

## PCSI

### Room Keauhou II - Session PCSI-MoA

#### Wide Bandgap/Organic Spintronics/New Approaches to Epitaxy I/Nanowires and Nanostructures

**Moderators:** Leonard Brillson, Ohio State University, Danna Freedman, Northwestern University, Fengyuan Yang, The Ohio State University, Erik Lind, Lund University

**2:00pm PCSI-MoA-1 Use of Electrografted Aryldiazonium Salts to Control the Surface Conductivity and Reactivity of ZnO, Alexandra McNeill,** University of Canterbury, New Zealand; *K Bell,* MacDiarmid Institute for Advanced Materials and Nanotechnology; *R Gazoni, R Reeves, A Downard, M Allen,* University of Canterbury, New Zealand

Zinc oxide (ZnO) is a transparent, earth-abundant, wide band-gap semiconductor with high surface sensitivity and reactivity that must be controlled for use in electronic applications, in particular transparent thin film transistors and UV photodetectors. In ambient conditions, the ZnO surface is terminated by hydroxyl groups that cause the conduction and valence bands to bend downwards, creating an electron accumulation layer that renders the surface highly susceptible to unwanted atmospheric adsorbates [1]. The surface hydroxyl termination can be deliberately replaced with covalently bonded organic functional groups. In doing so, the surface band bending and surface conductivity can be directly manipulated. In this work, nitro- and trifluoromethyl-phenyl multilayered films have been attached to ZnO by electrografting from aryldiazonium salt solutions. Synchrotron X-ray photoemission spectroscopy confirms that both surface modifiers remove the native downward band bending, with the nitro-phenyl termination producing a large upwards band bending consistent with an electron-depleted surface. It was also observed that X-ray-induced reduction of the nitro-terminated film serves to further increase the upward band bending, which is an unexpected and as yet unexplained phenomenon. Diazonium salt chemistry has been rarely used to modify ZnO, yet this work indicates that it is a highly promising surface modification strategy for controlling the surface conductivity and reactivity of this technologically-important transparent semiconductor.

[1] R. Heinhold et al., *Phys. Rev. B* **88**, 23 (2013)

**2:15pm PCSI-MoA-4 Influence of Interface State and Band Bending on In and N Polar InN from Angle-resolved XPS, T Honda, Yusuke Nakajima,** Kogakuin University, Japan

Indium nitride (InN) has a smallest bandgap and a largest mobility among III-V nitride semiconductors[1]. However, the epitaxially grown InN layer contains a surface-charge-accumulation-layer, in which the Fermi-level is pinning at an energy position sufficiently higher than the conduction band minimum, resulting in a degradation of device performance[2]. The surface-charge-accumulation-layer induces a band bending and subsequent influences on the electrical properties in the surface region [3]. In this paper, surface band bending in In and N polar InN films was observed using angle-resolved X-ray photoelectron spectroscopy (AR-XPS) to discuss the surface states.

In and N polar InN layers were grown on (0001)GaN templates and free-standing (0001)GaN by RF-MBE. AR-XPS (JEOL, JPS9000) spectra were observed using a Mg K $\alpha$  line (1253.6 eV) as an excitation source. The binding energies in the spectra were corrected using the C1s core level emission peak. The background intensities based on a white noise were considered. The observation was performed at RT. Before the observation, the surface oxides on the samples were removed using a HCl solution. The AR-XPS spectra near the valence band maximum at detection angles of 0 and 40 degrees are shown in Fig. 1 (a) and (b). Both figures are normalizing the spectrum. Both spectra are similar to those in a previous report[4], but slightly changed each other. Difference in between the spectra is shown in inset. The observed angle is defined as the tilt angle from the normal direction of the detector and is related to the average excitation depth in XPS. The result shows that the band bending is downward on the surface. Here, "downward" means that some holes in a bulk region move to its surface states [2]. The XPS spectra around the valence bands (VBs) of In- and N-polar InN layers are shown in Fig. 1 (c) (d). The tailing states are observed around the VBs, which will be due to the surface states occupied by electrons

**2:20pm PCSI-MoA-5 Influence of Al<sub>2</sub>O<sub>3</sub>/ In<sub>0.76</sub>Si<sub>0.24</sub>O<sub>0.99</sub>C<sub>0.01</sub> Interface on Reliability for Oxide Thin Film Transistor, Kazunori Kurishima,** Meiji University, National Institute for Materials Science, Japan; *T Nabatame,* National Institute for Materials Science, Japan; *T Onaya,* Meiji University, National Institute for Materials Science; *T Kizu, K Tsukagoshi, A Ohi, N Ikeda, T Chikyow,* National Institute for Materials Science, Japan; *A Ogura,* Meiji University, Japan

Recently, influence of dipole and fixed charge of SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> interface on threshold voltage ( $V_{th}$ ) control has been reported in back-gate-type Indium oxide (InO<sub>x</sub>)-based thin film transistors (TFTs) with SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> dielectrics[1]. Previously, effect of In-Si-O film as a new InO<sub>x</sub>-based channel material on stability of transistor properties was demonstrated [2]. Here, we pay attention to characteristics at interface between the Al<sub>2</sub>O<sub>3</sub> dielectric and In<sub>0.76</sub>Si<sub>0.24</sub>O<sub>0.99</sub>C<sub>0.01</sub> (ISOC) channel of ISOC TFT with Al<sub>2</sub>O<sub>3</sub> dielectric. In this paper, we focus on the reliability of bottom-gate-type ISOC TFT with Al<sub>2</sub>O<sub>3</sub> dielectric.

The bottom-gate-type ISOC TFTs were fabricated as follows. At first, Pt gate electrode was patterned on Si/SiO<sub>2</sub> substrate using photolithographic process. Next, a 30-nm-thick Al<sub>2</sub>O<sub>3</sub> film was deposited on Pt gate electrode by ALD at 300 °C using TMA precursor and H<sub>2</sub>O gas and was annealed at 300 °C in O<sub>2</sub>. A 10-nm-thick ISOC film was subsequently deposited on Al<sub>2</sub>O<sub>3</sub> film by sputtering using SiC and In<sub>2</sub>O<sub>3</sub> targets and was annealed at 300 °C in air. The Au (100 nm)/Ti (10 nm) source/drain electrodes were patterned on ISOC film and was finally annealed at 250 °C in O<sub>3</sub>.

Fig. 1 shows typical  $I_d$ - $V_g$  properties of the TFT with Al<sub>2</sub>O<sub>3</sub> dielectric. The  $V_{th}$ , on/off current ration and field-effect-mobility value of Al<sub>2</sub>O<sub>3</sub>/ISOC TFT were -0.3 V, 6.4 $\times$ 10<sup>8</sup> and 15.2 cm<sup>2</sup>/Vs, respectively. The lower subthreshold swing (SS) of 88.5 mV/decade was obtained. Negative gate bias stress was applied to examine stability of transistor properties of Al<sub>2</sub>O<sub>3</sub>/ISOC TFT. The change of  $V_{th}$  ( $\Delta V_{th}$ ) increased with increasing the  $V_g$ - $V_{th}$  (Fig. 2 (a)). The  $\Delta V_{th}$  in Al<sub>2</sub>O<sub>3</sub>/ISOC TFT was -4.6 V at a stress time of 3 h when  $V_g$ - $V_{th}$  was applied -10 V. This suggested that the ISOC channel body was depleted, and the holes near the Al<sub>2</sub>O<sub>3</sub>/ISOC interface were trapped by deep donor-like trap states, which were oxygen-vacancy-related defect states, as shown in Fig. 2(b) [3].

[1] K. Kurishima et al., *J. Vac. Sci. Technol.* **A33**, 061506 (2015).

[2] N. Mitoma et al., *Appl. Phys. Lett.* **104**, 102103 (2014).

[3] W-T. Chen et al., *IEEE Electron Device Lett.*, vol. **32**, no. 3, pp. 1552-1554, Nov. (2011).

**2:25pm PCSI-MoA-6 Thermodynamic Analysis of 3Ga-H Surface Reaction Process for GaN(0001), Kazuki Sekiguchi, H Shirakawa, K Chokawa, M Araidai,** Nagoya University, Japan; *Y Kangawa, K Kakimoto,* Kyushu University; *K Shiraishi,* Nagoya University, Japan

Clarification of the growth mechanism during GaN MOVPE is crucial for the practical realization of GaN power devices, with which significant energy savings can be achieved. In our previous study, we analyzed the TMG decomposition process based on a calculation of the formation free energy and the activation energy [1]. It has been reported that TMG loses methyl groups one by one which react with H<sub>2</sub> and finally decomposes into GaH in the vapor phase. We concluded that the main reaction gases on the surface of the substrate are GaH and NH<sub>3</sub>, which are the gallium and nitrogen sources, respectively. So, we have been investigating the behavior of GaH and NH<sub>3</sub> on the surface of GaN. According to a previous study [2], the reconstructed surface is a 3Ga-H surface, which means the hydrogen terminates 3 out of the 4 top Ga, under the growth conditions of our previous study [1]. Therefore, in this study, we clarify the reactions of GaH and NH<sub>3</sub> and the growth process on a 3Ga-H surface.

In the analysis of the reactions given by GaH and NH<sub>3</sub> at a 3Ga-H surface, we calculated the formation energy of the various surface reactions such as the adsorption reactions of NH<sub>3</sub>, NH<sub>2</sub>, GaH, and so on. As a result, on a 3Ga-H surface, GaH decomposition occurs, and Ga atom is adsorbed while H<sub>2</sub> is desorbed in the vapor phase. Only this reaction can occur at 1300 K, which is the substrate temperature. With this reaction, the surface of the substrate changes from Fig.1 (a) to (b). Moreover, this reaction is repeated. Therefore, at a 3Ga-H surface, GaH decomposes into Ga and H atoms, and the Ga atoms are adsorbed one after another as shown in the following figure; Fig.1 (a) to (b) to (c) to (d). Finally, all 3 H atoms on the surface are desorbed in the vapor phase and 3 Ga atoms are adsorbed onto the GaN surface, forming a Ga-rich layer. This is also considered to correspond to the formation of Ga droplets.

2:30pm **PCSI-MoA-7 Effects of Incorporating Si into Al<sub>2</sub>O<sub>3</sub> Gate Oxides in GaN-MOSFETs**, *Eiji Kojima, K Chokawa, H Shirakawa, M Araidai, K Shiraishi, K Shiozaki, T Kachi*, Nagoya University, Japan

There has been a growing interest in gallium nitride (GaN) as a material for next-generation power conversion devices. In order to realize GaN-MOSFETs, it is important to determine the most suitable gate oxide. Among the various materials for gate oxides, Al<sub>2</sub>O<sub>3</sub> is one of the best owing to its relatively large conduction band offset (CBO) for GaN. However, the CBO of Al<sub>2</sub>O<sub>3</sub> is smaller than that of SiO<sub>2</sub>, which means the leakage current of GaN devices with Al<sub>2</sub>O<sub>3</sub> gate oxides are higher than those with SiO<sub>2</sub> gate oxides. Leakage current can lead to instability of the threshold voltage. Kikuta et al. have reported that Al<sub>1-x</sub>Si<sub>x</sub>O<sub>3</sub> mixed oxides deposited by plasma-enhanced atomic layer deposition might achieve high reliability MOSFET devices with reduced leakage current.<sup>1</sup> In this study, we investigated the effect of incorporating Si at oxygen vacancies in Al<sub>2</sub>O<sub>3</sub>. We calculated the atomic and electronic structures of oxygen vacancies in amorphous Al<sub>1-x</sub>Si<sub>x</sub>O<sub>y</sub> using first-principles calculations.

The calculations were performed using the VASP code<sup>2</sup>, which is based on density-functional theory with the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation.<sup>3</sup> We prepared amorphous Al<sub>2</sub>O<sub>3</sub> with 120 atoms and constructed Al<sub>0.8</sub>Si<sub>0.2</sub>O<sub>3</sub>, Al<sub>0.46</sub>Si<sub>0.54</sub>O<sub>3</sub> and Al<sub>0.23</sub>Si<sub>0.77</sub>O<sub>3</sub> models. Next, we removed an oxygen atom and calculated the atomic and electronic structures. In Al<sub>2</sub>O<sub>3</sub>, we found the well-known oxygen vacancy structures. However, a new Si-Si bond was formed in Al<sub>0.8</sub>Si<sub>0.2</sub>O<sub>3</sub>, Al<sub>0.46</sub>Si<sub>0.54</sub>O<sub>3</sub> and Al<sub>0.23</sub>Si<sub>0.77</sub>O<sub>3</sub>. As a result, no deep defect levels were formed in the bandgap with the Al<sub>1-x</sub>Si<sub>x</sub>O<sub>3</sub> mixed oxides, although deep defect levels originating from oxygen vacancies were formed in amorphous Al<sub>2</sub>O<sub>3</sub> (Fig. 1 (a)-(d)). These results indicate that gate leakage would be reduced in MOSFETs with Al<sub>1-x</sub>Si<sub>x</sub>O<sub>y</sub> mixed oxides. Thus, Al<sub>1-x</sub>Si<sub>x</sub>O<sub>3</sub> is one of the best candidates for GaN-MOSFETs.

2:35pm **PCSI-MoA-8 Native Point Defect Measurement, Processing, and Identification Near Ga<sub>2</sub>O<sub>3</sub> Surfaces**, *H Gao, G Foster*, The Ohio State University; *H Von Wenckstern*, University of Leipzig, Germany; *M Grundmann*, Universität Leipzig Institut für Experimentelle Physik II, Germany; *M Higashiwaki*, National Institute of Information and Communications Technology, Japan; *Leonard Brillson, H Zhao*, The Ohio State University

Ga<sub>2</sub>O<sub>3</sub> research has expanded rapidly due to its wide band gap enabling very high breakdown fields and n-type doping ranging from intrinsic to degenerate, both features which lead to numerous solid state electronics applications. However, it is not yet known what defects form to compensate free carriers, reduce their mobilities, and limit their densities. We used a combination of depth - resolved cathodoluminescence spectroscopy (DRCLS), surface photovoltage spectroscopy (SPS), and remote oxygen plasma (ROP) processing to measure and begin to identify native point defects within the outer tens of nanometers of Ga<sub>2</sub>O<sub>3</sub> grown by pulsed laser deposition (PLD), low pressure chemical vapor deposition (LPCVD), and edge- defined film- fed growth (EFG). All three growth methods exhibit common optical features corresponding to transitions into and out of multiple deep level defect states within the Ga<sub>2</sub>O<sub>3</sub> band gap. (Fig.1.) DRCLS permits measurements of defect states from the free semiconductor surface into the bulk with depth resolution of tens of nanometers or less [1]. (Fig.2.) This capability permits us to measure how near-surface chemical processing changes DRCLS features, initially, how ROP filling of oxygen vacancies (V<sub>O</sub>) reduces specific V<sub>O</sub>-related deep level features, as found for other oxide semiconductors [2,3]. ROP processing produces clear reductions in specific defect features corresponding to V<sub>O</sub>-related features, largest near the surface and extending more than 40 nm below. (Fig. 3) SPS features determine deep level energies corresponding to DRCLS transitions. (Fig. 4.) These SPS energies complement DRCLS transition energies and correlate with defect energies predicted theoretically for V<sub>O</sub> in different lattice configurations (VDW) [4] and with energy levels extracted experimentally from deep level transient and optical spectroscopies DLTS and DLOS (SAR), respectively [5]. (Fig.5.)

These results indicate that oxygen vacancies in Ga<sub>2</sub>O<sub>3</sub> form multiple defect levels in the range of 2.5 – 3.5 eV above the valence band maximum (E<sub>v</sub>). More near-surface processing and characterization methods are available to probe the defect nature of other deep level features now observed. The combined near-surface detection and processing of Ga<sub>2</sub>O<sub>3</sub> opens a new avenue for identifying and controlling native point defects in this and other semiconductors too. Supported by NSF Grants No. DMR-1305193 and DMR-1755479 with thanks to Tamura Corp.

2:40pm **PCSI-MoA-9 Geometry Effects in Spin Pumping through Thin Organic Films**, *Georg Schmidt*, Martin-Luther-Universität Halle-Wittenberg, Germany

INVITED

We have investigated spin pumping from yttrium iron garnet (YIG) into Pt through ultrathin organic films (C<sub>60</sub>, DH<sub>4</sub>T) by measuring the damping in ferromagnetic resonance (FMR) by spin pumping and the DC inverse spin-Hall effect (ISHE) in the Pt. With increasing thickness d<sub>o</sub> of the organic the damping drops monotonically from a maximum for zero interlayer thickness to zero for 10 nm or more. The ISHE, however, changes in a non-monotonic way. Maximum ISHE is observed for d<sub>o</sub>=0. For d<sub>o</sub> of 1 or 2 nm the ISHE drops to less than 50% (Fig. 1). Further increase leads to a reversal of this trend for both organic materials and only after a second maximum is reached a drop to zero is observed which is approx. exponential with interlayer thickness. The origin of this effect can be found in the growth mode of the organic layers. In very thin films the organic molecules grow as islands which can ideally be regarded as half spheres. Magnitude and direction of the ISHE depend on the absolute directions of pumped spins and spin current and their relative orientation. The spin current enters through the bottom of the islands but exits perpendicular to the organic/Pt interface. Only the spin current through the top of the island causes a maximum signal (Fig. 2) while currents flowing almost in plane barely contribute. They either do not cause any ISHE or they cause an ISHE-voltage perpendicular to the measurement direction. With increasing thickness the islands coalesce to a closed layer and all spin currents again pass the interface perpendicular to the layer. The original effect is then restored, except for a decrease by spin flip in the organic film. Simulations and transmission electron microscopy show that this model fully describes our findings. The results are important because they show that especially for spin pumping through very thin films the morphology is extremely important and many different layer thicknesses need to be investigated to get a coherent picture. Due to the purely geometrical origin the effect is universal for all conducting interlayer materials.

3:10pm **PCSI-MoA-15 Controlling Anisotropy in Organic-Based Magnets for Microwave Electronics and Quantum Magnonics**, *Michael Chilcote, M Harberts, Y Lu, I Froning, H Yu*, The Ohio State University; *B Fuhrmann*, IZM, Martin-Luther-Universität Halle-Wittenberg; *K Lehmann*, Institute für Physik, Martin-Luther-Universität Halle-Wittenberg; *A Franson*, The Ohio State University; *N Zhu, H Tang*, Yale University; *G Schmidt*, Martin-Luther-Universität Halle-Wittenberg, Germany; *E Johnston-Halperin*, The Ohio State University

Progress in the field of organic electronics has yielded significant advances in the development and application of organic light emitting diodes, organic photovoltaics, and organic field effect transistors. The success of these device applications suggests that further expansion of the field to include magnetic functionality may be promising. At the same time, the emergence of optimized thin film growth of and successful encapsulation strategies for organic magnets allows for long term stability of high quality magnets under ambient conditions. Organic-based magnets of the form M[Acceptor]<sub>x</sub> (M = transition metal, x ≈ 2) exhibit room temperature magnetic ordering and provide the opportunity to tailor magnetic properties through the careful selection of the transition metal ions and organic ligands. However, despite the promise of these systems, important outstanding questions remain. For example, while these materials are typically considered to be globally disordered structurally, the canonical magnet of this materials class, vanadium tetracyanoethylene (V[TCNE]<sub>x</sub>), exhibits robust magnetism, has a single-peaked, ultra-narrow magnetic resonance feature (approximately 1 G at 10 GHz), and has been shown to have a Curie temperature as high as 600 K.

We present work that illustrates strategies to control the anisotropy in this material system through growth morphology or temperature-dependent structural changes. We present the facile synthesis of a new class of organic-based magnetic nanostructures consisting of nanowires of V[TCNE]<sub>x</sub>. These nanowires exhibit uniaxial magnetic anisotropy in direct contrast to the isotropic in-plane response of typical thin-films. Furthermore, the magnetic anisotropy persists to the point of re-coalescence of the nanowires into a thin film, suggesting that dipole fields arising from shape anisotropy do not play a dominant role, instead pointing to interface-templated structural ordering as the origin of this anisotropy. Moreover, isolated films of V[TCNE]<sub>x</sub> analogs show a temperature-dependent switch in the easy axis, pointing towards the presence of an additional contribution to the uniaxial anisotropy. These results introduce a new degree of freedom for organic-based magnetism, allowing for the engineering of magnetic anisotropy in materials that exhibits both robust room-temperature magnetic order and the benefits typically found in other

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organic materials. Together with recent demonstration of encapsulation technologies and demonstrated functional microwave devices that exhibit high quality factors across a frequency range, these results suggest future promising applications in microwave electronics and quantum magnonics.

3:15pm **PCSI-MoA-16 Controlling the Self-Assembly and Optoelectronic Properties of Porphyrin Nanostructures**, *James Batteas, A Wan, T Reyes, M Elinski, M Buzbee*, Texas A&M University; *C Drain*, Hunter College of CUNY

Porphyryns are highly conjugated macrocyclic organic compounds which, due to their rich photophysical properties, have found numerous applications in areas ranging from catalysis, to optoelectronics, to photodynamic cancer therapies.[1,2] To tune their described structural and electronic properties, self-organizing porphyryns into hierarchical structures is often desirable.[3] Here, utilizing simply electrostatic interactions via the acidification of tetra(*p*-carboxyphenyl)porphyryn (TCPP) using hydrochloric acid, we have created porphyryn nanostructures, whose structural and optical properties are found to be pH dependent. From combinations of UV-visible absorption spectroscopy and atomic force microscopy (AFM) we have observed that after the carboxylate groups of TCPP were protonated (at ca. pH 5), the porphyryns form J-aggregate nanoplatelets. These structures further evolve, and by lowering pH to ca. pH 2, nanotubes ranging from ca. 30 - 300 nm in diameter with aspect ratios of > 400:1 are formed, with the absorption spectrum of the porphyryn nanotubes showing a collapse of the Q bands, revealing that protonation of the central nitrogens on the porphyryn macrocycle has occurred. Both in solution and on surfaces, these structures can be formed and cycled between, simply by changing solution pH. The porphyryn nanotubes have been observed by cryo-TEM to exhibit a highly organized lattice, and elemental mapping, as well as X-ray photoelectron spectroscopy (XPS) shows that chloride is intercalated within the porphyryn nanotubes at low pH, but not in the mid-pH range platelet structures. Photoconductivity of the porphyryn nanofibers was measured by four point probe and two-terminal current voltage (I-V) measurements and show the material to be semi-conducting in nature. As in solution, the structures on the surface can be tuned from platelet to nanofiber structures, simply by local pH changes, and using capillary condensation around an AFM tip, we can pattern these structures spatially on the surface.

4:30pm **PCSI-MoA-31 Tailoring Semiconductor Growth with Light**, *Kirstin Alberi*, National Renewable Energy Laboratory **INVITED**

The development of new semiconductor materials, heterostructures and interfaces critically relies on our ability to direct their synthesis. Vapor phase epitaxy methods generally allow crystal growth to be controlled to a high degree through parameters such as substrate temperature, atomic or molecular fluxes and substrate properties (crystallographic orientation, atomic step density, etc). Yet, these parameters alone may not always provide sufficient degrees of freedom to regulate the resulting material phase, compositional profiles and defect populations. Here we examine the mechanisms by which photons can affect semiconductor growth processes and may thus be used as an independent, externally controlled growth parameter. Many of the changes are driven by the influence of excess free carriers on adatom incorporation and desorption processes or a change in the electron potential at the growth surface. We discuss our recent work on how light can be used to address two specific growth challenges: 1) the incorporation of large Bi atoms into GaAs [1] and 2) the formation of heterovalent GaAs/ZnSe interfaces [2]. Based on our understanding of photo-assisted growth mechanisms, we also highlight other areas where light may provide additional control over end material properties.

[1] D.A. Beaton, A. Mascarenhas and K.Alberi, *J. Appl. Phys.*, **118**, 235701 (2015)

[2] K. Park and K. Alberi, *Scientific Reports*, **7**, 8516 (2017)

5:00pm **PCSI-MoA-37 Confined Lateral Overgrowth of Epitaxial InP Layers by Chemical Beam Epitaxy**, *Sukgeun Choi, B Markman, H Tseng, S Brunelli, A Goswami, D Pennachio, J Klamkin*, University of California, Santa Barbara; *M Rodwell*, University of California, Santa Barabara; *C Palmstrom*, University of California, Santa Barbara

Recently, tunnel field-effect transistors (T-FET) have received considerable attention as a promising candidate for next-generation logic devices beyond metal-oxide-semiconductor FETs. T-FETs offer a fast transition between *on* and *off* device states with low power consumption. However, since charge carriers must “tunnel” through the bandgap of the transistor source, T-FETs tend to suffer low *on*-state current, which in turn slows device operation. In an attempt to mitigate the issue with low *on*-state

current by increasing the tunnel probability, a confined hetero-junction T-FET has recently been proposed [1].

Here, we demonstrate lateral overgrowths of epitaxial InP thin layers inside three-dimensional confined structures defined by SiO<sub>2</sub> walls in chemical beam epitaxy on InP substrates for the development of high-performance III-V hetero-junction T-FETs. Figure 1 shows a schematic of substrate structure, growth process, and a resulting top-view scanning-electron micrograph.

Suppression of undesired parasitic nucleation on SiO<sub>2</sub> surfaces and growth of high-quality InP layers inside the confined structure are strongly influenced by surface chemistry and chemical reactions between precursor molecules and surfaces. Dependencies of structural properties of InP layers on growth parameters such as substrate crystallographic orientation, direction of lateral growth, growth temperature, and V/III ratio are discussed. Technical challenges in the substrate preparation procedures and characterization of thin layers formed inside confined structures are also addressed. Success of confined epitaxial lateral overgrowth would pave a pathway toward the monolithic three-dimensional integration of semiconductor hetero-structures for advanced electronic and photonic device technologies.

[1] P. Long et al., *IEEE Electron. Dev. Lett.* **37**, 345(2016).

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5:05pm **PCSI-MoA-38 Epitaxial Wafer Scale Growth of Tungsten Dichalcogenides**, *Tanushree Choudhury, M Chubarov, X Zhang, J Robinson, J Redwing*, The Pennsylvania State University

Transition metal dichalcogenides (TMDs) have been a focus of interest due to the direct band gap of the monolayers in the range of 1.6 – 2.0 eV and large exciton binding energies, which leads to interesting electronic and optical properties. One major challenge in harnessing the potential of these materials is the growth of high quality epitaxial mono- and few-layer films over large areas. The growth on C-plane sapphire is expected to lock the domain orientations at 0° and 60° due to the hexagonal symmetry, which can result in epitaxial TMD films with reduced high-angle grain boundaries.<sup>1</sup> Oriented growth for TMDs like MoS<sub>2</sub><sup>1</sup> and WSe<sub>2</sub><sup>2</sup> has been demonstrated by powder vapor transport on C-plane sapphire previously. However, we find that in a cold-wall metal organic chemical vapor deposition (MOCVD) process, even though this orientation relation is maintained for WSe<sub>2</sub>, this locking does not extend universally to WS<sub>2</sub>. The reason for this difference is crucial in not only obtaining oriented films but also understanding the basic interactions between the TMDs themselves and/or the precursors involved and the sapphire substrate.

In this work, WS<sub>2</sub> and WSe<sub>2</sub> mono- and few-layer films were deposited by MOCVD system on 2” C-plane sapphire wafers using tungsten hexacarbonyl (W(CO)<sub>6</sub>), hydrogen selenide (H<sub>2</sub>Se) and purified hydrogen sulfide (H<sub>2</sub>S). The growth was carried out for 1 h at 800- 900°C for WSe<sub>2</sub> and 850-1000°C for WS<sub>2</sub> to achieve fully coalesced films with domains on the order of 1 mm in size. The results show that there is a distinct difference in the growth of WSe<sub>2</sub> and WS<sub>2</sub> films. Though both WSe<sub>2</sub> and WS<sub>2</sub> have an epitaxial relation with the underlying sapphire substrate, the WSe<sub>2</sub> domains are predominantly oriented at 0° and 60°, but the WS<sub>2</sub> films show presence of domains at other angles as well. In case of WSe<sub>2</sub>, the orientation relation is maintained at all the growth temperatures investigated, but for WS<sub>2</sub>, the orientation is maintained at 0° and 30° at lower temperatures between 750-850°C. Additional orientations emerge at 900-1000°C. Further details about the epitaxial relation, the interface interaction and the differences in the growth of WS<sub>2</sub> and WSe<sub>2</sub> will be presented.

[1] D. Dumcenco, .D. Ovchinnikov, K. Marinov, P. Lazi, M. Gibertini, N. Marzari, O. L Sanchez, Y. C. Kung, D. Krasnozhan, M. W. Chen, S. Bertolazzi, P. Gillet, A. F. Morral, A. Radenovic, A. Kis, *ACS Nano*, **9**(4), **2015**, 4611–4620.

[2] L. Chen, B. Liu, M. Ge, Y. Ma, A. N. Abbas, C. Zhou\*, *ACS Nano*, **9** (8),**2015**, 8368–8375.

5:10pm **PCSI-MoA-39 Structural Phenomena at the 3D/2D Interface: Epitaxy of Metals on Transition Metal Dichalcogenides**, *Kayla Cooley, A Domask, R Alsaadi, S Mohney*, The Pennsylvania State University

Of the many emerging 2D materials, transition metal dichalcogenides (TMDs) are interesting for electronic and photonic devices as many of them are semiconducting when only a few layers thick, and they can be transferred onto flexible substrates. Successful application of these

materials relies on building a fundamental understanding of the interfaces between TMDs and other materials, such as metals. Although metal/TMD epitaxy has been reported in literature, it has been observed in only a few systems to date. Much remains to be learned about this interesting phenomenon, which could offer new insights into quasi-van der Waals epitaxy for the development of novel heterostructures and for electrical contacts that may be altered or improved through epitaxy.

This work investigates a series of transition metals deposited on TMDs ( $\text{MoS}_2$ ,  $\text{WSe}_2$ ) at room temperature to identify metals exhibiting epitaxy on TMDs and to determine factors controlling this growth. Each metal/TMD system was analyzed by transmission electron microscopy and selected area electron diffraction to identify phases present and their crystallographic orientation. Annealed samples (4h @ 400°C) were also examined to determine if thermal processing induced structural or chemical changes.

On  $\text{MoS}_2$ , many FCC metals from our work (Ag, Al, and Pd) and literature (Au, Pt, and Pb) - along with an HCP metal (Zn) from our work—were epitaxial with the following relationships:  $(111)_{\text{FCC}} \parallel (001)_{\text{TMD}}$  and  $\langle 110 \rangle_{\text{FCC}} \parallel \langle 110 \rangle_{\text{TMD}}$  or  $(0001)_{\text{HCP}} \parallel (0001)_{\text{TMD}}$  and  $\langle 11-20 \rangle_{\text{HCP}} \parallel \langle 11-20 \rangle_{\text{TMD}}$ . In all cases, the close-packed plane with hexagonal symmetry grows on the basal plane of  $\text{MoS}_2$ , although lattice mismatches range from 9.4-18.6%. Like all tested BCC metals (Mo and Mn), the FCC Ni and HCP Ru and Re metals were not epitaxial on  $\text{MoS}_2$ , despite providing similar symmetry and lattice mismatches. We have discovered a strong correlation between activation energy to surface diffusion available from DFT calculations [1] and metal epitaxy on  $\text{MoS}_2$ . Our work also suggests that additional variables, such as homologous temperature, correlate almost as well.

In expanding the study to include metal/ $\text{WSe}_2$  systems, a number of interesting differences were observed. Some metals were epitaxial on  $\text{WSe}_2$  but not on  $\text{MoS}_2$ . Conversely, FCC Pd was epitaxial on  $\text{MoS}_2$  after deposition, but it was epitaxial on  $\text{WSe}_2$  only after annealing. More modeling of the surface of  $\text{WSe}_2$  is needed to better understand these differences. Our ongoing work opens pathways for fundamental studies of Schottky barrier heights and the effect of atomic arrangement at the contact interface on this important parameter.

[1] W. A. Saidi, *J. Chem. Phys.* **141**, 094707 (2014)

**5:15pm PCSI-MoA-40 Temperature Dependence of Photoinduced Hydrogen Production and Simultaneous Purification in  $\text{TiO}_2$  Nanotubes/Palladium Bilayer Membrane**, *J. Asai, Kei Noda*, Keio University, Japan

Photocatalytic hydrogen ( $\text{H}_2$ ) production with widegap semiconductor materials has been expected as one of the new clean energy sources. To provide  $\text{H}_2$  gases for practical uses, all the  $\text{H}_2$  reforming units must be followed by hydrogen purification units for separating generated  $\text{H}_2$  from other byproduct and residual gases such as carbon dioxide and oxygen. This issue can limit the miniaturization of  $\text{H}_2$  production systems and the further development of on-site reformers toward mobile application of hydrogen energy. With this background, we have developed photoactive hydrogen production/separation membrane with a bilayer structure of an oxidized titanium dioxide ( $\text{TiO}_2$ ) nanotube array (TNA) and a hydrogen permeation film of palladium (TNA/Pd membrane) [1,2].

In this work, the temperature dependence of photoinduced  $\text{H}_2$  production and purification in the TNA/Pd membrane was examined. This membrane was fabricated by transferring a TNA embedded in a titanium foil onto an electrodeless-plated 10- $\mu\text{m}$ -thick palladium film. This membrane can reform a methanol/water (1:1) mixture photocatalytically under ultraviolet (UV) irradiation and concurrently purify generated hydrogen gas through the Pd layer. The  $\text{H}_2$  production rate ( $r_{\text{H}_2}$ ) with the membrane at various temperatures was evaluated by using a home-made characterization system (Fig. 1(a)). As shown in Fig. 1(b), the measured  $r_{\text{H}_2}$  showed larger values at higher temperature of the membrane.  $r_{\text{H}_2}$  increased abruptly after several hours of UV irradiation and this inflection point appeared faster at higher temperature of the membrane. These behaviors can be probably related to the permeation characteristics of hydrogen through the Pd layer.

[1] M. Hattori, K. Noda, and K. Matsushige, *Appl. Phys. Lett.* **99**, 123107 (2011).

[2] M. Hattori and K. Noda, *Appl. Surf. Sci.* **357**, 214 (2015).

**5:20pm PCSI-MoA-41 Structural Properties and Carrier Transport in Axial Silicon-Germanium Nanowire Heterojunctions**, *X Wang, Leonid Tsybeskov*, New Jersey Institute of Technology; *T Kamins*, Stanford University; *X Wu*, D Lockwood, National Research Council Canada, Canada

Recent advances in forming semiconductor heterojunctions within spatially confined nanoscale objects, including nanowires (NWs), show that the traditional limitations in the lattice-mismatched hetero-growth can be challenged. In various III-V semiconductor NWs, abrupt heterojunctions have been successfully demonstrated using the vapor-liquid-solid (VLS) growth for GaAs/InAs (7% mismatch) and InAs/InP (3% mismatch) heterojunctions. In group IV semiconductors, the approach is complicated not only by the 4.2% lattice mismatch between Si and Ge but also because Si and Ge both have a quite high solubility in the Au-Si catalyst. During chemical vapor deposition (CVD) based VLS growth using  $\text{SiH}_4$  and  $\text{GeH}_4$  (or similar gases), a supply of Si remains effectively "on" in the catalyst, and Si effectively intermixes with the arriving Ge even if the  $\text{SiH}_4$  flow is already switched "off". One way to address this problem is to choose a catalyst with a lower Si solubility, e.g. AlAu<sub>2</sub> and AgAu. Another possibility is to significantly reduce growth temperature before turning a  $\text{GeH}_4$  source "on". Using the latter technique, we demonstrated Si-Ge heterojunction NWs with nearly ideal interface (Fig. 1) and only an 8 nm thick SiGe transition layer between straight and nearly micron-long Si and Ge NW segments [1].

In this work, we analyzed structural and electrical properties of axial Si-Ge heterojunction nanowires (NWs). The observed non-linear and rectifying current-voltage characteristics, strong flicker noise and damped current oscillations with frequencies of 20-30 MHz are explained using the proposed SiGe heterojunction NW energy band diagram including the energy states associated with the NW surface (and near-surface) structural imperfections revealed by transmission electron microscopy.

[1] Wang, X., et al. *Journal of Applied Physics* **118**.23 (2015): 234301.

**5:25pm PCSI-MoA-42 High Performance InAs Quantum Dot Lasers Grown on on-axis (001) Si with Low Threading Dislocation Density**, *Daehwan Jung, J Norman, M Kennedy, C Shang*, University of California, Santa Barbara; *R Herrick*, Intel Corp.; *Y Wan, B Shin, I MacFarlane, C Jan, A Gossard, J Bowers*, University of California, Santa Barbara

InAs quantum dots (QDs) epitaxially grown on Si are promising for efficient, scalable, and reliable light source for Si-based photonic integrated circuits. The effective lateral carrier confinement in QDs makes themselves less sensitive to threading dislocations that inevitably occur from the growth of GaAs on Si. Most of the previous research on QD lasers on Si employed intentional off-cut (4-6 °) substrates to circumvent electrically active antiphase domains that arise at the polar/non-polar interface. To be fully compatible with CMOS foundries, on-axis Si substrates have been recently used via various growth techniques, but the QD laser performance has been considerably diminished mainly due to the high threading dislocation density (TDD).

In this work, we demonstrate high performance 1.3  $\mu\text{m}$  quantum dot lasers epitaxially grown on on-axis (001) Si using molecular beam epitaxy [1]. Thermal cycle annealing and strained-layer superlattices were performed, and the TDD was reduced from  $\sim 3 \times 10^8 \text{ cm}^{-2}$  to  $\sim 8 \times 10^6 \text{ cm}^{-2}$  in the metamorphic GaAs buffer layer on Si. A sample with one QD layer for photoluminescence was grown, and a very small full-width at half-maximum of 28 meV was measured at room temperature (Figure 1-a). Uncapped QDs also revealed a highly homogeneous height distribution with a density of  $\sim 5.2 \times 10^{10} \text{ cm}^{-2}$ . The high quality GaAs/Si template enabled record-low threshold current of 6.2 mA (Figure 1-b) at 20 °C. Lifetime tests were performed at Intel Corp., and the devices revealed extrapolated mean-time-to-failure (double initial threshold current) of more than one million hours for CW operation at 35 °C, which is a record-long lifetime for any lasers grown on on-axis (001) Si.

**5:30pm PCSI-MoA-43 Atomistic Mechanisms of Orientation and Temperature Dependence in Gold-Catalyzed Silicon Growth**, *Yanming Wang*, Massachusetts Institute of Technology; *A Santana*, Beijing Computational Science Research Center; *W Cai*, Stanford University

Gold-catalyzed vapor-liquid-solid (VLS) growth is widely used in the synthesis of silicon-based low-dimensional nano-structures. However, growth anomalies are often observed [1, 2], whose formation is believed to highly depend on the growth orientation and temperature, but a complete understanding has not been achieved yet. In this talk, we present a systematic study on the orientation and temperature dependences in the VLS process [3], by means of long molecular dynamics (MD) simulations up to 100 ns using an MEAM potential that well reproduces the binary phase

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diagram [4]. The Si growth velocities are extracted from the simulations under various conditions for  $\langle 110 \rangle$  and  $\langle 111 \rangle$  orientations respectively. Our data suggest a linear dependence of the growth velocity on the Si supersaturation for  $\langle 110 \rangle$  growth, in contrast to a non-linear dependence for  $\langle 111 \rangle$  growth. By analyzing the surface morphologies, this difference is linked to the continuous growth mechanism on  $\{110\}$  substrate and the island nucleation controlled growth on  $\{111\}$  substrate. Furthermore, we find that the  $\langle 111 \rangle$  growth in our MD simulations operates in the regime where the nucleation rate is higher than the island expansion rate. This is traced to the formation of a gold saturated monolayer above the nucleated Si island, impeding its further growth. Also, it is found that the temperature dependent atom activity near the  $\{111\}$  interface is lower, explaining the smaller growth velocity of the  $\{111\}$  surface than that of the  $\{110\}$  surface.

[1] V. Schmidt, S. Senz and U. Gösele, *Nano letters***5**, 931 (2015).

[2] Y. Li, Y. Wang, S. Ryu, A. F. Marshall, W. Cai, and P. C. McIntyre, *Nano letters* **16**, 1713 (2016).

[3] Y. Wang, A. Santana and W. Cai, *Journal of Applied Physics*, **122**(8), 085106 (2017).

[4] S. Ryu and W. Cai, *Journal of Physics: Condensed Matter***22**, 055401 (2010).

5:35pm **PCSI-MoA-44 Evaluation of Strain in the Oxide Covered Silicon Nanowires for Thermoelectric Devices by Raman Spectroscopy**, *Ryo Yokogawa*, Meiji University, Japan; *S Hashimoto, M Tomita, T Watanabe*, Waseda University, Japan; *A Ogura*, Meiji University, Japan

Silicon nanowires (SiNWs) are promising candidates for the thermoelectric devices as well as next-generation channel materials of surrounding gate field-effect transistors. Especially SiNWs with cover oxide is recognized as a promising new thermoelectric material owing to their low dimensionality and the disorder strain induced at the  $\text{SiO}_2/\text{SiNWs}$  interface. To realize SiNW devices with high electric and thermoelectric performances, further improvements through the optimization of strain in the NWs are necessary to achieve a higher mobility and a lower thermal conductivity. Raman spectroscopy is a powerful strain evaluation technique in the nanostructures, because it has advantages such as a high spatial resolution and a nondestructive measurement. In this study, we evaluated the strain in the oxide covered SiNWs. We fabricated SiNWs using silicon-on-insulator (SOI) wafers with thermal oxidation under various conditions. We also performed small amount of  $\text{Ar}^+$  ion irradiation to modify the  $\text{SiO}_2/\text{SiNW}$  interface (25 keV,  $1.0 \times 10^{14} \text{ cm}^{-2}$ ).

As a result, before  $\text{Ar}^+$  ion irradiation, the anisotropic biaxial stresses of the along the SiNW length and width directions were confirmed to be compressive and tensile stress, respectively. On the other hand, after  $\text{Ar}^+$  ion irradiation, we confirmed that the stress of the along the SiNW length direction became tensile stress, and the stress of the along the SiNW width direction was almost completely relaxed. We consider that an oxide-induced lattice disorder of the SiNW is relaxed by breaking strained bonds at  $\text{SiO}_2/\text{SiNW}$  interface by the ion irradiation, and tensile stress along the long direction in the SiNW is induced by SiNW lattice disorder. In conclusion, we evaluated the strain induction mechanism in the SiNW by Raman spectroscopy, sensitively.

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