PCSI
Room Canyon/Sugarloaf - Session PCSI-2WeA

Synthesis of Materials for Devices
Moderator: Alec Talin, Sandia National Laboratories

4:30pm **PCSI-2WeA-31 Nitrogen Doping of Gallium Oxide by Ion Implantation and its Application to Vertical Transistors**, *Masataka Higashiwaki,* National Institute of Information and Communications Technology, Japan*; M Wong,* National Institute of Information and Communications Technology*; K Goto, H Murakami, Y Kumagai,* Tokyo University of Agriculture and Technology, Japan   **INVITED**
β-gallium oxide (β-Ga_2O_3) has a very large bandgap (~4.5 eV) and a breakdown electric field exceeding 6 MV/cm, making it an attractive candidate for next-generation power electronics. However, Ga_2O_3 has a fundamental physical drawback, namely a lack of hole-conductive *p*-type material, because of unavailability of shallow acceptors, a valence band structure mostly formed by O $2p$ orbitals, and a self-trapping effect of free holes. Recently, we succeeded in developing a nitrogen (N)-ion-implantation doping process for Ga_2O_3 to form an energy barrier in a device structure [1] and then fabricating vertical Ga_2O_3 transistors by using a device process based on the N-ion implantation doping [2, 3].

N atoms are theoretically expected to be a deep acceptor in Ga_2O_3. We performed N-ion implantation doping into an *n*-Ga_2O_3 layer to fabricate a current blocking layer by forming a Si-doped–N-doped–Si-doped Ga_2O_3*n-p-n* junction. Note that Si is a shallow donor with an activation energy of about 50 meV in Ga_2O_3. Then, depletion-mode (D-mode) and enhancement-mode (E-mode) vertical Ga_2O_3 transistors with a current aperture were fabricated by using a manufacturable all-ion-implanted process, which is similar to commercial Si and SiC power device technologies, with Si and N doping. Both the D-mode and E-mode devices demonstrated successful transistor action and decent device characteristics.

[1] M. H. Wong, M. Higashiwaki *et al.*, Appl. Phys. Lett. **113**, 102103 (2018).

[2] M. H. Wong, M. Higashiwaki *et al.*, IEEE Electron Device Lett. **40**, 431 (2019).

[3] M. H. Wong, M. Higashiwaki *et al.*, in *Abstract of 77th Device Research Conference, 2019.*

5:10pm **PCSI-2WeA-39 Studying the Nucleation of GaP on v-Grooved Si for III-V/Si Device Integration**, *Emily Warren,* National Renewable Energy Laboratory*; T Saenz,* Colorado School of Mines*; A Norman,* National Renewable Energy Laboratory*; J Zimmerman,* Colorado School of Mines
The direct heteroepitaxy of III-V materials on Si for high efficiency optoelectronic and photovoltaic applications has progressed greatly in recent years, but most studies have focused on polished wafers, that are compatible with microelectronics (e.g. CMOS) fabrication, but not photovoltaic technologies. There has been recent interest in growing III-Vs on "v-grooved" surfaces, where nanoscale patterning and facet selective etching is used to pattern nominally (001) Si surfaces with linear (111)-facetted v-groove structures. This v-grooved geometry suppresses antiphase boundaries (APBs), thereby enabling defect-free nucleation of polar III-V materials on non-polar Si. However, for applications where cost is important, it also brings with it the challenge of creating the v-grooved pattern in a cost-effective way, without an expensive wafer-polishing step.

In this work, we show how v-groove structures can be prepared with cost-effective patterning approaches (nanoimprint lithography and interference lithography) on unpolished Si surfaces.[1] Unlike prior studies of growth of III-Vs on v-groove structures, which have focused on lattice mismatched heteroepitaxy of III-Vs (GaAs, InP, etc.), we have focused on GaP, which has a very small lattice mismatch with Si and enables us to understand the fundamentals of III-V nucleation on partially v-grooved surfaces, where multiple facets are exposed during growth. This is also an excellent platform to investigate the coalescence of selective area growth, a topic that is important for large-area applications such as photovoltaics.[2] We have systematically studied the nucleation conditions for GaP on v-groove Si and identified conditions that enable facet-selective nucleation without the formation of APBs, and lead to smooth, planar coalesced films.

5:15pm **PCSI-2WeA-40 Improving Heterointerfaces in Rapidly Grown III-V Electronic Devices using Dynamic Hydride Vapor Phase Epitaxy (D-HVPE)**, *Dennice Roberts, J Simon, K Schulte, A Ptak,* National Renewable Energy Laboratory
High growth rates and precursor utilization make hydride vapor phase epitaxy (HVPE) a powerful tool for the growth of homoepitaxial III-V materials, particularly GaN and GaAs [1,2]. However, most applications are limited to thick single layers rather than electronic devices that require multiple heterointerfaces. Single-chamber HVPE systems are hampered by the long residence times of vapor phase constituents, typically requiring a growth interrupt to create abrupt interfaces. The non-abrupt nature of interfaces created in single-growth-chamber systems limits the use of HVPE in heteroepitaxial devices. The recent development of dynamic HVPE (D-HVPE) addressed this issue by introducing a second, largely isolated growth chamber, allowing a sample to be shuttled between growth chambers with established steady-state reactions to produce high quality, chemically- and structurally-abrupt interfaces. D-HVPE-grown single- and dual-junction GaAs and GaAs/GaInP solar cell devices show efficiencies approaching that of materials grown by more conventional means such as MOVPE. [3]

Here we present an assessment of improved interface quality between isostructural samples grown by traditional HVPE and D-HVPE in a custom reactor. Time-resolved photoluminescence measurements reveal samples grown by D-HVPE have significantly higher lifetimes than samples grown by HVPE. Trap-assisted recombination is also present in samples grown by traditional HVPE, resulting in different calculated lifetimes at high- and low-level injection. We compare structure and morphology differences and discuss growth mechanisms of D-HVPE grown solar cells.

[1] E. Gil-Lafon, J. Cryst. Growth **222** 3 (2001) [2] K. Motoki, Jpn J. Appl. Phys. **40** (2001) [3] J. Simon, Crystals **9** 3 (2019)

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5:20pm **PCSI-2WeA-41 Real-Time Optical Monitoring of the Epitaxial Growth of Zincblende Semiconductors**, *Alfonso Lastras-Martinez,* Universidad Autónoma de San Luis Potosi, México
Non-invasive optical probes such as reflectance anisotropy spectroscopy (RAS) are attractive for real-time monitoring of the epitaxial growth of cubic semiconductors given their high sensitivity and instrumental simplicity. RAS enhances the surface response against the bulk signal by taking advantage of the reduced symmetry of the near-surface region of cubic crystals. Nevertheless, although the surface specificity of RAS has been known for long time, its use for monitoring epitaxial growth had been hampered by the lack of both a rapid spectrometer to follow epitaxial growth and a full understanding of the physics underlining RAS line shapes.

In this talk we demonstrate the power of RAS to elucidate phenomena occurring during the very first stage of the MBE homoepitaxial growth of GaAs (first half monolayer (ML)). We present real-time RAS spectra acquired during growth, taking advantage of a recently developed rapid RAS spectrometer. On the basis of a singular value decomposition analysis, we show that RAS spectra for As-rich surfaces (corresponding to c(4x4) and (2x4) surface reconstructions) comprise two independent components with contrasting evolutions along growth. A first component, associated to the orthorhombic strain induced by surface reconstruction, rises sharply upon starting growth and its amplitude changes sign as the surface reconstruction shifts from c(4x4) to (2x4). All this takes place during the growth of the first half ML. Afterwards, the amplitude of the first component oscillates following layer-by-layer growth. In contrast, the amplitude of the second component shows relatively small changes along growth which suggests that it is characteristic of As-terminated surfaces, regardless of their specific reconstruction.

5:25pm **PCSI-2WeA-42 Pulsed Laser Deposition of Epitaxial $Sr_3Al_2O_6$ as a Water-Soluble Sacrificial Layer for GaAs Deposition**, *Imran Khan, B McMahon, A Norman, A Zakutayev,* National Renewable Energy Laboratory
Despite the record high efficiency for GaAs solar cells, its terrestrial application is limited due to both the particularly high costs related to the required single crystal substrates and the epitaxial growth. Significant substrate reuse is one strategy that has been heavily explored by the PV community, however, the usefulness of all the existing techniques is limited due to the need for toxic etchants, substrate re-polishing and/or expensive intermediate process steps. A water-soluble lift off layer could reduce costs by avoiding these potential downsides.

$Sr_3Al_2O_6$ (SAO) is a water soluble, cubic oxide (space group *Pa-3*), with lattice constant 15.84Å. This is close to $(2\sqrt{2})a_{GaAs}$ = 15.99Å, giving a close lattice match between SAO <100> and GaAs <100> after 45° lattice

rotation. We investigated the epitaxial growth of high structural quality SAO on single crystal $SrTiO_3$ (STO) substrates by Pulsed Laser Deposition (PLD), and the feasibility of subsequently growing GaAs epitaxially on top of it.

We identified that pulsed laser deposited SAO on STO is polycrystalline for substrate temperatures lower than 650°C, however the films could be epitaxially crystallized partially by high temperature annealing. Careful optimization of the growth parameters for obtaining epitaxial SAO on STO was explored, and we identified that the SAO film quality is strongly dependent on the growth temperature and O_2 partial pressure. An STO capping layer was grown on the SAO to protect from moisture induced degradation, which was also epitaxial.

XRD spectra for the films with optimized deposition parameters showed SAO (400) and SAO (800) peaks that were epitaxially aligned to the STO (100) and STO (200) substrate peaks. TEM analysis revealed that the grown SAO films are epitaxially crystalline throughout the thickness. The epitaxial growth of the STO capping layer is a qualitative indication for the high quality of the SAO surface. Research activity is ongoing to experiment the practicability of growing GaAs on these sacrificial SAO films.

5:35pm **PCSI-2WeA-44 Epitaxial Relationship of Cu3N Grown on YSZ(001) Substrate by Mist CVD Method**, *Nao Wakabayashi,* Kogakuin University, Japan

Copper nitride (Cu3N) is Anti-ReO3 type cubic structure. It is reported that the bandgap energy of single crystal Cu3N is about 1.4 eV and this can be applied as a solar energy conversion material [1]. Cu3N has typically grown by physical vapor deposition (PVD) using vacuum pressure [2]. Mist chemical vapor deposition (mist CVD) method is one of the cost-effective growth techniques and is possible to grow in atmospheric pressure [3]. Recently, we have succeeded in the epitaxial growth of Cu3N on *c*-plane sapphire by mist CVD method using NH3 aqueous solution as a solvent. The epitaxial relationship in in-plane direction of this Cu3N film was Cu3N(100)//a-Al2O3(11-20). This indicates that the film had multi-domain structure, since a-Al_2O_3 has not cubic but corundum structure. [4]. In this study, Cu3N was grown on a YSZ(001) substrate by mist CVD method. The epitaxial relationship was evaluated.

Cu3N thin film was grown on a YSZ(100) substrate by vertical-type mist CVD method. Copper (II) acetylacetonate was used as a source material for the growth. The Cu (II) acetylacetonate was solved in NH3 aqueous solution of 28%. The concentration of Cu was 0.1 mol/L. The mist, formed by the 2.4 MHz ultrasonic transducer, was transferred to the reaction area by nitrogen carrier gas. The Cu3N film was grown totally for 2 hours at the temperatures of 300°C.

The XRD θ-2θ pattern, shown in Fig. 1(a), indicates that the film has the epitaxial relationship of Cu3N(001)//YSZ(001) in the growth direction. The XRD f scan patterns, shown in Fig. 1(b), indicates that the film has the epitaxial relationship of Cu3N(100)//YSZ(100) in the in-plane direction. Thus, we have succeeded in the suppression of multi-domain structure, which is observed in the growth on a-Al_2O_3, using the YSZ substrate with cubic structure.

In the presentation**,** different growth phenomena for Cu3N on a-Al2O3 and YSZ substrates are also discussed.

[1] K. Matsuzaki *et al.*, Appl. Phys. Lett. **105**, 222102 (2014).

[2] Z.Q. Liu *et al.*, Thin Solid Films. **325,** 55 (1998).

[3] T. Kawaharamura *et al.*, J. Appl. Phys. Lett. **47**, 4669 (2008).

[4] T. Yamaguchi *et al.*, *in preparation*.

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5:40pm **PCSI-2WeA-45 UPGRADED: Halogen Surface Chemistries for Atomically Precise Manufacturing on Si(100)***, Kevin Dwyer,* M Dreyer, K Gaskell, University of Maryland*; R Butera,* Laboratory for Physical Sciences

Atomic-scale fabrication of electronic devices in silicon has been widely demonstrated using a scanning tunneling microscope (STM) and hydrogen-based surface chemistries to precisely place phosphorous donor atoms on the surface. Incorporation of PH3 precursors into lithographic patterns formed from a hydrogen resist in a Si surface can produce metallic wires, quantum dots defined by electrostatic gates, and single donor atom qubits for quantum information (QI) research[1]. However, interest in acceptor dopants and hole-based devices necessitates the development of alternate precursor and/or resist chemistries for device fabrication. Halogen chemistry is potentially more favorable for acceptor incorporation than hydrogen[2], and to that end we explore halogen-based resists including Cl, Br, and I, along with metal-halide precursors to deposit acceptor dopants.

Here, we present results on the complete surface passivation of Si(100) using Cl, Br, and I, and demonstrate STM lithography at cryogenic and elevated temperatures [3]. We further study the stability of halogen-terminated Si(100) in ambient environments using x-ray photoelectron spectroscopy (XPS) to facilitate transport of samples outside of ultra-high vacuum environments. Finally, we present results of metal-halide adsorption on Si(100) as a viable path towards acceptor doping.

6:00pm **PCSI-2WeA-49 Novel Growth Mechanisms in van der Waals Epitaxy: 3D Morphologies of Bi₂Se₃***, Theresa Ginley, S Law,* University of Delaware

Van der Waals (vdW) materials, such as graphene, transition metal dichalcogenides, and bismuth chalcogenides, are an increasingly popular research topic due to their wide variety of applications. They are characterized by strongly bonded layers in the *a-b* plane and weak vdW bonds between layers in the *c*-direction. Careful control of vdW materials could create designer stacks of 2D materials or unlock the unique physics of 3D topological insulators, resulting in improved optoelectronic, spintronic, and valleytronic technologies. Growth via Molecular Beam Epitaxy (MBE) is a promising avenue for improved material quality due to its' highly customizable growth conditions. Unlike traditional MBE, which relies on the strong interaction between the growth material and a lattice matched substrate, vdW epitaxy takes advantage of the weak vdW bonds to grow on substrates with vastly different crystal structures. Unfortunately, vdW epitaxy cannot be fully explained via the well-known mechanics of traditional MBE. Growth of atomically smooth layers remains challenging as vdW materials tend to grow in terraced "wedding cake" morphologies. Also, vdW materials favor the (001) orientation with the vdW gaps parallel to the growth surface. Other orientations have been reported via MBE but require extensive substrate pretreatment or prepatterning. Improved understanding of the growth mechanisms involved in vdW epitaxy could allow for improved material quality as well as exotic growth morphologies.

In this study, we use the topological insulator Bi₂Se₃ as a prototypical vdW material for the exploration of growth mechanics. We chose to grow on GaAs(001) substrates as the interaction of adatoms with the post deoxidization reconstructed surface may provide greater insight than a less complex growth surface, such as previous work on sapphire substrates. It was found that growth at a substrate temperature of 425°C produced a significant amount of growth in the elusive (0015) orientation, with domains aligned along the GaAs[110] axis (Sample A). It is believed that bismuth aggregation due to thermal degradation as well as fast diffusion of bismuth along GaAs[110] combine to push growth into this orientation. A film grown on a 10nm $(Bi_{0.5}In_{0.5})_2Se_3$ buffer layer results in the formation of Bi₂Se₃ platelets with sheer walls and flat tops (Sample B). Based on this research it is believed that vdW growth dynamics are dominated by the relative strength of film/adatom and substrate/adatom interactions. The morphologies reported here differ significantly from those reported on sapphire, implying that substrate interaction is key to understanding novel morphologies in vdW materials.

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