silicon photonics wafers—using metalorganic chemical vapor deposition (MOCVD), followed by non-selective QDL epitaxial growth via molecular beam epitaxy (MBE). The MOCVD selective GaAs buffer layer exhibits a total defect density as low as 1.4×10^7 cm^{-2}. A seven-layer QD stack was optimized to enhance QD material gain and optical confinement.

Efficient light coupling from the monolithically integrated QDL into silicon nitride (SiN) waveguides has been demonstrated, achieving a coupling loss of 5.4 dB and a rear-facet output power of 4.7 mW. This state-of-the-art coupling performance, compared to previous all-MBE non-selective epitaxy approaches, is primarily attributed to the reduced facet gap enabled by the MOCVD-grown selective GaAs buffer. The devices operate at temperatures up to 105 °C, with an extrapolated operational lifetime of 6.2 years at 35 °C.

Furthermore, single-mode laser operation was realized by leveraging butt-coupling of the QD gain section into external SiN distributed Bragg reflectors (DBRs) and cascaded Si microrings. The monolithically integrated DBR QD laser exhibited a side-mode suppression ratio (SMSR) of 32 dB at 1299 nm. These promising results are currently being scaled for 300 mm wafer production, including securing a 300 mm MOCVD–MBE growth pathway, with subsequent transfer to AIM Photonics for full 300 mm silicon photonics wafer processing.

The advances presented in this work open new pathways toward truly monolithic silicon photonics with significantly reduced cost, size, weight, and power (C-SWaP).

OPTIMIZATION OF TIMING PARAMETERS OF CE-DOPED GARNETS BY COMPLEX CODOPING

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The study is driven by the demands of next-generation particle physics experiments, particularly the High-Luminosity LHC at CERN [1]. In addition to requiring radiation hardness of up to 1 MGy, scintillation detectors must generate a sufficient number of “prompt” photons to prevent detector pileup during particle collision events occurring every 25 ns. Ce-doped garnets are among the most promising materials for meeting these requirements. Meanwhile, our Czochralski growth process for YAG-based crystals using tungsten (W) crucibles is significantly more cost-efficient than the growth of Ga-containing crystals such as GAGG:Ce, which require expensive iridium (Ir) crucibles. This study focuses on codoping strategies for Ce-doped YAG to reduce scintillation rise and decay times while maintaining high light output. Specifically, codoping with Sc^{3+} and aliovalent cations enhances carrier transport to Ce luminescence centers and influences the thermal ionization of electrons from $Ce^{3+}/^{4+}$ $5d_1$ levels to the conduction band.

The first research direction focuses on dual Ca^{2+}/Mg^{2+}-codoped YAG:Ce, which offers an optimal combination of high light output (exceeding 22,000 ph/MeV) and a decay time of 26–28 ns—nearly twice as fast as the intrinsic Ce^{3+} lifetime in garnets. Another approach involves Sc^{3+}-codoped YAG:Ce, achieving a light output of 14,000–18,000 ph/MeV with a decay time of 21–23 ns. Further acceleration of scintillation decay may be possible through heavy codoping of YAG with Ce and additional dopants, as this reduces carrier path lengths to luminescence centers. However, this remains a technological challenge. Additionally, since YAG has a moderate density of 4.4 g/cm³, which limits its scintillation efficiency, crystals of Y/Gd/Lu-substituted garnet solid solutions were grown, achieving densities of up to 6.44 g/cm³.

Finally, large YAG:Ce,Ca,Mg crystals up to 200 mm in length were successfully grown, and a set of 1×1×100 mm³ fibers was fabricated for testing in SPACAL-W at CERN. Despite some longitudinal variations in dopant concentrations, the homogeneity of scintillation parameters along the crystals was confirmed.

This work was made in the frame of Horizon Europe ERA Widening Project no. 101078960 “TWISMA”.

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STUDY ON THE GROWTH OF NITI USING THE MICRO PULLING DOWN METHOD AND THE DEVELOPMENT OF A FLOATING ZONE FURNACE

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Nickel titanium has an austenite to martensite phase transition and has been studied extensively in the past as a shape memory alloy, but a lot can still be learned from such phase transitions. Crystals of high quality are hardly accessible for intermetallic phases, especially for NiTi. Often, the Bridgman- or Czochralski-method are used. However, these established single crystal growth methods require relatively long process times and thus the variation of parameters is time consuming. We offer the solution to this problem with the micro pulling down (µpd) method. The µpd process is a fast and flexible method for the fabrication of small, in the best case, single crystalline samples. By pulling the melt down through a hole in the crucible bottom, it is possible to reduce oxygen contamination, since oxides float on top of the melt due to their low density. In this work, we show the developed µpd setup together with the optimized fabrication parameters, as well as structural, chemical, morphological and electronic data of the obtained NiTi crystals. The carbon uptake due to the use of a graphite crucible in the µpd-method is analyzed over multiple pulling procedures.

To eliminate any contamination of the melt by the crucible a floating zone (FZ) furnace is being designed and manufactured. The current development state of the FZ system is also presented here. Here we show the chamber design, linear drives, induction heating system, which were all built from scratch, and first overall testing. The combination of both methods should provide a strong basis for synthesizing NiTi and other intermetallic phases.

THE IMPACT OF HYDRODYNAMIC INTERACTIONS ON COLLOIDAL CRYSTAL NUCLEATION

Talid Sinno (University of Pennsylvania), Ying-Shuo Peng (University of Pennsylvania)

Although molecular simulations have been extremely useful for unraveling some of the mechanistic details of colloidal crystal nucleation, a longstanding issue is that simulations consistently under-predict nucleation rates in weakly supersaturated hard-sphere systems, sometimes by orders-of-magnitude [1]. This is true for both direct simulations of crystal nucleation and enhanced sampling approaches [2,3]. Recently, hydrodynamic correlations between particles due to the solvent have drawn attention as a potential explanation for this mystery. Yet, computational studies that include hydrodynamic interactions (HIs) have mostly shown relatively small effects that arise due to the impact of HIs on single particle attachment kinetics on an already-formed critical nucleus [4,5].

Here, we consider the impact of HIs on density fluctuations in a metastable colloidal fluid as a potential explanation for the discrepancy between simulation and experiment. Specifically, we employ the total intermediate scattering function, $F(k,t)$, to study the impact of HIs on density fluctuations. Brownian Dynamics (BD) simulations are used to simulate systems without HIs, while Multiparticle Collision Dynamics (MPCD) [6] simulations are used to capture the effect of HIs. Our results reveal that in MPCD, density fluctuations decay much more slowly than in BD. This observation leads to a key insight: the enhanced lifetime of pre-critical density fluctuations due to HIs may be crucial for forming large nuclei, especially under weak supersaturation conditions. Moreover, we find that the density-field-stabilizing effect from HIs becomes even more pronounced at larger length scales (lower wavevectors), higher volume fractions, and weaker interparticle interactions—all of which are characteristic of the weakly supersaturated hard-sphere regime where simulation-experiment discrepancies are most severe [1]. Finally, we interpret the impact of this effect on nucleation rates using an analytical model.

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COMPUTATIONAL ANALYSIS OF THE EFFECT OF INTERACTION HETEROGENEITY ON COLLOIDAL FLUID-CRYSTAL COEXISTENCE

Talid Sinno (University of Pennsylvania), Po-Ting Wu (University of Pennsylvania), John Crocker (University of Pennsylvania)

Micron-scale colloidal particles with short-ranged attractions, such as spherical colloids functionalized with single-stranded DNA oligomers, have emerged as a powerful platform for studying colloidal self-assembly phenomena with the long-term goal of identifying routes for metamaterial fabrication. Although these systems have been investigated extensively both experimentally and computationally, certain features have generally been ignored to preserve simplicity. One example of an important, yet underappreciated, such feature is interaction heterogeneity (IH), namely variability in the interparticle interaction strengths across a population of colloidal particles. In the case of DNA-functionalized particles, this variability can arise from statistical variability in the DNA strand areal density grafted on particle surfaces during fabrication.

In a previous study, we demonstrated that IH can modulate nucleation and gelation kinetics under non-equilibrium conditions. Here, we investigate in detail the dependence of equilibrium fluid-crystal coexistence on IH using a multicomponent coexistence tracing approach. We first examine the thermodynamic impact of IH by constructing fluid-crystal bulk phase diagrams for systems exhibiting different extents of ‘natural’ IH, i.e., that which is expected to arise naturally from the DNA-grafting process. Overall, we find that the presence of natural IH stabilizes the fluid phase, while the crystal phase tends to be enriched in ‘stronger’ colloids, i.e., those exhibiting larger binding energies. Next, using a highly idealized model of IH in which only two types of particles are present—strong and weak—we further explore the possibility of using intentionally designed IH to modulate nucleation and crystallization of colloids. Our results demonstrate that IH significantly impacts crystallization behavior even under equilibrium conditions and provide a new perspective on tuning IH as a controllable parameter for optimizing colloidal self-assembly.

IN-SITU BORON NITRIDE DIELECTRIC FOR GAN HIGH ELECTRON MOBILITY TRANSISTORS

Michael Snure (Air Force Research Laboratory, Sensors Directorate), Eric Blanton (KBR), Laura Davidson (KBR), Gordon Grzybowski (KBR), Kyle Liddy (Air Force Research Laboratory, Sensors Directorate), Bita Pourbahari (McMaster University, Department of Materials Science and Engineering), Nabil Bassim (McMaster University, Department of Materials Science and Engineering)

Gallium nitride based high electron mobility transistors (HEMTs) have become a leading technology for radio frequency and power conversion devices. However, HEMT performance is limited by surface defects, interface traps, and gate leakage resulting in devices with threshold voltage shifts, current collapse, high off-state current, and low break down voltages. To suppress these effects, dielectric layers including SiN, SiO2, and Al2O3 are implemented. Ex-situ deposition of dielectrics can result in interface traps limiting performance. In-situ deposition of nitride dielectrics, like SiN, can improve interfaces, but since Si is a shallow n-type dopant it has been shown to result in leakage at the surface. As an alternative, BN has shown excellent results as a dielectric, in particular for two-dimensional semiconductors, due to its van der Waals (vdW) bonding, ultra-wide band gap, dielectric and breakdown properties. Due to the vdW bonding of BN atomically smooth and abrupt interface can be achieved. Here we present work on in-situ metal organic chemical vapor deposition (MOCVD) of thin BN layers on GaN and AlGaN/GaN as a potential gate dielectric and passivation layer. To achieve high quality interfaces BN growth temperature and time were optimized. Ultra-thin (~4nm) and smooth (>0.4 nm RMS) sp2 bonded BN was grown in-situ on GaN and AlGaN/GaN structures with no damage to the bulk or surface properties. BN capped AlGaN/GaN two-dimensional electron gas (2DEG) structures achieved mobilities of nearly 2000 cm2/Vs and sheet electron concentrations (ns) of > 1.1 x 1013 cm-2. Compared to uncapped AlGaN/GaN 2DEG structures BN results in an increase in ns due to lowering of the surface barrier height. Using x-ray photoelectron spectroscopy, the valence band minimum and band alignments of GaN and BN were measured with a 2.2 eV conduction band off-set consistent with the measured barrier height for BN/GaN diodes. BN/AlGaN/GaN showed a reduced gate leakage current compared to control samples without in-situ BN. Capacitance voltage characterization showed minimal hysteresis indicating excellent interface quality. This work demonstrates 2D BN as a potential dielectric and passivation layer for AlGaN/GaN HEMTs.

VAN DER WAALS EPITAXY OF GAN FOR TRANSFER OF HIGH ELECTRON MOBILITY TRANSISTORS

Michael Snure (Air Force Research Laboratory, Sensors Directorate), Eric Blanton (KBR), Nicholas Glavin (Air Force Research Laboratory, Materials and Manufacturing Directorate)

Epitaxial growth on van der Waals surfaces (vdW), such as graphene and hBN, offers a unique route to epitaxial lift-off (ELO) of thin film materials and devices. Unlike Si and III-Vs, which have established ELO methods, ELO of GaN layers and devices from the growth substrate is particularly challenging. van der Waals ELO offers great promise but is still in the laboratory stages of development and has yet to demonstrate the scale and yield of other technologies. As the need for efficient power and RF electronics continues to expand transfer and integration of GaN based devices, like high electron mobility transistors (HEMTs), will continue to grow. For GaN, sp2 bonded BN is an ideal vdW buffer due to its atomically flat and smooth surface, high temperature and chemical stability, excellent insulating and dielectric properties, and ability to be grown in the same metal organic chemical vapor deposition reactor (MOCVD) in the same process. Here we will describe vdW epitaxy and lift-off of AlGaN/GaN films and HEMTs with excellent properties. We will show the impact of the epitaxy process, BN template morphology, GaN nucleation and strain have on the ELO. The morphology of the BN template layer will affect adhesion and lift-off, which in extreme cases can result in spontaneous lift-off, while strain leads to bowing of released films impacting cracking and bonding. We will show that with a well-controlled epitaxial process vdW assisted ELO can be a versatile high yield technology that can be used to transfer a full 4” wafer or isolated HEMTs. This ELO process is even suitable for complex high-performance devices like air bridged multi-finger HEMTs. Finally, the impact of this transfer method on GaN HEMT performance will be discussed.

EPITAXIAL SYNTHESIS OF CORRELATED TOPOLOGICAL OXIDE

Ryan (Jeongkeun) Song (Oak Ridge National Laboratory), Ho Nyung Lee (Oak Ridge National Laboratory)

Oxide heterostructure engineering provides a powerful platform for tuning the physical properties of transition metal oxides (TMOs), which host unique quantum states due to strong electron correlations. Among these, 4d niobates (ANbO3, A = Sr & Ca) have attracted significant attention in oxide electronics because of their exceptional optoelectronic properties and high-mobility electrical conductivity. Furthermore, the recent introduction of topology into them has enabled new insights into creating novel topological states. However, despite extensive research, the existence and nature of such topological states in 4d niobate films remain elusive, primarily due to the instability nature of their perovskite phase. In this talk, we will discuss about the growth of perovskite 4d niobates films by controlling kinetic energy during the growth process [1,2]. By tuning the oxygen partial pressure, we demonstrate the ability to control topotactic transitions between the metallic perovskite phase (ANbO3) and its insulating phase (ANbO3.5). Additionally, we will explore the physical properties emerging from topological fermions in these films, [3-5].

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THEORETICAL STUDY ON THE ROLE OF INTERFACIAL DIPOLAR INTERACTIONS IN DIRECTING GROWTH PATHWAYS AND DIMENSIONALITY OF THE CRYSTAL

Duo Song (Pacific Northwest National Laboratory), Lili Liu (Pacific Northwest National Laboratory), Andrew Ritchhart (Pacific Northwest National Laboratory), Maria Sushko (Pacific Northwest National Laboratory)

Precise control over morphology and dimensionality during homogeneous and heterogeneous nucleation is critical for functional materials because atomic arrangement defines their electronic structure and properties. The formation of mineral surfaces during nucleation in solution introduces several interfacial interactions, including the dipolar forces, which can significantly affect growth pathways by altering interactions in the electric double layer. However, the absence of a clear correlation between particle morphology and the polarity of the solvent suggests that the solvent effect is more complicated than a dielectric screening of surface dipoles. The solvent-driven mechanism of morphological control at the nanoscale was investigated in the model metal oxide prone to branching through secondary nucleation. We showed that in aqueous solution branching in ZnO nanocrystals is triggered by dipole accumulation along the slow growth direction. Experimental observation of crystal morphology and DFT calculations performed for a large ZnO cluster in vacuum, water, ethylene glycol (EG), and ethanol demonstrate that solvent interactions with nanoparticle faces can compensate or enhance surface dipole and control crystal dimensionality and hierarchy development. Additionally, the calculated adsorption energies of water, EG, and ethanol molecules on ZnO (0001), $(10\bar{1}0)$, and $(2\bar{1}\bar{1}0)$ surfaces suggest that enthalpic solvation controls the relative growth rates of these faces. These studies reveal the role of interfacial polarization of solvated nanocrystals in morphological control during solution growth.

DEVELOPMENT OF DUAL-MODE HALIDE SCINTILLATOR: 6LISR2I5 AND 6LI-DOPED CS3CU2I5.

Luis Stand (University of Tennessee, Department of Nuclear Engineering, Scintillation Materials Research Center), Ketaki Joshi (University of Tennessee, Department of Nuclear Engineering), Xianfei Wen (University of Tennessee, Department of Nuclear Engineering), Jason Hayward (University of Tennessee, Department of Nuclear Engineering), Charles Melcher, (Scintillation Materials Research Center), Jarek Glodo (Radiation Monitoring Devices, Inc), Edgar van Loef (Radiation Monitoring Devices, Inc), Mariya Zhuravleva (Department of Material Science and Engineering, Scintillation Materials Research Center)

Dual-mode scintillators for nuclear nonproliferation applications must effectively identify and differentiate between gamma and neutron signatures without sacrificing their high sensitivity to X-rays and gamma rays to accurately distiguish between dangerous and non-threatening radioactive sources. In this work, we investigate 6LiSr2I5 and 6Li-doped Cs3Cu2I5 as promising dual-mode scintillators. Their melting points, well below 500°C, allow us to grow high-quality single crystals from the melt via the vertical Bridgman technique. For 6LiSr2I5, we investigated Ce3+ and Eu2+ as luminescence centers, both have excellent properties with light yields between 45,000 and 75,000 photons per MeV and energy resolutions as good as 3.2% at 662 keV. For Cs3Cu2I5, 6Li was added to undoped and Tl-doped Cs3Cu2I5 crystals to enable thermal neutron detection via the 6Li(n, α)t reaction. Under 662 keV gamma-ray excitation, 6Li-Cs3Cu2I5 crystals have absolute light yields of up to 65,900 photons per MeV and energy resolutions as good as 3.5% at 662 keV. When exposed to a moderated 252Cf source, our crystals achieve light yields of up to 167,200 photons per neutron, with a full energy thermal neutron peaking at 3 MeV in gamma equivalent energy. Gamma-neutron pulse shape discrimination studies reveal well-separated gamma and neutron events, resulting in Figure-Of-Merits (FOM) as high as 3.7. Our findings show that 6LiSr2I5 and 6Li-Cs3Cu2I5 scintillator materials are promising prospects for research and development for national security and other applications.

GROWTH OF BULK HEXAGONAL BORON NITRIDE FROM A LITHIUM FLUX

Nathan Stoddard (Lehigh University Dept. of Materials Science and Engineering), Florian Metzger (Lehigh University Dept. of Materials Science and Engineering), Tenzin Sherpa (Lehigh University Dept. of Materials Science and Engineering), Jonathan Valenzuela (Lehigh University Dept. of Materials Science and Engineering), Siddha Pimputkar (Lehigh University Dept. of Materials Science and Engineering)

The hexagonal polymorph of boron nitride (hBN) is a material of great interest for electronic and optoelectronic applications. There is a demand for large area single crystals both as a bulk material and as a source of 2D monolayers for quantum and 2D devices. Recent work has produced mm scale lateral dimensions but thicknesses only in the range of 10’s to low 100’s of micrometers. The temperature (1400-1800 ºC) and/or pressure conditions (2.5-2500 MPa) for crystal growth by existing methods provide significant limitations to upscaling and tend to produce very thin crystals. This study describes the growth of hBN crystals via two routes from a flux of lithium boron nitride in a novel parameter space: around 1200 ºC with 0.1-1.5 MPa of nitrogen overpressure. Analysis of the hBN crystals provide evidence for optical transparency, phase purity, chemical purity narrow Raman peak width, while the aspect ratios of 0.1-0.2 for crystals with lateral widths of 0.5-1.5 mm are promising for the attainment of thicker crystals.

TEMPLATED GRAIN GROWTH OF PMN-PT-PZ CERAMICS: EFFECT OF SINTERING ATMOSPHERE

Gerald Stranford (CTS Corporation), Zhongming Fan (CTS Corporation)

Textured piezoelectric ceramics based on the lead magnesium niobate-lead zirconate-lead titanate (PMN-PT-PZ) system offer superior performance relative to traditional piezoelectric ceramic materials. Manufacturing of textured ceramics involves orienting single crystal platelets within the ceramic powder matrix that act as templates for oriented grain growth during sintering in a process known as templated grain growth (TGG). Alignment of the templates is typically achieved using processes such as tape casting where the flow of the slurry under the doctor blade creates high shear forces that align the platelet shaped templates. Tape cast sheets are laminated together to form cross-sections of the desired thickness. The matrix initially densifies during sintering followed by growth of the matrix around the templates. Matrix material is transported to the template and growing grain through a liquid phase. Therefore, successful texturing requires the presence of a liquid phase during sintering, which is typically provided by the addition of PbO to the ceramic matrix powder and creating a PbO-rich environment around the part.

We observe an inverse relationship between the piezoelectric d33 constant and the thickness of the cross-section. Our investigation shows a significant interaction between the surface of the part and the powder bed and cover wafers used to provide the PbO-rich atmosphere during sintering. These interactions effectively alter the crystalline phase near the surface, reducing the depolarization temperature (Td) and increasing the d33 for a thin layer at the surface of the part. The effect of this thin surface layer decreases as the thickness of the cross-section increases and the higher Td and lower d33 below the thin surface layer dominate the properties.

DRIVING UP THE QUALITY OF MOCVD (OMVPE) – GROWN STRAINED BALANCED QUANTUM CASCADE LASERS (QCLS) EPI-STRUCTURES AT LARGE SCALE PRODUCTION

Wlodek Strupiński (VIGO Photonics S.A.), Maciej Bugajski (Łukasiewicz Institute of Microelectronics and Photonics), Andrzej Kolek (Department of Electronics Fundamentals, Rzeszow University of Technology), Grzegorz Hałdas (Department of Electronics Fundamentals, Rzeszow University of Technology), Kamil Pierściński (Łukasiewicz Institute of Microelectronics and Photonics), Iwona Pasternak (Faculty of Physics, Warsaw University of Technology). Walery Kołkowski (VIGO Photonics), Justyna Kurek (VIGO Photonics), Dawid Dembowski (VIGO Photonics), ddembowski@vigo.com.pl

This paper highlights the complexity of growing high-quality InGaAs/InAlAs strain-balanced quantum cascade lasers (QCLs) using the low-pressure OMVPE (MOVPE) method. QCL epi-growth, in particular, presents significant challenges for OMVPE technology. We address the quality and scaled manufacturing issues and demonstrate the commercial viability of quantum cascade laser heterostructures developed in the production-type MOCVD multi-wafer planetary reactor. Various lasers were designed for emission in the range from 3.8 to 12 µm.

We paid special attention to achieving the abrupt interfaces, optimizing the interruption growth time, and time of exposure of the InAlAs layer to oxygen contamination in the reactor to work out a compromise. Another challenge was controlling the precision level's thickness and composition, enabling device fabrication of the expected wavelength and optical power. Consequently, the growth of quantum cascade laser structures with high crystallographic quality and repeatability resulted in high-performance, high-power continuous-wave operation devices. We introduced innovative solutions to these challenges, resulting in a significant advancement in QCL OMVPE growth technology. This paper describes the case 7.7 µm based on In0.59Ga0.41As/In0.37Al0.63As material system in detail. The active region is built on a diagonal two-phonon resonance design with 40 cascade stages. Strain-balanced material compositions with net strain -0.001% were used to increase the conduction band offset to ~ 770 meV, improving carrier confinement. For epitaxial process control, we used high-resolution X-ray diffraction (HR XRD) and transmission electron microscopy (TEM) to characterize the structural quality of the QCL samples. The grown structures were processed into mesa Fabry-Perot lasers using dry etching RIE ICP processing technology. The basic electro-optical characterization of the lasers was provided. We also presented the results of Green's function modelling of QCLs and demonstrated the capability of the non-equilibrium Green's function (NEGF) approach for sophisticated yet computationally effective simulations of laser characteristics. Simulations revealed the spurious state within the device's active region, which is responsible for generating leakage at the structure output. This knowledge opens the way for further improvement of device design, underlining the significance of our findings.

THE CZOCHRALSKI GROWTH AND SCINTILLATION PROPERTIES OF CE AND MG CO-DOPED Y3(GA,AL)5O12 SINGLE CRYSTALS

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[Introduction] Complex garnet scintillators such as Ce doped (Gd,Y,Lu)3(Ga,Al)5O12 [1] have diverse range of applications such as environmental monitoring, industrial inspection, and medical diagnostics, as well as in high-energy physics experiments. Among them, Gd3Ga3Al2O12 (GAGG) have attractive scintillation properties such as the highest light yield of about 56000 photons/MeV, a fast decay time of around 90 ns.[2] And the development of scintillator-based photon-counting X-ray computed tomography (PCCT) using the garnet scintillators has considerably been focused on in recent years. [3,4] In the case of GAGG, the K-absorption edge of Gd situated ~50 keV makes energy discrimination in this energy region of PCCT difficult. On the other hand, Mg,Ce: Y3(Ga,Al)5O12 (YAGG) grown was reported with a high light yield of ~36000 photons/MeV and fast decay time of ~20 ns. Since YAGG does not contain Gd and its Y K-absorption edge is as low as ~20 keV, it has no adverse effects on PCCT. Alkali earth ions (AE2+) co-doping enhances the light yield and accelerates the decay time [5] and Mg,Ce:YAGG is promising scintillator for PCCT. In this research Mg and Ce co-doped YAGG single crystals were grown by the Cz method with a view to practical application. The dopants and host composition were optimized considering the segregation of each cation and the scintillator properties.

[Results] Single crystals of Mg,Ce:YAGG were grown by the Cz□method with a radio frequency heating system. Typical growth and rotation rates were 1 mm/hr and 10 rpm, respectively. Crystals were grown from a 50 mm diameter Ir crucible under the N2 with 30% CO2 atmosphere. Yellow colored bulk single crystals with 24 mm diameter and 70 mm length were grown. Mg,Ce:YAGG showed a light yield of 50,000 photons/MeV and decay time of ~50 ns. Details of scintillation properties, segregation of the cations, and the effects of gallium oxide evaporation will be discussed in our presentation.

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CRYSTAL GROWTH OF FUNCTIONAL MATERIALS AT THE AIR FORCE MATERIALS AND MANUFACTURING DIRECTORATE

Michael Susner (Materials and Manufacturing Directorate, Air Force Research Laboratory), Pijush Bhattacharya (Materials and Manufacturing Directorate, Air Force Research Laboratory; Core4ce Inc), Benjamin S. Conner (Materials and Manufacturing Directorate, Air Force Research Laboratory; Core4ce Inc), Ryan Siebenaller (Materials and Manufacturing Directorate, Air Force Research Laboratory; Department of Materials Science and Engineering, The Ohio State University), Emanuel Rowe (Materials and Manufacturing Directorate, Air Force Research Laboratory)

The Air Force Crystal Growth Center (AFCGC) at the Materials and Manufacturing Directorate was established in 2020 as a facility where novel single crystalline materials can be synthesized and developed for specific Air Force applications. Since instantiation, we have focused on enhancing three core competencies for the synthesis of novel functional materials: 1) flux growth, 2) vapor transport growth, and 3) Bridgman growth. In this presentation we will cover the breadth of growth capabilities present at AFRL as well as our successes with the growth of materials exhibiting unique optical, ferroelectric, and magnetic properties that have helped pushed the envelope for DoD advancements in a variety of technological areas. These include novel approaches to synthesis and growth of halide perovskite materials, synthesis of kagome magnets for possible spintronic applications, and the novel manipulation of light-matter interactions in van der Waals materials.

HETEROEPITAXY OF NONLINEAR TERNARY MATERIALS FOR FREQUENCY CONVERSION IN THE MLWIR REGION

Vladimir Tassev (Air Force Research Laboratory), Shivashankar Vangala (Air Force Research Laboratory), Michael Snure (Air Force Research Laboratory), Harris Hall (Air Force Research Laboratory), Samuel Linser (KBR), Duane Brinegar (KBR)

High-power, tunable sources in the MLWIR region are in great demand for various applications in defense, security, science, industry, and medicine, such as aircraft protection, remote sensing, airport scanners, breath analysis, ultrafast spectroscopy of chemical reaction dynamics, etc. Since the available direct sources in this range do not satisfy essential requirements, frequency conversion via phase or quasi-phase matching (QPM) in nonlinear optical materials was suggested as a solution. Unfortunately, all materials studied to date have achieved fundamental or technological limits. Such limits include the strong two-photon absorption of GaAs in the 1.0–1.7 μm range, which deteriorates any device performance, or the low quality of the commercial GaP wafers, which leads to the fabrication of low-quality orientation-patterned (OP) GaP templates and, thus, to subsequent poor growth on them. All this led to the search of alternative material solutions. Involving a new material, however, is associated with large investments as facing new limitations is not unusual. Instead, we propose to combine two of the most studied and, so far, most successful QPM materials, GaAs and GaP, expecting in one material to obtain the best of both. Modifying the material properties by changing the chemical composition x = 0.32–0.93 resulted in widening the transmission range of GaAs towards the shorter wavelengths, eliminating the additional absorption band between 2-4 μm in GaP, increasing the hardness, melting point, and, from there, the laser damage threshold, etc. Growth of OP-GaAs substrates were also performed on patterns with domain widths ranging 18–62 μm, facilitated by the decrease of the refractive index (strictly correlated with the nonlinear figure of merit and the domain width). In addition, a significant improvement of layer quality was achieved by growth on simplified OP templates without a second MBE encapsulating layer, where their (periodically) rougher surfaces result in a more uniform layer nucleation. Finally, frequency conversion in the mid infrared was demonstrating by SHG using, for the first time, a pump-source from the telecommunication band generating SH radiation above 5 μm which is the upper limit for all available direct solid-state lasers and also the upper transparency limit for oxide-based birefringent crystals and in ferroelectric periodically poled LiNbO3. The maximum SH power for OP-GaAsP was 56 mW, achieved at conversion efficiency of 19%.

CRYSTAL GROWTH OF PMN-PT BASED SINGLE CRYSTALS

Jian Tian (CTS Corporation), Weiguo Zhang (CTS Corporation), Kyle Grove (CTS Corporation), Tom Vencill (CTS Corporation)

Piezoelectric single crystals PMN-PT and PIN-PMN-PT have excellent dielectric and piezoelectric properties. Both crystals have been widely used in premium medical ultrasound. However, the adoption in other industries has been limited due to concerns regarding certain properties, property variations or higher cost compared to PZT ceramics. To address these challenges and further expand the potential applications of crystals, we have been developing crystal growth techniques to increase crystal growth efficiency and production capacity, as well as to improve crystal property with new crystal compositions to meet diverse application requirements.

Bridgman growth is used to grow PMN-PT and PIN-PMN-PT crystals. With growing demand for single crystals and need for cost reduction, manufacturers have dedicated significant resources to growing crystals of larger diameter and longer length. Over the past 20+ years, crystal boule diameter has increased from 25mm to 100mm, with 125mm crystal growth under development. At the same time, the usable length of crystals has increased from 20mm to 50mm. Advancements in crystal diameter and length significantly boost the efficiency in crystal growth, crystal availability and affordability.

To further extend crystal usable length beyond 50mm, continuous feed (CF) crystal growth is required. Unlike Bridgman growth where all materials are loaded into crucible before growth, CF growth adds materials to crucible gradually during crystal growth. This allows crystals to grow longer with reduced risks from high hydrostatic pressure or prolonged chemical attack from melt. Using CF growth, crystals of 150mm usable length have been grown.

Another notable benefit of CF growth is that crystal compositions and thus properties can be regulated through materials feeding and crystal growth. The compositional segregation is greatly compensated with CF growth, making it practical to grow crystals with severe segregation. Mn doping to PMN-PT or PIN-PMN-PT crystals can significantly increase the mechanical quality factor of crystal, which is an important parameter for high power transducer applications. However, Mn is known to have a large segregation coefficient during crystal growth, leading to significant gradient in Mn and thus properties in a typical Bridgman grown crystal. CF growth helps to achieve a more uniform distribution of Mn in the crystal along growth direction. Results of Mn-doped PIN-PMN-PT crystal will be presented.

SINGLE CRYSTAL GROWTH OF LITAO3 FROM THE MELT WITHOUT PRECIOUS METAL CRUCIBLES

Taketoshi TOMIDA (C & A Corporation), Vladimir Kochurikhin (C&A Corporation), Yuji Ohashi (Tohoku University), Masanori Kitahara (C&A Corporation), Yasuhiro Shoji (C&A Corporation), Hiroki Sato (Tohoku University), Kei Kamada (Tohoku University), Koichi Kakimoto (Tohoku University), Akira Yoshikawa (Tohoku University)

Functional complex oxide single crystals of lithium tantalate (LiTaO3) are mainly produced by the Czochralski (Cz) method using an iridium crucible. In the crystal growth process of materials with high melting temperature, volume change caused by the melting and solidification of raw materials damage expensive iridium crucibles.

Under the background of rising prices in the precious metal market, there is a lot of interest in crystal production methods such as replacing expensive crucibles (Ir to Pt-Rh) and floating zone methods. In Japan, one of the crucible-free crystal growth method, the Oxide Crystal growth from a Cold Crucible (OCCC) method, has been proposed as a crystal growth method without using precious metal crucibles in 2019. Then, crystal growth of LiTaO3, as piezoelectric materials, and β-Ga2O3, as semiconductor material, have been reported.

During crystal growth process by the OCCC method, the electrical resistivity of the molten oxide is very important. Lithium oxides are insulators at room temperature. However, their electrical resistivity decreases at high temperatures, then dramatically changes in the temperature range of solid-liquid transition. Some molten oxide materials can be heated directly with high frequency power in the same way as metallic materials. The electrical resistivity of Gd-Al-Ga garnet and lithium tantalate have also been reported to decrease significantly near the melting point. On the other hand, molten silicon oxide and molten boron oxide are insulating. The nature of the carriers responsible for the conductivity of molten oxides has not been clarified.

This study reports on the cause of crack appearance in LiTaO3 crystal with stoichiometric composition grown by the OCCC method. Compositional variation in grown crystal and the temperature environment of the crystal growth process will be discussed.

EVALUATION OF CRYSTAL PROPERTIES OF Β-GA2O3 CRYSTALS GROWN UNDER AIR ATMOSPHERE USING OXIDE CRYSTAL GROWTH FROM A COLD CRUCIBLE METHOD

Taketoshi Tomida (C&A Corporation), Vladimir Kochurikhin (C&A Corporation), Liudmila Gushchina (C&A Corporation), Masanori Kitahara (C&A Corporation), Yasuhiro Shoji (C&A Corporation), Yongzhao Yao (Mie University), Kei Kamada (Tohoku University), Koichi Kakimoto (Tohoku University), Akira Yoshikawa (Tohoku University)

Beta-gallium oxide (β-Ga2O3) is the only wide band gap material that can be grown from a melt, and it is expected that bulk single crystal growth will be possible, similar to silicon semiconductor material. β-Ga2O3 crystals, ranging from 2 to 6 inches, are produced by the Czochralski (Cz) method or Edge-defined Film-fed Growth (EFG) method using iridium crucibles, and by the Bridgeman method using Pt-Rh crucibles. Recently, crucible-free crystal growth methods such as the floating zone (FZ) method or Oxide Crystal growth from a Cold Crucible (OCCC) method have gained attention due to the rising prices of precious metals.

This study reports on the crystal properties of β-Ga2O3 crystals grown under air atmosphere using the OCCC method, which does not use precious metal crucibles. The OCCC method enables crystal growth under high oxygen partial pressures due to direct induction heating of the oxide melt with low electrical resistivity. In the OCCC method, the area of high-frequency heating around the periphery of the oxide melt is influenced by the height of the heating coil and its position relative to the melt surface. The results of heat and mass transfer calculations of direct induction heating of the gallium oxide melt and the actual crystal growth results are compared. The changes in the temperature field inside the gallium oxide melt due to the coil height and the observed dislocation density of the obtained crystals are discussed.

CRYSTAL GROWTH AND PROPERTIES OF KGD(WO4)2

Joshua Tower (Radiation Monitoring Devices, Inc.), Huicong Hong (Radiation Monitoring Devices, Inc.)

Single crystals of KGd(WO4)2 (KGW) were grown by Top Seeded Solution Growth (TSSG) for laser applications. Crystal growth was done in a Czochralski puller with a platinum crucible. Flux of K2WO4 was used to lower the growth temperature below the structural phase transition that occurs at 1005 degrees Celsius. High purity chemicals of K2CO3, Gd2O3, and WO3 were purchased from Thermo Fisher. Crystals were grown in the [010] direction. Resulting crystals have rectangular growth morphology and cross-sectional size up to 25 by 35 mm. Initial growth runs were made undoped, as the growth conditions were optimized. KGW crystals thus produced are colorless and highly transparent after polishing. Optical transmission spectra of the undoped crystals show a sharp cutoff around 315 nm with no apparent absorption bands up to the limit of the spectrometer at 900 nm. Powder x-ray diffraction confirmed a single phase of crystalline KGW without impurities. No precipitates were observed by optical microscopy or by HeNe laser scattering.

LITHIUM MOLYBDATE PURIFICATION AND CRYSTAL GROWTH FOR SCINTILLATING BOLOMETERS

Joshua Tower (Radiation Monitoring Devices, Inc.), Huicong Hong (Radiation Monitoring Devices, Inc.), Lindley Winslow (Massachusetts Institute of Technology), Michael Squillante (Radiation Monitoring Devices, Inc.)

The Majorana nature of neutrinos is one of the most important questions being pursued in physics today. This has given the search for neutrinoless double beta decay (0νββ) a high priority among proposed nuclear physics experiments. Recent advances in cryogenic bolometer technology have significantly improved detector sensitivity and background rejection. The research reported here investigates the synthesis, purification, and crystal growth of lithium molybdate, and the testing of these crystals as scintillating bolometers at cryogenic temperatures.

Single-crystals of lithium molybdate (Li2MoO4 or LMO) were grown by Czochralski in sizes up to 65 mm diameter. The crystal compounds were synthesized in a separate step prior to crystal growth. Transparent colorless crystals were produced when materials of suitable purity were used. Crystal purity is crucial for the scintillation light output, as well as the low radioactivity background required for the rare event detection. Purification of MoO3 was done in a two-step process of sublimation followed by wet chemistry co-precipitation. Wet chemistry was also used to recover molybdenum isotopes from the LMO scraps after crystal cutting.

Scintillating bolometer data were measured from LMO crystals at around 20 mK at the Canfranc underground laboratory in Spain. Strong scintillation light output was found at low-temperature, enabling good discrimination between alpha and beta/gamma emissions in light-vs-heat analysis. This particle discrimination capability is crucial for background reduction in 0νββ research. Radioactive contaminations were also determined through the heat spectra.

This work has been supported by the US Department of Energy SBIR grant No. DE-SC0023588.

ANALYSYS OF EFFECTS OF STACKING FAULTS AND FORMATION MECHANISM OF BASAL PLANE DISLOCATIONS IN 4H-SIC

Hidekazu Tsuchida (Central Research Institute of Electric Power Industry (CRIEPI)), Satoshi Asada (Central Research Institute of Electric Power Industry (CRIEPI)), Fumihiro Fujie (Central Research Institute of Electric Power Industry (CRIEPI))

This paper overviews the defect formation in 4H-SiC wafers and discusses the effects of stacking faults (SFs) in epilayers on device performance, as well as the formation mechanism of basal plane dislocations (BPDs) during epitaxial growth.

To investigate the effects of various types of SFs on current conduction, φ100 μm Schottky barrier diodes (SBDs) containing a SF with a covering ratio of unity were fabricated on ~30 μm-thick 4H-SiC epilayers. The type of SF in the SBDs was identified based on the photoluminescence (PL) spectrum. The electrical measurements confirmed that the conductance of the SBDs declines with increasing SF-originated PL peak wavelength, in the order of 420 nm ((31) SF), 460 nm ((42) SF), 490 nm ((50) SF), and 513 nm ((62) SF) [1]. Our simulation analysis showed that the potential barrier created by the SF-induced quantum well (QW) becomes higher and fewer electrons surpass the potential barrier in the order of (31), (42), (50), and (62) SFs [2]. Accordingly, the experimental results showing smaller conductance in the SBDs covered by the SF with the longer SF-originated PL peak are attributed to a higher potential barrier formed by the SF creating a deeper QW.

The formation of BPDs in the 4H-SiC wafers with epilayer thickness of 10-100 μm was investigated using X-ray topography [3]. It was confirmed that BPD half-loops generated near the triangular 3C-SiC defects and from the wafer edge, extending to several mm in width for the wafers with an epilayer thickness of 50 μm and above. Analyzing the topography contrast, Type-A BPDs having a dislocation segment with an extra half-plane above the core were found to extend into the substrate side, while Type-B BPDs with the opposite sign were present in the epilayer and formed interfacial dislocations. The stress acting on the wafer at the growth temperature was examined using finite element method, considering the differences in lattice constants and coefficients of thermal expansion of the n+ substrate, n− epilayer, and 3C-SiC. Based on the results, the driving force for the formation of Type-A BPDs is attributed to misfit induced tensile stress in the substrate and local tensile stress around 3C-SiC defects, while the formation of Type-B BPDs is attributed to misfit induced compressive stress in the epilayer.

[1] S. Asada et al., Appl. Phys. Express 15, 045502, 2022, [2] S. Asada et al., IEEE Trans. Electron Devices 70, 1757, 2023, [3] F. Fujie et al., J. Appl. Phys. 135, 235706, 2024.

COMPUTATIONAL AND THEORETICAL INVESTIGATIONS INTO THE ORIGIN OF ULTRA WIDE-BAND GAP IN ETCHED SILICON NANOWIRES

Moneesh Upmanyu ()

Silicon nanowires (SiNWs) remain promising candidates for confinement-induced engineering for silicon optoelectronics as the 2D confinement in these 1D nanostructures can drive transitions from indirect to a direct bandgap. Recent catalyst-free chemical vapor etching routes have shown the feasibility of sub-5 nm SiNWs with a direct bandgap of 4.75\,eV. The electronic response is consistent with an ultrawide bandgap (UWBG) semiconductor, a first in the world of silicon, and is the response is attributed to the large residual strains within the nanowires. Here, a combination of classical atomic-scale simulations and continuum analyses are used to study the interplay between bulk and surface mechanics and surface chemistry that stabilizes the large lattice compression of the diamond cubic lattice within the etched nanowires. We find that stabilization of large hydrostatic strains entail stresses at the silicon-oxide interfaces at the nanowire surfaces, implicating the surface constructions and silicon-rich oxide chemistry. The understanding offers modified etching pathways for scalable synthesis of ultrawide bandgap silicon nanostructures.

CRYSTAL GROWTH AND SCALE-UP OF TLCABR3 FOR HIGH-ENERGY X-RAY RADIOGRAPHY APPLICATIONS

Edgar van Loef (Radiation Monitoring Devices, Inc.), Myles Inniss (Radiation Monitoring Devices, Inc.), Mariya Zhuravleva (Scintillation Materials Research Center, University of Tennessee), Kimberly Pestovich (Materials Science and Engineering, University of Tennessee), Luis Stand (Scintillation Materials Research Center, University of Tennessee), Jaroslaw Glodo (Radiation Monitoring Devices, Inc.), Chuck Melcher (Materials Science and Engineering, University of Tennessee), Lakshmi Soundara-Pandian (Radiation Monitoring Devices, Inc.)

Crystals of TlCaBr3 of up to 38 mm diameter and 100 mm long were grown by the Vertical Bridgman technique. TlCaBr3 has orthorhombic crystal structure with space group Cmcm (63). Its density and Zeff are 4.69 g/cm3 and 65, respectively. The radioluminescence spectrum of TlCaBr3 features a broad emission band peaking at 470 nm with a corresponding light yield of about 42,000 ph/MeV.

To perform X-Ray Radiography, one or more TlCaBr3 crystals were cut into 4.5 x 4.5 x 26.8 mm pixels and assembled into an array. Measurements performed with this array show promising results.

CRYSTAL GROWTH AND CHARACTERIZATION OF THALLIUM-BASED PEROVSKITE SEMICONDUCTORS

Edgar van Loef (Radiation Monitoring Devices, Inc.), Myles Inniss (Radiation Monitoring Devices, Inc.), Mariya Zhuravleva (Scintillation Materials Research Center, University of Tennessee), Kimberly Pestovich (Scintillation Materials Research Center, University of Tennessee), Luis Stand (Scintillation Materials Research Center, University of Tennessee), Jaroslaw Glodo (Radiation Monitoring Devices, Inc.), Chuck Melcher (Materials Science and Engineering, University of Tennessee), Lakshmi (Soundara-Pandian, Radiation Monitoring Devices, Inc.)

Perovskite single crystal halide semiconductors are a versatile group of materials with a unique set of properties that cause these materials to be of great interest for advanced applications in optoelectronics and radiation detection. They offer several advantages over traditional semiconductors like silicon and germanium, such as having a relatively low melting point, allowing for Bridgman and Czochralski crystal growth, can be operated at room temperature, have tunable bandgap properties, and typically have high density and effective atomic number allowing for efficient radiation detection.

For example, the recently developed Perovskite semiconductor CsPbBr3 has a reasonably high density of 4.85 g/cm3, exhibits excellent charge transport properties, shows good defect tolerance, and can be grown as bulk crystal and thin film at temperatures below 600°C.

In this paper we present a new family of Perovskite halide semiconductors based on the thallium cation. This family of materials combine the structural versatility of Perovskites with the high atomic number and exceptional charge transport characteristics of thallium. Our research shows that these materials can be grown by the Bridgman technique, have high density and effective Z, and show interesting optoelectronic properties.

GROWTH OF TERNARY SULFIDES BY MIRCO-PULLING-DOWN METHOD

Vojtěch Vaněček (FZU - Institute of Physics of the Czech Academy of Sciences), Robert Král (FZU - Institute of Physics of the Czech Academy of Sciences), Vítězslav Jarý (FZU - Institute of Physics of the Czech Academy of Sciences), Lubomír Havlák (FZU - Institute of Physics of the Czech Academy of Sciences), Romana Kučerková (FZU - Institute of Physics of the Czech Academy of Sciences), Vladimir Babin (FZU - Institute of Physics of the Czech Academy of Sciences)

Luminescence properties of sulfide-based materials were extensively investigated toward the end of the twentieth century, establishing their utility across various applications including electroluminescent phosphors, color-conversion phosphors, and persistent luminescent materials1. However, prior research primarily focused on powdered sulfide materials due to significant technical challenges associated with bulk crystal growth. Technologically, sulfides exhibit the unfavorable characteristics of both halides and oxides. Similar to halides, many sulfides are unstable in air—particularly at elevated temperatures—requiring crystal growth under inert or sulphidizing atmosphere. Like oxides, sulfides generally possess high melting points; however, their chemical reactivity with refractory metals complicates the selection of suitable crucible materials. Despite these challenges, sulfides offer several compelling properties, including comparatively narrower band gaps than oxides, high refractive indices, low phonon energies, and pronounced covalent bonding. These attributes make sulfide crystals promising candidates for applications in ionizing radiation detection, active media for solid-state infrared lasers, and near infrared luminophores. Motivated by these opportunities, we adapted our micro-pulling-down (μ-PD) apparatus, originally designed for halide crystal growth, to accommodate high-temperature sulfide crystal growth. Using this setup, we successfully grew Lu_2S_3 crystals as a model system of high-melting sulfide (~ 1750 °C)2. However, degradation of graphite crucible at high temperatures resulted in suboptimal crystal quality. To address this limitation, we extended our study to alkaline earth thiogallates, which melt at lower temperatures (~1200 °C) and are compatible with graphite crucibles. Additionally, we explored the use of glassy carbon crucibles for crystal growth of higher-melting (> 1700 °C) thiogallate analogues, wherein gallium is substituted by lanthanides, demonstrating the adaptability and potential of our approach.

1. Smet, P. F., Moreels, I., Hens, Z. & Poelman, D. Luminescence in sulfides: a rich history and a bright future. Materials 3, 2834–2883 (2010).
2. Vaněček, V. et al. Growth and Spectroscopic Properties of Pr3+ Doped Lu2S3 Single Crystals. Crystal Growth & Design 24, 4736–4742 (2024).

NONCLASSICAL MECHANISMS TO INHIBIT BETA-HEMATIN CRYSTALLIZATION INFORM STRATEGIES TO SUPPRESS BLOOD-STAGE MALARIA PARASITES

Peter Vekilov (University of Houston), Huan-Jui Lee (University of Houston), Hamidreza Azargoshasb (University of Houston), David Sullivan (Johns Hopkins University)

Malaria remains a significant public health challenge in equatorial regions of the world largely owing to the parasite's emerging resistance to the recently introduced drugs of the artemisinin (ART) family. In the human body most ART-derivative drugs are metabolized to dihydroartemisinin (DHA), which, in the parasite residing in the red blood cells is activated by heme to form an adduct with hematin (H-DHA). In search of strategies to circumvent malaria parasites drug resistance, we explore the mechanism employed by H-DHA to inhibit the synthesis of hemozoin crystals, the main constituent of the heme detoxification pathway of the parasites. We also examine how tafenoquine (TQ), an antimalarial introduced in 2018, interacts with hemozoin formation. We show that both H-DHA and TQ block a fraction of the crystal growth sites, the kinks, and mildly inhibit the classical growth mode of □-hematin, the synthetic analogue of hemozoin, by generation and spreading of layers. H-DHA and TQ exert opposing effects on the nucleation of hematin crystals: H-DHA strongly enhances crystal nucleation, whereas TQ potently suppresses it. The two drugs accomplish their nucleation control missions by enhancing or impeding the formation of mesoscopic hematin-rich clusters, the precursors of hematin crystal nucleation. The diverging effects on crystal nucleation and the nucleation precursors trigger in two distinct nonclassical pathways to suppress hematin crystal growth that transform H-DHA and TQ into potent hematin growth inhibitors. With H-DHA we find that hematin crystallites, whose nucleation is promoted by H-DHA, incorporate into large hematin crystals and suppress their growth, likely by straining the crystal lattice. Importantly, the induced growth suppression is irreversible and persists even in the absence of H-DHA. TQ suppresses a nonclassical growth mode, which activates at elevated hematin concentrations, by impeding the formation of the hematin-rich clusters, the shared precursors of both crystal nucleation and nonclassical growth. Measurements of TQ parasite killing potency reveal that, consistently with the mechanistic insights, this drug exerts a stage-specific inhibitory effect and suppresses both ring stage parasites, when hemozoin crystals nucleate, and trophozoites, when the crystals grow. This dual-action mechanism highlights TQ’s ability to disrupt parasite survival at multiple points during the blood stage of infection.

TAILORING PIEZOELECTRICITY AND DIELECTRIC RESPONSE OF TEXTURED PBTIO3-BASED CERAMICS FOR SENSORS

Beecher Watson (Pennsylvania State University), Casey Zhang (Pennsylvania State University), Susan Trolier-McKinstry (Pennsylvania State University), Scott J. Brumbaugh (Pennsylvania State University), Richard J. Meyer Jr. (Pennsylvania State University), Mark A. Fanton (Pennsylvania State University)

Piezoelectric sensors require materials that leverage high piezoelectric charge coefficients (dij) and sufficiently large dielectric permittivity (εij) to generate voltage in response to applied stress. In this work, we select a modified-lead titanate composition as a model system for exploring the key factors controlling densification, epitaxial growth, and subsequent templated-grain growth processes. The impacts of matrix powder characteristics on the epitaxial development process are also explored such as perovskite A-site chemistry and powder crystallinity. Template particle chemistries are discussed as they relate to the piezoelectric, ferroelectric, and dielectric properties derived from final material solid solutions and symmetry. IEEE properties for textured Mn-doped PbTiO3 ceramics are reported demonstrating high piezoelectric g33 coefficients over 0.100 Vm/N. Rayleigh analysis demonstrates that the piezoelectric response is dominated by intrinsic contributions as a result of the high stability and low mobility of domain walls in a crystallographically textured tetragonal material system.

PROBING VACANCY TYPE DEFECTS WITH POSITRON ANNIHILATION SPECTROSCOPY IN THIN FILMS AND SINGLE CRYSTALS

Marc Weber (Washington State University), John S. McCloy (Washington State University)

Single crystals and thin epitaxial single crystal films are used in a wide range of applications including semiconductors, scintillators, solar cells and more.

In many cases Additional layers are deposited on a substrate. The substrate surface preparation and the quality of the grown layers are influenced by point defects like vacancies.

Positrons, the antiparticle to electrons, are uniquely suited to detect vacancies and vacancy-impurity complexes.

Future new materials are expected to withstand harsh environments such as radiation by swift ions, neutrons and cosmic rays. Again, vacancies form a significant component of the generated damage.

With the use of a variable energy beam of positrons depth profiles of vacancies can be measured and correlated with crystal growth and surface preparation conditions.

In this presentation the strengths and weaknesses of the technique will be explored based on examples from recent work on gallium oxide single crystals.

The evolution of near surface damage due to cutting and intermediate polishing steps as well as chemical surface preparation will be demonstrated for the example case of CdZnTe single crystals.

USE OF OXIDE DISPERSION STABILIZED PLATINUM CRUCIBLES FOR HIGH TEMPERATURE CRYSTAL GROWTH APPLICATIONS

Matthias Wegner (Heraeus Precious Metals), Luca Krohn (Heraeus Precious Metals)

Utilization of Platinum DPH-Strong crucibles in the crystal growth of high melting point materials, such as lithium tantalate, represents a significant advancement in materials science. Platinum, with a melting point only slightly higher than lithium tantalate, offers unique advantages in the crystal growth process. Our experiments have demonstrated that Pt DPH-Strong materials enable successful melting and growth of lithium tantalate crystals, highlighting their robustness and versatility.

A remarkable feature of Platinum DPH-Strong crucibles is their ability to be repaired multiple times via cold working after heavy usage and consequent warpage/deformation, ensuring long-term usability and cost-effectiveness. The ability to repair and reuse these crucibles without compromising structural integrity or performance is a significant benefit, reducing overall cost of crystal growth operations.

Furthermore, our studies confirm that no measurable platinum contamination occurs in the crystal melt, maintaining the purity and integrity of the grown crystals. This is critical for ensuring high quality of the final product, as contamination could adversely affect the crystal's properties, underscoring the suitability of Platinum DPH-Strong crucibles for applications where material purity is paramount.

Platinum crucibles offer a significant commercial advantage over traditionally used iridium crucibles. The cost of platinum is considerably lower than iridium, making it a more economical choice for large-scale crystal growth operations. This cost advantage is particularly important in industries requiring large quantities of high-purity crystals, such as electronic component production.

Additionally, the quality of the crystals can be enhanced using platinum crucibles, as they allow for melting in an oxidizing atmosphere. This prevents potential oxygen deficits that can arise with iridium crucibles, which require a reducing or inert atmosphere. An oxidizing environment is beneficial for maintaining the stoichiometry of the crystal, thus reducing defect densities in the grown crystals and ensuring the highest quality and property requirements.

The combination of cost-effectiveness, high material purity, and enhanced crystal quality positions Platinum DPH-Strong crucibles as a serious alternative to traditional iridium crucibles, driving innovation and efficiency in crystal growth processes.

2D AND 3D IN-SITU X-RAY VISUAIZATION OF THE PHYSICAL VAPOR TRANSPORT GROWTH PROCESS OF SILICON CARBIDE

Peter Wellmann (Crystal Growth Lab, MAterials Department 6, UNiversity of Erlangen-Nürnberg (FAU)),
Sven Strüber (FAU), Michael Salamon (EZRT), EZRT ()

Silicon carbide (SiC) is an example of a new semiconductor material used in power electronics where the growth process must be precisely controlled to achieve high crystalline quality. The state-of-the-art physical vapor transport method, performed at over 2000°C, uses a closed graphite crucible, which does not allow visual control as in the Czochralski melt growth process used for silicon. Normally, the crystal grower is limited to measuring the temperature at the top and bottom of the growth cell, which can be related to the applied heating power. By applying computer simulation of the temperature field (and optionally mass transport), a model of the growth conditions inside the cell is obtained and an estimate of the expected crystal evolution with growth time is possible. The 2D and 3D in-situ X-ray visualization developed in the authors' laboratory provides an extraordinary direct and quite detailed observation of the evolving SiC crystal and its consumption during the growth process.

In the case of 2D in-situ X-ray visualization, the monitored evolution of the SiC growth interface is linked to the thermal boundary conditions as well as to the morphological changes of the SiC source material. The experimental results allow the optimization of the hot zone design to improve the shape of the growth interface and, in addition, to evaluate whether the SiC source material used provides favorable boundary conditions for the growth process. Despite such fundamental issues, the 2D system can be used as a routine process monitoring tool to further improve the SiC PVT process yield.

The more advanced 3D in-situ X-ray visualization provides a more sophisticated view of the growth interface and allows, for example, precise monitoring of the occurrence and local movement of growth facets. For example, a deviation from a smooth, slightly convex growth interface can be related to a growth kinetic distortion such as the occurrence of unwanted polytype switching. Even initial nucleation of different local growth islands can be observed, which help to improve the seeding process by implementing adapted growth steps.

The aim of this presentation is to introduce the technical aspect of the 2D and 3D X-ray visualization tool and to point out different analysis methods that allow a deeper understanding of the SiC-PVT growth process.

Acknowledgements: This work was supported by the German Science Foundation (DFG) under contract number WE2107-12-2.

CLOSE SPACE PHYSICAL VAPOR TRANSPORT GROWTH OF INTRINSIC AND DOPED SIC LAYERS AND THIN CRYSTALS FOR PHOTONIC APPLICATIONS

Peter Wellmann (Crystal Growth Lab, Materials Department 6, University of Erlangen-Nürnberg (FAU), Germany), Sven Strüber (Crystal Growth Lab, Materials Department 6, University of Erlangen-Nürnberg (FAU), Germany), Cristina Grazzi (Crystal Growth Lab, Materials Department 6, University of Erlangen-Nürnberg (FAU), Germany)

Photonic applications of silicon carbide (SiC) include yellow phosphors, photocatalytic water splitting, intermediate band solar cells, waveguides, quantum information, and most recently, laser power converters. Close Space Physical Vapor Transport (CS-PVT) offers a variety of growth process features that are advantageous over standard PVT used for commercial fabrication of n-type doped 4H-SiC wafers for power electronics. Photonic applications often require very pure SiC materials or p-type doped or n/p-type co-doped crystals. In addition, the electronic band gap plays an important role for light absorption and emission, which requires the growth of high quality 3C-SiC and 6H-SiC in addition to the standard PVT 4H-SiC.

Historically, the CS-PVT growth method was a predecessor of the standard PVT method. While standard PVT is well suited for growing bulk crystals with a thickness of about 30 - 50 mm, CS-PVT focuses on much thinner SiC crystals (typical values 100 µm -1 mm, maximum thickness 5 - 10 mm, typical values 100) and allows a much more defined setting of growth process parameters such as supersaturation. In terms of growth rate, CS-PVT and standard PVT behave similarly: 25 - 200 µm/h (CS-PVT) and 100 – 300 µm (standard PVT).

One characteristic of the CS-PVT growth process is the possibility to precisely tailor the axial temperature gradient inside the growth cell and to reduce the radial temperature to basically negligible values. This way, SiC materials of various polytypes (3C-SiC, 4H-SiC, 6H-SiC and even 15R-SiC) can be grown with very low defect density. Additionally, the intrinsic point defect density (like carbon vacancies) can be tailored in CS-PVT.

Another characteristic is the possibility to switch from a diffusion/kinetically limited vapor growth mode (typical for standard PVT) to ballistic mass transport. The latter is of great importance to intentionally dope SiC with various dopants (like aluminum) which cause problems in standard PVT.

The presentation focusses on two issues. (i) The physical background of the CS-PVT method will be introduced with many details. As an application example, new results on the fabrication of 4H-SiC and 3C-SiC p-i-n layer stacks for laser power converters will be presented

Acknowledgements: This work was supported by the German Science Foundation (DFG) under contract number WE2107-15-2 and by the European Union under the Europe Horizon contract number 101160868 (RePowerSiC_Space).

HISTORY OF LARGE KDP AND KD*P TO SUPPORT FUSION LASERS

Matthew Whittaker (G&H Ohio)

The demands of larger laser systems required co-development of larger crystalline optics for Q-Switching and Frequency Conversion. The author will review the 50 year development of the largest KDP and KD*P crystals that were required to support these ever increasing laser sizes. Provide an overview of differences between rapid and conventional growth techniques and discuss current record crystal sizes.

CRYSTALLIZATION IN A MICROGRAVITY ENVIRONMENT

Anne Wilson (Buter University), Ken Savin (Redwire), Molly Mulligan (Redwire), Stephen Tuma (Redwire), Lillian Miller (Butler University)

Crystalline materials are present in dozens of everyday items like personal care items, medicines, electronics, buildings, and housewares. Improvements to crystal forms can lead to better absorption of medicines, reduced waste, more durable coatings, and faster electronics. Microgravity can be an excellent tool for the fabrication of improved crystal forms from semiconductors to proteins.

A review of the literature demonstrates that crystals grown in microgravity are larger, more uniform, structurally better, and have improved characteristics compared to their Earth-grown counterparts. In addition, this improvement is seen across material types (small molecules, large protein aggregates, metals, insulators, etc.). Given the breadth of examples, crystallization in a microgravity environment is likely to provide improvements to other materials as well.

We have recently partnered with Redwire to explore small molecule crystallization in microgravity aboard the International Space Station. The “small” molecules range from amino acids to macrolactone antibiotics and were selected for their broad-ranging applications to biochemistry and human health. Results from these studies will be shared.

MICROGRAVITY AS A TOOL FOR BETTER CRYSTALS

Anne Wilson (Butler University), Ken Savin (Redwire), Molly Mulligan (Redwire), Stephen Tuma (Redwire), Lillian Miller (Butler University)

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We have recently partnered with Redwire to explore small molecule crystallization in microgravity aboard the International Space Station. The “small” molecules range from amino acids to macrolactone antibiotics and were selected for their broad-ranging applications to biochemistry and human health. Results from these studies will be shared.

QUANTIFYING THE MICROSCOPIC DEGREES OF FREEDOM OF GRAIN BOUNDARIES

Ian Winter (Sandia National Laboratories)

For fixed macroscopic degrees of freedom of a grain boundary, there exists a large multiplicity of states characterized by different relative grain translations. More recently, another degree of freedom, the number of atoms at a grain boundary, has emerged as an equally important component as the relative grain translation to describe grain boundary structural multiplicity. We introduce a generalized grain boundary translation vector that can act as an effective descriptor of grain boundary structure and show that this vector provides a link between the previous disparate microscopic degrees of freedom of grain boundaries. We further show how the microscopic degrees of freedom of a grain boundary can be used to quantify structural transformations. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525 (SAND2022-1056 A). This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

THE ROLE OF ULTRATHIN TRANSITION METAL OXIDES IN ADVANCED FREESTANDING MEMBRANE

Katja Isabelle Wurster (Department of Energy Conversion and Storage, Technical University of Denmark)

Complex oxides exhibit a diverse array of intriguing properties, including ferroelectricity, piezoelectricity, and pyroelectricity, which continue to draw significant interest. To unlock and expand their range of functionalities, various strategies have been utilized to alter lattice symmetry. In this presentation, I will demonstrate how the deliberate manipulation of symmetry can unlock extraordinary possibilities. I will demonstrate innovative techniques that have enabled the production of ultrathin, freestanding oxide films approaching the two-dimensional limit. These advancements open new opportunities to explore the rich and novel functionalities of complex oxides and their interfaces. Additionally, I will present our latest results on the impact of stacking and twisting freestanding oxide membranes, including the fundamental principles behind these effects.

SINGLE CRYSTAL GROWTH OF FUNCTIONAL OXIDE CRYSTALS FROM THE MELT WITHOUT USING PRECIOUS METAL CRUCIBLE

Akira Yoshikawa (Tohoku University), Taketoshi Tomida (), Vladimir V. Kochurikhin (, Gushchina Liudmila (), Masanori Kitahara (), Yasuhiro Shoji (C&A Corporation, FOX Corporation), Kei Kamada (New Industry Creation Hatchery Center, Tohoku University, C&A Corporation, FOX Corporation), Rikito Murakami (Institute for Materials Research, Tohoku University, C&A Corporation), Takahiko Horiai (New Industry Creation Hatchery Center, Tohoku University, C&A Corporation), Yuji Ohashi (New Industry Creation Hatchery Center, Tohoku University), Hiroki Sato (New Industry Creation Hatchery Center, Tohoku University), Martin Nikl (Institute of Physics of the Czech Academy of Sciences), Koichi Kakimoto (Institute for Materials Research, Tohoku University)

Many of the functional oxide single crystals have been produced by the Czochralski method using expensive iridium crucibles. Iridium has been preferred over other crucible candidates such as Pt, Pt-Rh, W, and Mo because of its high melting point, which is far above 2000°C, as well as its ability to allow oxygen partial pressures of up to 2% and its ability to be recast.
However, with the recent rapid rise in the precious metal market, Mo and W are being reconsidered as alternatives to expensive precious metal crucibles, and precious metal crucible-free crystal growth methods are attracting attention. We are aiming to establish a precious metal crucible-free single crystal growth method by the Oxide Crystal growth from the Cold Crucible (OCCC) method, which is a melt growth method using a water-cooled copper crucible.
Sesquioxides such as zirconium oxide, gallium oxide, and lithium oxide are insulators at room temperature, but their electrical resistivity decreases at high temperatures, with a steep decrease in electrical resistivity above the melting point. The electrical resistivity of gallium oxide and composite oxides such as Gd-Al-Ga garnet and lithium tantalate, a composite oxide containing lithium oxide, also decreases significantly near the melting point. This feature makes direct heating of these oxide melts possible, but since their resistivity is higher than that of precious metals, high frequencies of several hundred kHz or higher are required. On the other hand, silicon oxide and boron oxide melts are insulating.
In this paper, single crystal growth of Ce:Gd3(Al,Ga)5O12, Ce:(La,Gd)2Si2O7, LiTaO3, and β-Ga2O3 by the OCCC method is reported and the difficulty of applying the OCCC method is discussed based on parameters such as melt electrical resistance. and other parameters such as the electrical resistivity of the melt.

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DEVELOPMENT OF FUNCTIONAL MATERIALS BASED ON EUTECTIC AND OTHER PHASE SEPARATION

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Eutectic eutectic crystals fabricated by unidirectional solidification are introduced for application as functional materials. Two types of scintillator applications are shown. (1) composite materials used in neutron scintillators: eutectic materials consisting of crystals with large neutron cross sections and efficient scintillator crystals (which do not require regular microstructures) and (2) high spatial resolution scintillators: regular rod/fiber structures in one phase immersed in a matrix of a second phase eutectic (one of which is a high-efficiency scintillator). In the latter case, the optical waveguide can be installed in either phase (cladding or core).

LiF/LiYF4 and LiF/CaF2:Eu eutectic crystals containing Li are suitable for (1) neutron scintillators, and CsI/NaCl and GdAlO3/α-Al2O3, which are eutectics with ordered rod/fiber structures, are suitable for (2) high spatial resolution scintillators. However, the in-plane temperature distribution at the solid-liquid interface must be homogeneous to a fairly high degree of accuracy in order to fabricate the eutectic of (2). Therefore, we have also developed an optical-guiding crystal scintillator plate, which consists of a core and a cladding similar to an optical fiber, where the core is a halide scintillator with high emission and the cladding is glass with a high refractive index difference, and the optical waveguiding scintillator fiber is made by reducing the diameter and bundling them together. We are also developing optical-guiding crystal scintillator plates made by bundling thin optical guiding scintillator fibers with a high refractive index difference in the cladding.

Possibilities for other functional eutectic crystals will also be presented.

ADVANCES IN CSP GROWTH AND CHARACTERIZATION RELATED TO GENERATION OF MID-IR LIGHT

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CdSiP2 (CSP) is a nonlinear optical chalcopyrite semiconductor developed as a wider-band-gap analog of ZnGeP2 (ZGP) enabling mid-infrared generation with widely-available 1- and 1.55-micron pump laser sources. CSP has a higher nonlinear coefficient (d36=84.5 pm/V) than ZGP (d36=79 pm/V), and its lower thermal conductivity (13.6 W/mK vs 35 W/mK for ZGP) is more than offset by nearly 10-fold lower absorption losses in the 1.06- to 2.1-micron wavelength range, thus, making CSP an attractive alternative to ZGP even for 2-micron-pumped OPOs.

CSP growth presents significant crystal growth challenges compared to ZGP, including twinning, cracking, and inclusions. Recent advances in crystal growth from stoichiometric melts using the horizontal gradient freeze (HGF) technique have resulted in the fabrication of phase match oriented parts with interaction lengths as long as 23 mm.

CSP crystals of different lengths and cut from different bulk grown boules were compared using a Q-switched Tm:YAP pump laser operating at 1.94 microns. Comparison of the performances (slope efficiency, threshold, etc) of different CSP crystals in an OPO configuration is presented.

Thermal lensing caused by optical absorption of the pump (which is lower than that of ZGP but still present at 1.94 microns for CSP) can be a concern in OPO design. Consequently, a comparison of thermal lensing behavior of several CSP crystals pumped at 1.94 microns is presented.

A MONTE CARLO STUDY OF THE EFFECT OF BUBBLES ON VOID SWELLING IN MATERIALS AGING

Luis Zepeda-Ruiz (Lawrence Livermore National Laboratory)

With the overall goal of predicting void swelling up to centuries of evolution, we have developed a first-passage kinetic Monte-Carlo approach for materials aging to investigate the sensitivity of void swelling to model parameters, including helium bubble density and size distribution. The results presented here consider the spatial distribution of individual point defects, bubbles, and voids, as well as differences in effective interaction radii and diffusion activation energies between vacancies and interstitials. Particular attention is paid to interaction (or lack of) between vacancy bubbles that seems to provide a more detailed information than previous rate-equation based approaches. Our results indicate that spatial effects that are not modeled in mean-field rate theories could play a significant role in bubble growth and void swelling for certain regimes of model parameters

OBSERVATION AND ANALYSIS OF THE “GALAXY” DEFECT IN 4H-SIC WAFER THROUGH X-RAY SYNCHROTRON TOPOGRAPHY

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Silicon Carbide has gained great interest for its high thermal conductivity, high saturation velocity, and high breakdown voltage and, therefore, its suitability to fabricate high-frequency, high-power electronic devices [1, 2]. It has been applied in various fields, including transportation and communication. However, the longevity and performance of SiC devices are hindered by defects within the substrate and epitaxial material. The observation of defects and understanding of their formation mechanism is critical for the improvement of crystal quality and, therefore, better device performance and production yield [3, 4].

In this study, we report the observation of a new arrangement of defects that we name the “galaxy” defect, which was observed on wafers from the same PVT-grown 6-inch 4˚ off-axis boule. Optical microscopy images show a region of a highly dense cluster of micrometer-level inclusions. Transmission XRT images indicate the formation of dislocation clusters with stronger contrast in (1-100) and (1-101) reflection images, while the contrast is weaker in (11-20) reflection images. Grazing images from the same region show a high density of BPDs within the “galaxy” defect region, as well as a high density of deflected Frank dislocations between the “galaxy” defect region and the periphery. A network of TED-LAGB is also observed on the (11-28) image of slices 25 and 49. SEM investigations were performed to identify the nature of the inclusions, but there was no contrast in the SEM images. Combining the results from these investigations, we propose that the optically visible inclusions are regions where threading dislocations are decorated with dopant atoms. The dopant concentration is possibly too small for a contrast in SEM images. Further investigations with various other characterizing methods, such as Raman mapping and TEM, are being utilized to confirm the nature of the inclusions in the “galaxy” defect and the formation mechanism of the dislocation cluster and LAGB observed on the XRT images. These results will also be discussed in this presentation.

DEVELOPMENT OF TEXTURED LEAD ZIRCONATE TITANATE (PZT) CERAMICS FOR PASSIVE ACOUSTIC SENSING APPLICATIONS

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Passive acoustic devices utilizing conventional ceramics, such as PZT-4, possess limited sensitivity due to a low hydrostatic piezoelectric voltage coefficient (gH). This work is developing [001] textured lead zirconate titanate (PZT) ceramics that display enhanced hydrostatic acoustic sensitivity. This work studies the key process conditions required to promote the templated grain growth (TGG) process in the PZT system. The viability of different lead titanate and lead zirconate titanate-based material systems is explored to maximize the effect of crystal anisotropy on the longitudinal and transverse piezoelectric properties. Densification and grain growth of templated-PbTiO3 and PZT structures are explored, and the influences of crystallographic structure and orientation on the longitudinal (g33) and transverse (g31) voltage sensitivity are discussed. Finally, the intrinsic and extrinsic contributions to the piezoelectric effect are characterized to set the stage for the discussion of the relationship between structure, hysteresis and domain wall motion in textured versus random ceramic PZT.

CONTINOUS FEED GROWTH OF MN:PIN-PMN-PT CRYSTALS

Weiguo Zhang (CTS Corporation), Kyle Grove (CTS Corporation), Patrick McGowan (CTS Corporation), Jian Tian (CTS Corporation)

Manganese doped Pb(In1/2Nb1/2)O3-Pb(Mg1/3Nb2/3)O3-PbTiO3 (Mn:PIN-PMN-PT) single crystal are promising candidates for high-power piezoelectric transducer applications because of their high mechanical quality factor (Qm). However, it is well-known that Mn:PIN-PMN-PT crystal grown by conventional Bridgman method exhibit property variation along the growth direction due to compositional segregation. In contrast, continuous feed growth has proven to be an effective technique for improving the uniformity of PT-based crystals compared to the Bridgman method. At CTS, we have developed the continuous feed growth for Mn:PIN-PMN-PT crystals in the industrial filed. Specifically, we have grown Mn:PIN-PMN-PT crystals of up to 100 mm usable length with homogenized physical properties along growth direction. Crystals grown by continuous feed method demonstrated properties satisfying industrial application requirements, based on our preliminary test. In addition, physical properties of as-grown crystals can be tailored by adjusting the composition of feeding materials to meet specific customer requirements.

SYNCHROTRON X-RAY TOPOGRAPHY ANALYSIS OF LOW ANGLE GRAIN BOUNDARIES INDUCED BY GROWTH STEP FLOW IN PVT-GROWN 4H-SIC CRYSTALS

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Low angle grain boundaries (LAGB) are aggregation of dislocations, usually threading edge dislocations (TEDs) or edge type basal plane dislocations (BPDs) to accommodate the misorientation of lattice planes[1-2], that lower yield of PVT 4H-SiC substrates and prevent the implementation of large size SiC devices. Therefore, establishing a clear understanding of the dislocation nature of LAGBs and their formation mechanisms is of great significance. Traditionally, LAGBs oriented along <1-100> have been linked to threading screw or mixed dislocations (TSDs/TMDs), which serve as spiral step sources during crystal growth[3]. When growth centers converge, misorientation is accommodated by the alignment of TEDs into LAGBs along <1-100>. A recently proposed step-flow model suggests that radial temperature gradients near the facet cause growth steps to propagate faster at boule edges than at the center, forming a horseshoe-shaped step morphology. As outer growth fronts meet, LAGBs form to accommodate misorientation; central fronts later meet these, forming LAGBs along the [1-100] direction[4]. In this study, unique distribution patterns of LAGBs observed are investigated by Synchrotron X-ray topography (XRT). For wafer A, LAGBs networks are observed near the facet region consisting of LAGB arrays with white and dark contrast TEDs extending from the facet region. All individual TED arrays set extend along the < 1-100 > directions, with identical 1/3<11-20> Burgers vectors perpendicular to the array direction. Ray-tracing simulations confirm their Burgers vectors and tilt directions. Three spikes are observed on the left edge of the facet. Based on the horseshoe-shaped mechanism, the outer spikes propagate faster than the inner one due to radial temperature gradients. When the growth fronts of the outer spikes encounter each other first, LAGBs are formed along [01-10] & [10-10] directions to accommodate misorientation in this region. The growth front associated with the central spike will keep moving forward and encounter the other two fronts to form the LAGBs along the [1-100] direction. Another LAGB set forms around micropipes (MPs) at the wafer's left edge, where step fronts merge similarly to the horseshoe model. For wafer B, LAGB networks originate in the facet area. TEDs arrays extending from the facet center. Several MPs on the right side suggest classical growth-center-driven formation, where TED arrays accommodate c-axis rotation caused by TSD clusters.

DEVELOPMENT OF B-GA2O3 FOR HIGH POWER ELECTRONIC DEVICES

Hongping Zhao (The Ohio State University)

Ultra-wide bandgap gallium oxide (Ga_2O_3), with a bandgap energy of 4.8 eV and a predicted critical field strength of 8 MV/cm, is emerging as a highly promising material for power electronics. Significant advancements have been made in the development of Ga_2O_3 substrates, thin film epitaxy, defects and doping control, and device demonstrations. However, challenges remain in achieving Ga2O3 power devices operating at 10-20 kV. This presentation will discuss recent progress in the MOCVD growth of Ga2O3, particularly for developing thick Ga2O3 drift layers, focusing on impurities and doping, phase stabilization, and progress in p-type oxides developments.

HALIDE SINGLE CRYSTAL SCINTILLATORS FOR X-RAY RADIOGRAPHY

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There is a growing need for scintillator materials with improved performance for national security technologies. For high energy X-ray radiography (0.5-9 MeV), scintillators must have high light yield, low afterglow, and radiation hardness, among other properties. In this presentation, several new inorganic halide perovskite single crystal scintillators (RbBX3, RbB2X5, Rb4BX6, B2+ = Ca, Sr, Eu; X- = Br, I) with promising properties are discussed. Namely, these crystals have very high light yield (>70,000 ph/MeV), promising X-ray afterglow and radiation hardness. In these applications, large volumes of crystal are needed for efficient screening for special nuclear materials. Therefore, we evaluate their feasibility for crystal growth scale up to ~1 inch in diameter using the Vertical Bridgman method.

BALANCING LIGHT YIELD AND ULTRAFAST DECAY IN CSCU$_2$I$_3$ SCINTILLATOR CRYSTALS GROWN BY SOLUTION METHODS

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The demand for novel scintillators with high light yield and ultrafast decay continues to rise, especially for time-of-flight PET and high-rate X-ray imaging [1]. In this context, lead-free perovskite-like $CsCu_2I_3$ has emerged as a promising candidate due to its broadband emission arising from self-trapped excitons and its ecofriendly composition [2,3] . However, achieving a simultaneous optimization of fast decay components and high scintillation light yield remains a significant challenge. In this work, we present a comprehensive study of $CsCu_2I_3$ single crystals grown via the antisolvent-assisted solution method, including both undoped and alkali-doped variants, aimed at tuning their scintillation response.

Through optimization of growth parameters, large, high-quality $CsCu_2I_3$ single crystals with dimensions ~7×5×3 mm were obtained. Undoped and doped (Na^+, K^+ <20 ppm) crystals were characterized structurally and optically. Photoluminescence, radioluminescence, and time-resolved luminescence studies confirmed the presence of broadband emission in the 500–700 nm range, attributed to self-trapped excitons. Notably, a 1-ns fast-decay component associated with a ~420 nm band was observed in “fast” samples. F rom pulse height measurements, the light yields are between 14 and 24 ph/keV with undoped crystals.SEM-EDS analysis revealed a cesium-deficient surface layer, possibly CuI or related copper-iodide phases, correlating with the emergence of this ultrafast decay channel.

Our analysis of “fast” and “slow” $CsCu_2I_3$ crystals revealed that the presence of the 420 nm band is strongly tied to the surface chemistry and defects introduced during crystal growth. However, this fast-decaying component is absent in “slow” samples. Moreover, thermoluminescence studies showed negligible afterglow in undoped crystals, while doped variants exhibited clear trap-related delayed emission. These findings indicate a complex interplay between doping, morphology, and defect states in governing both scintillation light yield and decay time.

In conclusion, o ur results provide valuable insight into the defect-related origins of ultrafast luminescence in this class of materials, offering a pathway for further development of low-cost, non-toxic, and fast-response scintillators for next-generation radiation detection systems [1].

[1] Wibowo et al. Commun Mater 4, 21 (2023)
[2] Yao et al, Adv Mater., 35, 2304938 (2023)
[3] Haposan et al. Phys Status Solidi (RRL), 19, 3, 2400298 (2025)

THE ROLE OF GAS PHASE NUCLEATION IN DIAMOND GROWTH PROCESS IN MPCVD CHAMBER

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Large area growth of nano- or polycrystalline diamonds with microwave plasma assisted chemical vapor deposition (MPCVD) is a promising technology for future microelectronics. Diamond nanoparticles nucleation is known to occur on the surface defects due to polishing and ion bombardment. The importance of the gas phase nucleation was reported in various studies, but the mechanism of diamond nanoparticles growth in the gas phase required further investigation. Numerical modeling, combined with the experiments targeting this phenomenon, enables fundamental insights into the growth mechanisms, optimization of the process conditions, and reactor design. A series of experiments was conducted to investigate the gas phase kinetics of nanodiamonds growth. In the standard setup of H2/CH4 in 2.45 GHz MPCVD reactor, particles formed in the gas phase were collected through the pinhole on the substrate at different pedestal heights. SEM and Raman analyses revealed complex trends in diamond particle size, re-nucleation, and growth rates. The model of MPCVD process included the gas phase nucleation of diamond particles coupled with CxHy species production, transport, and decay within the reactor. It was demonstrated that the pedestal height and process conditions affect the distribution of CxHy species, gas temperature, and diamond particles flux to the substrate. At low pressure under 40 Torr, nanoparticles concentration is localized in the center above the substrate. The gradual increase of pressure to 100 Torr shifts the concentration peak to the pedestal edge, which is consistent with the CH3 density. Considerable nanoparticles flux to the substrate is observed for the pressures below 100 Torr, since particles reach the size when they become driven by thermophoretic force from the plasma core to the relatively cold substrate. Thus, under typical PCD growth conditions, the defects formation should be expected near the substrate edge, where increased nanoparticles flux may contribute to formation of re-nucleation centers. Higher pressure regimes above 150 Torr are characterized by the gas temperature of 3000 K and large amount of H atoms. In the center of the reactor above the substrate, “ring shaped” concentration of CH3 has a minimum, while H mole fraction is maximal and no nanoparticles are formed. Model of MPCVD with gas phase nucleation enables choosing the growth conditions for diamond particles deposition on the substrate.