

Thursday Morning, December 6, 2018

Thin Films

Room Naupaka Salons 4 - Session TF-ThM

Nanostructured Surfaces and Thin Films: Synthesis and Characterization III

8:00am **TF-ThM-1 Interface and Surface Control of MoS₂-based Nanoelectronic Devices with Organic Treatment**, *Takhee Lee*, Seoul National University, Republic of Korea

Transition metal dichalcogenide (TMD) two-dimensional (2D) atomic layered materials have recently drawn considerable attention as promising semiconductors for future ultrathin layered nanoelectronic device applications. Unlike graphene, TMD materials have a semiconductor band gap, for example, molybdenum disulfide (MoS₂) that has been widely studied is known to have a direct band gap of ~1.9 eV as a single MoS₂ layer and an indirect band gap of ~1.2 eV as a bulk MoS₂ crystal.

In this talk, I will present our group research works on MoS₂-based nanoelectronic devices. In particular, I explain the following topics on the electrical properties of MoS₂ FETs; the effect by the environments such as oxygen and water [1], gate bias stress-dependent device instability [2], interface control by high energetic proton beam irradiation [3], surface treatment by molecules for sulfur vacancy passivation of MoS₂ [4], and hybrid devices of organic materials and MoS₂ [5].

References

- [1] W. Park et al., *Nanotechnology*, 24, 095202 (2013)
- [2] K. Cho et al., *ACS Nano*, 7, 7751 (2013).
- [3] T.-Y. Kim et al., *ACS Nano*, 8, 2774 (2014).
- [4] K. Cho et al., *ACS Nano*, 9, 8044 (2015); K. Cho et al. *Adv. Mater.* 30, 1705540 (2018).
- [5] J.-K. Kim et al., *Scientific Reports*, 6, 36775 (2016); J. Pak et al., *Nanoscale*, 7, 18780 (2015).

8:40am **TF-ThM-3 Epitaxial GdFe_{0.8}Ni_{0.2}O₃ Multiferroic Thin Films Grown Device Using Operando X-ray Technique**, *Shu-Jui Chang, M Chung*, National Chiao Tung University, Republic of China; *Y Liu, H Lee*, National Synchrotron Radiation Research Center; *Y Tseng*, National Chiao Tung University, Republic of China

Complex oxides have been extensively investigated due to complicated structural and electronic orbitals. The physical properties of these oxides may vary with growth mechanism. Among all the growing methods, radio frequency (RF) sputtering possesses advantages of good stoichiometry, great reproducibility and less pricy. This work demonstrates the fabrication of epitaxial GdFe_{0.8}Ni_{0.2}O₃ thin film (abbreviated as GFNO) by RF sputtering, analysis of fundamental physical properties and the application in the research in ferromagnetic and multiferroic layer heterostructure interface with in-situ spectroscopy technique. The epitaxial nature properties of thin film were examined by synchrotron radiation high resolution X-ray scattering at NSRRC. In addition to structure, the analysis on ferroelectricity (polarization and leakage), magnetism, electronic configuration and valence state have been also conducted with the result of room-temperature ferroelectricity and ferrimagnetism of GFNO thin film. Using in-situ XAS, XMCD and MOKE analysis have been conducted to investigate the effect of the electric field on the Co and GFNO interface. The native cobalt oxide in the interface has been found to transfer into metallic state due to the enhancement in the intensity of XAS absorption peak. Meanwhile, the intensity of XMCD also increases, indicating that the spin moment has also increases. In MOKE analysis, the coercivity of cobalt declines with rising applied electric field which comes from the increase in metallic state cobalt. This work was financially supported by the "Center for the Semiconductor Technology Research" from The Featured Areas Research Center Program within the framework of the Higher Education Sprout Project by the Ministry of Education (MOE) in Taiwan. Also supported in part by the Ministry of Science and Technology, Taiwan, under Grant MOST-107-3017-F-009-002.

9:00am **TF-ThM-4 Effect of the Ultrasonic Treatment on the Si-SiO₂ System Defects Structure**, *Daniel Kropman*, Tallinn University, Estonia; *V Seeman*, Tartu University, Estonia; *A Medvids*, Riga Technical University, Latvia; *P Onufrievs*, Riga Technicacal University, Latvia

The effect of ultrasonic treatment (UST) on the defect structure of the Si-SiO₂ system by means of electron spin resonance(ESR),selective etching, MOS capacitance technique and secondary ions mass-spectroscopy is

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presented. The non-monotonous dependence of the defect densities on the US wave intensity has been observed. The influence of the UST frequency on the ESR signal intensity of the defect centres depended on the defects type and may be caused by vibration energy dissipation, which are a function of defect centres type. In the ESR spectra of Si samples a signal with g=1.9996 (Pa centres) connected with vacancy complexes is observed. After UST appears another signal with g=2.0055 (broken bonds of Si atoms). The influence of the US frequency and sample orientation on the ESR signal intensity varies for different centres. The frequency and orientation dependence of the ESR signal with g=1.9996 and the lack of this dependence for the centres with g=2.0055 show that vibration energy dissipation depends on the type of defect centers. Defect density at the interface grows with an increase of US wave intencity or changes nonmonotonously depending on the oxide thickness and crystallographic orientation. In the samples with thick oxide/0,6 mkm there is a maximum in the dependence of the charge carriers lifetime on the US wave amplitude and in the samples with thin oxides /0,3 mkm/ there is a minimum. This shows that the structural defects form electrically active centres and their density can be varied by US. The density of point defects and absorbed impurities at the Si-SiO₂ interface can be reduced and its electrical parameters improved by an appropriate choice of the UST and oxidation condition. US is widely used not only for materials treatment but in medicine as well (cancer treatment).

References:

- [1] D.Kropman,V.Poll,L.Tambek,T.Karner,U.Abru.*Ultrasonics* 36(1998)10211025 [2] D.Kropman,S.Dolgov.*Physica satatus Solidi* © v.9,issue 10-11,pp.2173-2176

9:40am **TF-ThM-6 Charge Induced Disorder Controls the Thermal Conductivity of Entropy Stabilized Oxides**, *Jeffrey Braun, C Rost*, University of Virginia; *M Lim*, North Carolina State University; *A Giri, D Olson*, University of Virginia; *G Kotsonis*, Pennsylvania State University; *G Stan*, National Institute of Standards and Technology; *D Brenner*, North Carolina State University; *J Maria*, Pennsylvania State University; *P Hopkins*, University of Virginia

Manipulating a crystalline material's configurational entropy through the introduction of unique atomic species can produce novel materials with desirable mechanical and electrical properties. From a thermal transport perspective, large differences between elemental properties such as mass and interatomic force can reduce the rate at which phonons carry heat and thus reduce the thermal conductivity. Recent advances in materials synthesis have enabled the fabrication of entropy-stabilized ceramics, opening the door for understanding the implications of extreme disorder on thermal transport. Measuring the structural, mechanical, and thermal properties of single-crystal entropy stabilized oxides, we show that local ionic charge disorder can effectively reduce thermal conductivity without compromising mechanical stiffness. These materials demonstrate similar thermal conductivities to their amorphous counterparts, in agreement with the theoretical minimum limit, resulting in this class of material possessing the highest ratio of elastic modulus to thermal conductivity of any isotropic crystal.

10:20am **TF-ThM-8 Thermal Boundary Conductance Across Heteroepitaxial ZnO/GaN Interfaces: Experimental Assessment of the Phonon Gas Model**, *John Gaskins*, University of Virginia; *G Kotsonis*, Pennsylvania State University; *A Giri*, University of Virginia; *S Ju*, University of Tokyo, Japan; *A Rohskopf*, Massachusetts Institute of Technology; *Y Wang, T Bai*, University of California, Los Angeles; *E Sachet, C Shelton*, North Carolina State University; *Z Liu*, University of Notre Dame; *Z Cheng*, Georgia Institute of Technology; *B Foley*, Pennsylvania State University; *S Graham*, Georgia Institute of Technology; *T Luo*, University of Notre Dame; *A Henry*, Massachusetts Institute of Technology; *M Goorsky*, University of California, Los Angeles; *J Shiomi*, University of Tokyo, Japan; *J Maria*, Pennsylvania State University; *P Hopkins*, University of Virginia

We present experimental measurements of the thermal boundary conductance (TBC) from 77 – 500 K across isolated heteroepitaxially grown ZnO films on GaN substrates. This data provides an assessment of the underlying assumptions driving phonon gas based models, such as the diffuse mismatch model (DMM), and atomistic Green's function (AGF) formalisms used to predict TBC. Our measurements, when compared to previous experimental data, suggest that TBC can be influenced by long wavelength, zone center modes in a material on one side of the interface as opposed to the "vibrational mismatch" concept assumed in the DMM; this disagreement is pronounced at high temperatures. At room temperature, we measure the ZnO/GaN TBC as 490[+150, -110] MW m⁻²

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K^{-1} . The disagreement among the DMM and A GF, and the experimental data at these elevated temperatures, suggests a non-negligible contribution from other types of modes that are not accounted for in the fundamental assumptions of these harmonic based formalisms, which may rely on anharmonicity. Given the high quality of these ZnO/GaN interfaces, these results provide an invaluable, critical, and quantitative assessment of the accuracy of assumptions in the current state of the art computational approaches used to predict phonon TBC across interfaces.

10:40am TF-ThM-9 Studies on Hot-wall Deposited Cadmium Sulphide (CdS) Thin Films for Buffer Layers in Thin Film Solar Cell, Balaji Gururajan, B Rangasamy, P Sankaran, P Nagarajan, S Kaliappan, K Dhonan, PSG College of Technology, India; V Asokan, Chalmers University of Technology, Sweden; M Natarajan, Coimbatore Institute of Technology, India; D Velauthapillai, Western Norway University of Applied Sciences, Norway

Cadmium Sulphide (CdS) thin films were deposited onto well-cleaned soda lime glass substrates using hot wall deposition technique at room temperature. The structure of the as-deposited CdS thin films was found to be hexagonal and oriented along $<0\ 0\ 2>$ direction. The CdS films were then annealed to 300 °C and crystallinity of the films was found to improve with the presence of additional diffraction peaks along $<0\ 0\ 2>$, $<1\ 0\ 1>$, $<1\ 0\ 2>$, $<1\ 1\ 2>$ directions. Raman Spectroscopy of the annealed films confirmed the hexagonal structure with a shift observed at 312 cm⁻¹. Selected area electron diffraction (SAED) pattern acquired from transmission electron microscopy analysis substantiated the hexagonal phase formation. X-ray photoelectron spectroscopy (XPS) confirmed the stoichiometric nature of CdS thin films with Cd:S atomic ratio of 1. Field emission scanning electron microscopy (FESEM) images revealed smooth morphology of the CdS films with distinctive grains. Atomic force microscopy (AFM) results indicated a surface roughness of 4.47 nm. Transmission spectra of the films were studied and the transparency was found to be above 80%. The optical band gap was found to be around 2.4 eV in accordance with the reported values. The results obtained clearly show that device quality CdS buffer layers can be effectively deposited using Hot-wall deposition.

11:00am TF-ThM-10 Intrinsec Photoluminiscent Properties of Crystalline and Amorphous Cd₂V₂O₇, Erika Cervantes Juárez, R Lozada Morales, A Meza Rocha, R Licona Ibarra, BUAP, Mexico

Cd₂V₂O₇ compounds in crystalline and amorphous phases were fabricated by the melt-quenching process. Characterizations such as X-ray diffraction, Raman spectroscopy and photoluminescence were performed. X-ray diffraction patterns of the crystalline sample showed peaks associated with a pure Cd₂V₂O₇ monoclinic structure, in agreement with the Raman vibrational spectrum. In the case of the amorphous sample, X-ray diffraction patterns only exhibited a broad band, typical of a glassy structure, whereas its Raman spectrum displayed two broad vibrational modes centered at 350 and 850 cm⁻¹, attributed to stretching vibrations of VO₃ groups. In spite of the structural differences, both samples presented similar photoluminescence features, consisting of a wide band in the 375–525 nm range with two peaks at 411 and 432 nm, associated respectively with the ³T₂ → ¹A₁ and ³T₁ → ¹A₁ electronic transitions in the VO₄ tetrahedron, under 340 nm excitation. Thus, blue light emission with CIE1931 chromaticity coordinates x~ 0.200 and y~ 0.145, and color purity of 62–63%, is achieved from the crystalline and amorphous Cd₂V₂O₇ compounds. The emission decay time profiles were well fitted to a bi-exponential function from which the calculated average lifetime values resulted to be 112 ± 13 and 99 ± 4 ns for the crystalline and amorphous Cd₂V₂O₇ samples, respectively. Theoretical calculations based on the density of electronic states revealed that the photoluminescence arises through charge transference processes from 3d orbitals of four-fold coordinated vanadiums to 2p orbitals of three-fold coordinated oxygens in the VO₄ tetrahedron, being the basic unit of Cd₂V₂O₇ in crystalline and amorphous phases.

11:20am TF-ThM-11 The Effect of Tin Impurities on CdTe Thin Films Solar Cell, J Ríos-González, CINVESTAV-Unidad Mérida, Mexico; R Mis-Fernández, I Rimmaudo, E Camacho-Espinosa, Juan Luis Peña, CINVESTAV-Unidad Mérida, Mexico, México

The doping of CdTe has been investigated with different materials such as Sb, As, Mg, Se, Bi. Sn-doped CdTe is a promising intermediate band photovoltaic material, therefore the optoelectronic and structural properties have been investigated in this work. Tin was co-sublimated with CdTe films by close-spaced sublimation (CSS) process in Ar environment to avoid Sn oxidation. CdTe:Sn was deposited on a superstrate structure, glass/ITO/ZnO/CdS, and Cu/Mo bi-layer was used as back contact. The amount of tin doping was kept constant. Well shaped and uniform grains

were found by Field Emission Scanning Electron Microscopy (FE-SEM) analysis (about ~ 3 μm). Also it was observed a morphological changes between as-deposited CdTe and Sn-doping CdTe. Energy Dispersive X-ray Spectroscopy (EDS) and X-ray Photoelectron Spectroscopy (XPS) showed presence of tin in the CdTe films. Xrays Diffraction (XRD) revealed peaks corresponding to the SnTe compound, as well as CdTe peaks strongly orientated along the (220) and (311) directions. The CdTe:Sn and as-deposited films showed a band gap of 1.49 eV. The measured efficiency of CdTe:Sn solar cell was 5.4%.

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