Tuesday Morning, January 21, 2025

PCSI
Room Keahou I - Session PCSI-TuM1
Oxide Semiconductor Materials I

Moderator: Bharat Jalan, University of Minnesota

8:30am **PCSI-TuM1-1 Atomistic Simulations for Understanding the Behavior of Dopants and Impurities in Ga2O3 and Related Alloys***, **Joel Varley**,* Lawrence Livermore National Laboratory **INVITED**

Gallium oxide (Ga_2O_3) is rapidly developing as one of the most promising ultra-wide bandgap platforms for next-generation power electronics owing to properties like a high breakdown field, controllable (*n*-type) electrical conductivity, and commercially-available single-crystal substrates that can be grown via a number of industrially-scalable processes. Beyond exhibiting a number of polymorphs with similarly attractive properties, alloying with Al into Ga_2O_3 to form $(Al_xGa_{1-x})_2O_3$ (AGO) alloys can lead to a significant increase of the band gap to potentially access higher power device figures of merit, analogous to the AlGaN system but spanning a much larger rage of ~4.8 eV-8.6 eV. Despite the progress with Ga_2O_3 and related alloys, a number of open questions remain on the nature of fundamental defects and the role of impurities and dopants in determining the observed optical and electrical properties of these materials. This is even more of an open question in the lesser studied alloys like AGO, particularly regarding the effectiveness of donor doping and how to overcome the possibility of compensation in the limit high Al-contents. In this work we survey the current understanding of point defects in Ga_2O_3, focusing on their potential optical and electrical consequences from insights gained through first-principles-based calculations employing hybrid functionals. We discuss what is known about donor and acceptor dopants, as well as their interactions with native defects and impurities incorporated through growth and processing steps. These results provide guidance for controlling defect populations and the electrical conductivity in Ga_2O_3 and related alloys and for facilitating next-generation power electronics based on this ultra-wide bandgap semiconductor family.

This work was partially performed under the auspices of the U.S. DOE by Lawrence Livermore National Laboratory (LLNL) under contract DE-AC52-07NA27344 and partially supported by Laboratory Directed Research and Development funding under project number 22-SI-003 and by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. DOE EERE AMMTO.

9:10am **PCSI-TuM1-9 UPGRADED: What Happens When a Dopant Doesn'T Go Where You Expect It to Go? The Case of MBE-Grown Yb-Doped $SrTiO_3$ on Si(001)***, **Scott Chambers**,* Pacific Northwest National Laboratory*; E. Ramerez, D. Guragain, J. Ngai,* University of Texas at Arlington*; P. Sushko, K. Koirala, Y. Du, N. Govind, M. Bowden,* Pacific Northwest National Laboratory*; D. Biswas, T. Lee,* Diamond Light Source, UK*; C. Weiland,* National Institute of Standards and Technology (NIST)*; J. Woicik,* National Institute for Science and Technology (NIST)

We present the structural and electronic properties of Yb-doped $SrTiO_3$/Si(001) grown by molecular beam epitaxy. Other rare-earth dopants that result in *n*-type conductivity in the ABO_3 perovskite lattice typically substitute for Sr at the *A*-sites. In contrast, Yb is shown to substitute predominantly for Ti at the perovskite *B*-sites based on data from atomically resolved scanning transmission electron microscopy and energy dispersive spectroscopy, as well as extended x-ray absorption fine structure measurements. An atom beam flux (f) mismatch was present during film deposition because it was *assumed* that Yb would occupy *A*-sites. As a result, the fluxes were set such that $f_{Yb} + f_{Sr} = f_{Ti}$. The formation of Yb_{Ti} rather than Yb_{Sr} results in Sr vacancies and extraneous (i.e. non-lattice) Ti atoms in the films. Yb exhibits two distinct charge states as determined by x-ray absorption spectroscopy and associated theoretical modeling, +2.7 and +2.1. These aliovalent dopants are compensated by donor electrons from oxygen vacancies that form during epitaxial film growth. The defect complexes resulting from the flux mismatch, together with oxygen vacancies, lead to deep-level electron traps that were detected by resonant photoemission and predicted to be stable by *ab initio* theory, as well as much higher sheet resistance than that associated with, for instance, La-doped $SrTiO_3$ films. *Ab initio* calculations show that the preference for *B*-site occupancy is driven by low oxygen chemical potential at the growth front as required to successfully deposit epitaxial STO on Si without amorphous SiO_2 formation at the interface.

9:30am **PCSI-TuM1-13 Thickness-Dependent Optical Constants of SnO_2 Thin Films on Si Grown by Atomic Layer Deposition***, **Yoshitha Hettige**, S. Zollner,* New Mexico State University*; A. Pratap Singh, B. Dutta, S. Chattopadhyay,* Indian Institute of Technology Indore, India

Zinc oxide (ZnO) and strontium titanate ($SrTiO_3$) have tunable optical constants that can be useful for optoelectronic applications. We study a third oxide, tin oxide (SnO_2), and investigate if its optical constants are also tunable. SnO_2 is a wide band gap semiconductor with attractive electrical, optical, *etc* properties. It is commonly used in gas sensors, solar cells, batteries, and energy-saving coatings. SnO_2 thin films were grown on a Si substrate using atomic layer deposition.

X-ray reflectivity (XRR) was performed for each SnO_2 thin film on Si. It was found that the SnO_2 thin film thicknesses are around 10-60 nm with an approximately 2 nm thick SiO_2 interfacial layer due to the wet cleaning before the deposition. We measured the ellipsometric angles ψ and Δ of SnO_2 thin films on Si at room temperature on a J. A. Woollam UV ellipsometer at 65° to 75° angles of incidence from 0.5 to 6.5 eV. We used a Tauc Lorentz oscillator to model the data for SnO_2 thin films. After obtaining a reasonable fit for SnO_2, we also performed a uniqueness fit for the film thickness. We compared the film thickness from all three techniques; XRR, Tauc Lorentz fit, and uniqueness fit. Finally, we extracted the dielectric function (ε) of the SnO_2 thin film from the obtained Tauc-Lorentz fit and compared it with all samples. The results show that the dielectric function (real ε_1 and imaginary ε_2 part) varies with thickness by no more than 15%. This observation is probably because of the weaker excitonic effects in SnO_2 or because the excitonic effects are not screened as for ZnO or $SrTiO_3$.

9:35am **PCSI-TuM1-14 Regulating the Phase Transition of Vanadium Dioxide Thin Films***, **Manish Kumar**, S. Rani, H. Lee,* Pohang Accelerator Laboratory, POSTECH, Republic of Korea

Vanadium dioxide (VO_2) is a popular thermochromic material owing to its potential applications in intelligent windows, sensors, and diverse electronic devices. VO_2 displays a distinctive metal-insulator transition (MIT) that occurs around 68°C temperature, which is accompanied by a structural transition and a dramatic change in the optical properties [1]. During this transition, the material shifts between its low-temperature insulating (transparent to near infrared rays) monoclinic phase (M1) and its high-temperature metallic (opaque to near infrared rays) rutile phase (R). From application perspective, it is highly imperative to stabilize VO_2 thin films with control on the phase transition properties. Ion-implantation is one of the effective route to tune the properties of VO_2 thin films [2, 3]. In the present work, we have studied B+ ion implanted VO_2 thin films.

Thin films of VO_2 were prepared by radio frequency (RF) magnetron sputtering technique. Apart from the pristine sample, three samples were implanted by B+ ions at different fluence ranging 5×10^{13} ions/cm^2 to 5×10^{14} ions/cm^2. B+ ions implanted VO_2 thin films revealed modified structural, electrical and optical properties. Structural phase transition and MIT temperatures were found to decrease with increasing implantation dose. Moreover, for ion-implanted VO_2 thin films, temperature dependent transmittance measurements depicted the shift in optical transition towards room temperature side. Such control of phase transition in VO_2 thin films is very crucial for device applications.

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[3] Qi Jia, Jörg Grenzer, Huabing He, Wolfgang Anwand, Yanda Ji, Ye Yuan, Kai Huang, Tiangui You, Wenjie Yu, Wei Ren, Xinzhong Chen, Mengkun Liu, Stefan Facsko, Xi Wang, Xin Ou Adv. Mater. Interfaces 5(8), 1701268 (2018).

9:40am **PCSI-TuM1-15 Formation of Transparent and Conductive SWCNT/SiO2 Composite Thin-Films on Pet Substrates Using Molecular Precursor Method***, **Hiroki Nagai**, K. Igarashi, M. Sato,* Kogakuin University, Japan

Transparent conductive films (TCF) are essential for optoelectronic devices, such as transparent electrodes for light-emitting diodes and solar cells. Transparent thin films of indium tin oxide (ITO) and fluorine tin oxide (FTO) on glass substrates are the most widely used for these purposes [1]. These typical TCO thin films provide an electrical resistivity of 10^{-3} Ω·cm and a high transmittance of over 80% in the visible-light region. Carbon nanotubes (CNTs)/inorganic composites have received much attention due to their optical, mechanical, electrical, and thermal properties. However, the poor adhesion of CNTs onto the substrate becomes a problem during the usage. SiO_2 is a highly transparent insulating material in the UV, visible, and infrared regions. Therefore, if conductivity can be added to SiO_2, it will become a new transparent conductive film with high adhesion. The single-walled carbon nanotube (SWCNT)-silica composite thin film on a quartz glass was formed by ultraviolet irradiation (20–40 °C) onto a spin-coated precursor film. With 7.4 mass% SWCNTs, the electrical resistivity reached 7.7×10^{-3} Ω·cm after UV irradiation. The transmittance was >80% at 178–2600 nm and 79%–73% at 220–352 nm. Heat treatment increased the transparency and pencil hardness without affecting the low electrical resistivity. Raman spectroscopy and microscopic analyses revealed excellent film morphology with good SWCNT dispersal. The low refractive index (1.49) and haze value (<1.5%) are invaluable for transparent windows for novel optoelectronic devices. Herein, we also report a promising composite thin film as a transparent and conductive material on PET (polyethylene terephthalate) substrates for flexible transparent conductive films.

9:45am **PCSI-TuM1-16 Phototransistor Array Based on Plasma-Engineered Amorphous Metal Oxide Semiconductors with Ferroelectric Dielectrics***, **Uisik Jeong**, S. Kim,* Sungkyunkwan University (SKKU), Republic of Korea

The potential for next-generation electronic applications has expanded significantly with the development of energy-efficient, high-performance broadband photodetectors utilizing cost-effective amorphous metal oxide semiconductors. Current commercially available photodetectors use various semiconductors to detect light across different wavelengths, from ultraviolet (UV) to near-infrared (NIR). However, their versatility is limited by the need for specific materials to target different wavelengths. This study explores the use of indium gallium zinc oxide (IGZO) as a metal oxide semiconductor, eliminating the need for additional external photo absorption layers. To enhance charge carrier generation and create subgap states in the IGZO film, hydrogen (H2) plasma treatment was applied, enabling wide-spectrum detection from UV to NIR without extra layers. Furthermore, a ferroelectric and high-k dielectric was introduced as the gate dielectric to induce a strong electric field in the channel, resulting in low-power operation. The H2 plasma-treated IGZO phototransistors demonstrated ultra-high photoresponsivity and detectivity over a broad range of wavelengths (400 to 1000 nm), making them a promising candidate for next-generation optoelectronic devices. This study presents a favorable approach for advancing energy-efficient, cost-effective, and high-performance broadband photodetectors.

9:50am **PCSI-TuM1-17 Improvement of Electrical Properties and Low-Temperature Development of Sol-gel Processed In-Ga-Zn-O Thin-Film Transistors Using UV-DI***, **Giyoong Chung**, y. kim,* Sungkyunkwan University (SKKU), Republic of Korea

The vulnerability of solution-processed metal-oxide semiconductors is significantly influenced by organic chemical-induced defects such as voids, holes, and organic residues. Moreover, solution-processed Oxide TFTs require a high temperature process to vaporize various organic compounds. Hydroxyl radicals (OH•), known as strong oxidants, are effective in eliminating and decomposing organic compounds.

In this study, we introduced UV-DI with hydroxyl radicals into the IGZO Sol-Gel mixture to produce lower boiling points components and deposit IGZO active layers with fewer defects. Hydroxyl radicals were generated in deionized (DI) water through an O_3/UV process, confirmed via potassium iodide (KI) and ultraviolet-visible (UV-vis) spectroscopy analysis. The intensity of the absorbance peaks at wavelengths of 290 nm and 350 nm increased with longer UV irradiation times. Additionally, we found that the density of hydroxyl radicals in DI water could be modified by adjusting the initial volume of DI water while maintaining the same UV irradiation duration. A DI water volume of 4.5 ml resulted in a higher concentration of hydroxyl radicals compared to 1.5 ml of DI water. Thermogravimetric and differential scanning calorimetry (TG-DSC) analysis revealed that the organic materials in the IGZO solution mixture with UV-DI treatment began to decompose at a lower temperature (121.6℃) than those in the pristine IGZO mixture (144.5℃). An abrupt weight loss was also observed in the IGZO solution with UV-DI compared to the pristine IGZO solution.The field-effect mobility and sub-threshold slope of the a-IGZO TFTs made with ozonated water were improved compared to the conventional process, increasing from 1.37 to 1.44 cm^2/V·s and decreasing from 0.24 to 0.20 V/dec, respectively. In addition, threshold voltage shifts over 7000 seconds under negative-bias stress conditions (NBS) were -7.25 V and -5.67 V for pristine IGZO and IGZO with UV-DI, respectively.

These results suggest that the addition of ozonated water to the sol-gel mixture is a simple method to achieve high-performance TFTs by reducing organic chemical-induced defects through low-temperature processing.

9:55am **PCSI-TuM1-18 A Study on the Impact of Thin Metal Films on Contact Resistance in IGZO FET***, **Juseong Min,*** Sungkyunkwan University, Samsung Electronics, Republic of Korea

Indium gallium zinc oxide (IGZO) is regarded as a highly promising material in semiconductor applications such as thin-film transistors (TFTs) and memory devices, due to its excellent properties, including low leakage current and high electron mobility [1,2]. However, there are still unresolved issues with IGZO, one of which is the high contact resistance between IGZO and source/drain electrodes, which significantly affects the performance of miniaturized transistor devices. Therefore, understanding and improving the contact resistance of IGZO is essential [3]. Various factors influence the contact resistance between IGZO and metals, but the metal's work function and the interaction between the metal and IGZO are particularly critical [4,5].

In this study, various thin metal films with a thickness of less than 5 nm were inserted between the electrodes and IGZO in transmission line model (TLM) devices to investigate the effect of metal oxide formation on contact resistance (fig.1). Based on these results, we analyzed how the metal's work function, oxidation tendency, and the band structure of metal oxides influence the contact properties with IGZO, and proposed strategies to effectively reduce contact resistance. These findings are expected to serve as valuable foundational data for improving the performance of various IGZO-based semiconductor devices.

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10:00am **PCSI-TuM1-19 Exploration of VO_2 Thin Films with Oxygen Deficiency***, **SUNITA RANI**, M. KUMAR, H. LEE,* Pohang Accelerator Laboratory, POSTECH, Republic of Korea

VO_2 has captured the attention of researchers due to its thermochromic properties and rapid semiconductor-to-metal transition. The semiconductor-to-metal shift occurs within the monoclinic M1 phase around 343K, coupled with a transformation from monoclinic to rutile crystal structure. The transparency of the monoclinic phase to near-infrared (NIR) radiation stands in contrast to the NIR opaqueness of the rutile phase. Maintaining precise stoichiometry in VO_2 is crucial, as even slight adjustments in oxygen levels can lead to the stabilization of different VO_2 polymorphs. Additionally, fine-tuning the stoichiometry offers a means of controlling the characteristics of VO_2. With this motivation, we have prepared stoichiometric and oxygen deficient VO_2 thin films on differently oriented sapphire substrates by radio frequency (RF) sputtering technique. The stoichiometric VO_2 thin films depicted characteristic semiconductor to metal transition around 343K. We noticed a complete suppression of semiconductor to metal transition in oxygen deficient VO_2 thin films and a metallic behavior was seen throughout the studied temperature range i.e. 273K to 373K. Oxygen deficiency led to significant modifications in the structural, electronic and optical properties of VO_2 thin films.

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