PCSI

Room Canyon/Sugarloaf - Session PCSI-1MoM

Oxides

Moderator: Tohru Honda, Kogakuin University

8:30am **PCSI-1MoM-1 MOCVD Epitaxy and Doping for β-Ga_2O_3 and $(Al_xGa_{1-x})_2O_3$**, ***Hongping Zhao,*** The Ohio State University **INVITED**

Ultrawide bandgap (UWBG) gallium oxide (Ga_2O_3) represents an emerging semiconductor material with excellent chemical and thermal stability. It has a band gap of 4.5-4.9 eV, much higher than that of the GaN (3.4 eV) and 4H-SiC (3.2 eV). The monoclinic β-phase Ga_2O_3 represents the thermodynamically stable crystal among the known five phases (α, β, γ, d , ε). The breakdown field of β-Ga_2O_3 is estimated to be 6-8 MV/cm, which is much larger than that of the 4H-SiC and GaN. These unique properties make β-Ga_2O_3 a promising candidate for high power electronic device and solar blind photodetector applications. Single crystal β-Ga_2O_3 substrates can be synthesized by scalable and low cost melting based growth techniques. Metalorganic chemical vapor deposition (MOCVD) growth technique was used to develop high quality β-Ga_2O_3 thin films and its ternary alloy $(Al_xGa_{1-x})_2O_3$. Control of background and n-type doping in β-Ga_2O_3 will be discussed. Record carrier mobilities of 184 $cm^2/V{\cdot}s$ at room temperature and 4984 $cm^2/V{\cdot}s$ at low temperature (45 K) were measured for β-Ga_2O_3 thin films with room-temperature doping concentrations of $2.5{\times}10^{16}$ and $2.75{\times}10^{16}$ cm^{-3}, respectively [1]. Growth and fundamental understanding of $(Al_xGa_{1-x})_2O_3$ are still lacking. The limit of Al incorporation in beta-phase Ga_2O_3 has not been understood or experimentally verified, although it was predicted up to 60% of Al composition could be incorporated into β-Ga_2O_3. N-type doping capability as a function of Al composition in $(Al_xGa_{1-x})_2O_3$ is another important fundamental question. Carrier transport properties in $(Al_xGa_{1-x})_2O_3$ will be discussed.

Acknowledgement: The authors acknowledge the funding support from the Air Force Office of Scientific Research FA9550-18-1-0479 (AFOSR, Dr. Ali Sayir) and the National Science Foundation (1810041).

[1] Z. Feng, AFM Bhuiyan, M. R. Karim, H. Zhao, Appl. Phys. Letts, 114, 250601 (2019).

9:10am **PCSI-1MoM-9 Atomic Structure and Electronic Properties of the Non-Polar In_2O_3 and β-Ga_2O_3(100) Surfaces**, *C Schulze, R Zielinski, J Hofmann, C Bruckmann,* Technische Universität Berlin, Germany*; Z Galazka,* Leibniz-Institut für Kristallzüchtung Berlin, Germany*;* ***Holger Eisele,*** Technische Universität Berlin, Germany

In_2O_3 and β-Ga_2O_3 belong to the transparent conducting oxides (TCOs), being promising candidates for a wide field of applications like in solar cells, in detectors, and for high-power devices. In order to achieve high efficiency in electronic and opto-electronic devices a variety of prerequisites are necessary, as e.g., high crystal quality with low defect densities, adjustable conductivity by doping, controllable surfaces and interfaces, etc. Especially the doping mechanisms and the resulting high electron mobility are still under broad discussion for sesquioxide material: Mainly oxygen vacancies are under strong debate about their functionality [1]. We use scanning tunneling microscopy (STM) and spectroscopy (STS) in order to analyze the atomic structure of the non-polar surfaces. Since non-polar surfaces typically show no intrinsic surface states within the fundamental band gap of semiconductor materials, it is furthermore possible to study bulk and doping states using these methods [2].

Both semiconductors, In_2O_3(111) and β-Ga_2O_3(100) show at their respective non-polar surface a 1×1 surface unit cell without reconstruction upon *in situ* cleavage. We found the unreconstructed surface unit cell in the case of In_2O_3(111) in empty state images with atomic resolution. In respective room-temperature STS spectra we can identify the conduction band contribution, the direct and the indirect valence band as well as at least 3 intrinsic states being located within the band gap. Due to the variation of the growth parameter we can assign at least some of these states to charge transfer levels of impurities and vacancies. Since the Fermi level is located within the fundamental band gap, we can exclude an intrinsic electron accumulation for the freshly cleaved surface, while in air aged samples show a strongly different behavior, i.e. metallic appearance as in the case of a surface electron accumulation.

The β-Ga_2O_3(100) surface also shows atomic resolution in empty state images. Even more, we can identify single dopant atoms. In the corresponding STS spectra we can assign the conduction band contribution and again charge transfer levels, originating most likely from vacancies of the three differently coordinated oxygen atom positions within the unit cell. Even more, we can identify a charge transfer level, which we can assign to Si doping. Due to our findings from differently doped samples we conclude that the conductivity from unintentionally doped β-Ga_2O_3(100) can be assigned to background doping by Si.

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9:15am **PCSI-1MoM-10 Growth and Structures of Metal Dopant-Ceria Mixed Oxide Interfaces**, *E Ginting, L Du,* ***Jing Zhou,*** University of Wyoming

Ceria has been widely studied as an oxidation-reduction catalyst due to its unique redox properties and oxygen storage capacity [1]. The addition of other metal elements such as Ti and Mn into ceria could better enhance its thermal stability and improve its redox properties and oxygen storage capacity. To understand the chemistry of doped-ceria mixed oxides, it is of crucial importance to determine their surface structures at the fundamental level. We present our study on the growth of ceria thin films with Ti and Mn dopants and the understanding of their structures using X-ray photoelectron spectroscopy, low-energy electron diffraction, as well as scanning tunneling microscopy. Well-ordered CeO_x(111) with controlled degree of Ce reduction and atomic structures can be prepared on a Ru(0001) single crystal substrate [2]. Metal-doped ceria mixed oxide interfaces were prepared by depositing Ti or Mn over CeO_x(111) thin films. C o-deposition of Ce with metal dopants can produce well-ordered $Ce_{1-x}M_xO_{2-\delta}$(111) mixed oxide films (M=Ti, Mn) [3]. Dopant types and compositions can influence the surface structures, electronic structures, and redox properties of ceria. Effects of Mn and Ti dopants in ceria were investigated for Ni as steam reforming of ethanol catalysts for energy production . Compared to pure ceria, addition of metal dopants in ceria can provide unique anchoring sites and interaction for deposited Ni, which can significantly stabilize Ni as small metal nanoparticles upon heating. Additionally, modified structures and electronic properties of ceria by dopants offer alternative adsorption and reaction sites and provide promotional effects in the resistance of the coke formation over deposited Ni nanoparticles in the adsorption and reaction of ethanol. The research is sponsored by the National Science Foundation (Award Number: CHE1151846).

[1] A. Trovarelli, *Catalysis by Ceria and Related Materials*, Imperial College Press: London (2002).

[2] Y. H. Zhou, J. M. Perket, A. B. Crooks, J. Zhou, *J. Phys. Chem. Lett.***1, (9)**, 1447-1453 (2010).

[3] Y. H. Zhou, J. Zhou, *J. Phys. Chem. Lett.***1, (11)**, 1714-1720 (2010).

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9:20am **PCSI-1MoM-11 Freestanding Crystalline Oxide Membranes and Heterostructures**, ***Seung Sae Hong,*** Stanford University **INVITED**

The ability to create and manipulate materials in two-dimensional (2D) form has repeatedly had transformative impact on science and technology. In parallel with the exfoliation and stacking of intrinsically layered crystals, the atomic-scale thin film growth of complex materials has enabled the creation of artificial 2D heterostructures with novel functionality and emergent phenomena, as seen in perovskite oxides. We present a general method to create freestanding complex oxide membranes and heterostructures with millimeter-scale lateral dimensions and nanometer-scale thickness [1]. This facilitates many new opportunities we are beginning to explore, and here we focus on probing the nanomechanical response and the application of extreme strain states [2].

[1] D. Lu, D. J. Baek, S. S. Hong, L. F. Kourkoutis, Y. Hikita, and H. Y. Hwang, Nat. Mater. **15**, 1255 (2016).

[2] S. S. Hong, M. Gu, M. Verma, V. Harbola, B. Y. Wang, D. Lu, A. Vailionis, Y. Hikita, R. Pentcheva, J. M. Rondinelli, and H. Y. Hwang, *in revision*.

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10:00am **PCSI-1MoM-19 Effects of Annealing on Electronic Defects in β-Ga_2O_3 Revealed by Linearly-Polarized Photoluminescence (LPPL)**, *R Sun, Y Ooi, P Ranga,* University of Utah*; M Saleh, K Lynn,* Washington State University*; S Krishnamoorthy,* ***Mike A. Scarpulla,*** University of Utah

β-Ga_2O_3 is of high interest for high voltage and high-power DC and microwave applications. Annealing in different ambient environments can be used to manipulate the point defect populations as a function of depth, both to understand populations induced by growth processes and then to use this understanding to optimize properties for applications. Here, we report on our studies of electronic defects using unique linearly-polarized photoluminescence (LP-PL). We utilize annealing in different atmospheres to manipulate defects. We find intriguing differences between responses of bulk crystals and epilayers gown on various substrates, elucidating the

unanticipated confounding effects of substrates. We use these comparisons to help to sort out the myriad possible hypotheses for which combinations of defects produce the observed changes. We attempt to unify our results with prior literature and interpretations.

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