PCSI

Room Ballroom South - Session PCSI-WeM

Spintronics II/Van der Waals Heterostructures II/Semiconductor Interfaces/Complex Oxides II

Moderators: Aaron Arehart, The Ohio State University, Michael Flatte, University of Iowa, Masataka Higashiwaki, National Institute of Information and Communications Technology, Chakrapani Varanasi, ARO

8:30am **PCSI-WeM-1 Current Switching of a Single Ferromagnetic Layer**, ***Chia-Ling Chien,*** Johns Hopkins University **INVITED**

Spin Hall effect (SHE) switching allows current switching of a single ferromagnetic (FM) layer in contact with a heavy metal (HM), where the pure spin current from the HM exerts a spin orbit torque to switch the adjacent FM layer. However, this highly attractive pure current switching scheme cannot occur unless a magnetic field is also applied along the current direction, thus greatly diminishing its prowess. In this work, we describe the essential role of the necessary magnetic field, which not only breaks geometrical symmetry and but also causes asymmetrical domain wall motion that accomplishes switching. More importantly, we demonstrate a new method of pure current switching by exploiting HMs with opposite spin Hall angles, different Dzyaloshinskii-Moriya interaction constants and competing pure spin current. We describe the intricate physics that accomplishes pure current switching of a single ferromagnetic layer without external field, built-in exchange bias or asymmetrical structure.

9:00am **PCSI-WeM-7 Epitaxial Heusler Superlattices with Perpendicular Magnetization**, ***Tobias Brown-Heft,*** *A McFadden, J Logan, C Palmstrom,* University of California, Santa Barbara

Magnetic tunnel junctions for use in system-on-chip memory require ferromagnetic electrodes with four key ingredients. First, single crystal thin film contacts must grow epitaxially on a variety of substrates to facilitate uniform performance across large arrays of devices. Second, perpendicular magnetic anisotropy (PMA) is desired to reduce spin transfer torque critical current, which reduces Joule losses for electrically switched devices. Perpendicular contacts also possess higher magnetic thermal stability as compared with in-plane magnetized contacts, which serves to preserve the magnetic state for technologically useful timescales. Third, Fermi level spin polarization must be high to enhance the tunnel magnetoresistance ratio and thereby improve state discrimination during read operations. Fourth, the contact must have low Gilbert damping, which further decreases spin transfer torque critical current.

Recently, J.G. Azadani *et al.* utilized theory calculations to argue that superlattices composed of alternating layers of certain full-Heusler compounds produce materials with all four of the properties mentioned above [1]. Specifically, epitaxial Co_2MnAl – Fe_2MnAl (CMA-FMA) superlattices are predicted to be half-metallic with 100% spin polarization, possess dominant PMA, and are composed of low Z elements with low damping coefficients. Furthermore, the spin polarization and PMA depend strongly on the superlattice periodicity, which is on the order of a single unit cell.

In this work, we utilize molecular beam epitaxy with computer controlled source shutters to grow CMA-FMA superlattices of varying periodicity on both GaAs(001) and MgO(001) substrates. High resolution x-ray diffraction is used to verify epitaxial growth. SQUID magnetometry and anomalous Hall effect are used to probe the magnetic and electronic properties of the films. We show that CMA-FMA films with a periodicity of 1.5 unit cells grown on GaAs(001) have lattice parameter a ≈ c = 5.98Å, and exhibit dominant PMA below 200K. Similar films grown on MgO(001) are epitaxial with a = 5.74Å and c = 5.80Å, and work is in progress to find conditions giving strong perpendicular behavior. Future work includes spin-resolved photoemission and point contact Andreev reflection spectroscopy to probe the spin polarization of the films.

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[1] J.G. Azadani, *Jour. of App. Phys.*, *119*(4), 43904 (2016)

9:05am **PCSI-WeM-8 Interface-dependent Spin Transfer Torque at Ferromagnetic Topological-Insulator Contacts**, ***Sarmita Majumder,*** University of Texas, Austin

In previous work, we have shown large magnetoresistances at room temperature (RT) for three Ferromagnet/Topological Insulator (FM/TI) devices (Fe/Bi_2Te_3-based devices with and without an evaporated SiO_2 oxide, and an Fe/Bi_2Se_3-based device without evaporated oxide) [1]. The observed magnetoresistance was substantially larger than previously reported for the same system at RT [2] and at low temperatures [3, 4], and was particularly enhanced when an evaporated SiO_2 layer was introduced between the Fe and Bi_2Te_3, and when Bi_2Se_3 was used instead of Bi_2Te_3. We have speculated that the Fe deposition directly onto the TI might form an Fe-rich FeTI compound [5] which might have been prevented in the case when an evaporated oxide was present between Fe and Bi_2Te_3.

In this presentation, we will show large interface-dependent magnetoresistances in these devices due to spin polarization of the Fe bar via electron injection and extraction from the TI to the Fe (STT) at 2 K. The required switching current for STT in our case is comparable to the previous results in [6] for Cr-TI/TI contacts. Moreover, to support our speculation regarding the interfacial dependencies, we have performed cross-sectional transmission electron microscopy (XTEM) at the FM/TI interfaces. Cross-sectional samples were prepared using focussed Ga-ion beam milling. Fig. 2 shows XTEM images from (a) Fe/Bi_2Se_3, and (b) Fe/SiO_2/Bi_2Te_3 interfaces. The Fe/Bi_2Se_3 interface shows an extra crystalline layer at the interface with a slightly larger half period of 0.53 nm compared to the Bi_2Se_3 fringes (1.02 nm/2 = 0.50 nm). Energy dispersive X-ray spectroscopy (EDX) profiling using scanning transmission electron microscopy (STEM) imaging across the interface confirmed the inclusion of Se into Fe. Fig. 1(b) shows an abrupt interface between the crystalline Bi_2Te_3 and evaporated SiO_2.

9:10am **PCSI-WeM-9 Annealing Effects on Interfacial Electronic Structure in Epitaxial Co_2MnSi/MgO/CoFe Magnetic Tunnel Junctions**, ***Anthony McFadden,*** *T Brown-Heft, C Palmstrom,* University of California, Santa Barbara

We investigate the effects of post-growth annealing in ultrahigh vacuum on the temperature dependent transport properties and tunneling magnetoresistance (TMR) in single crystal CoFe/MgO/Co_2MnSi magnetic tunnel junctions (MTJ's) grown by molecular beam epitaxy. Full-Heusler Co_2MnSi(001) layers were grown at elevated temperature on Cr buffered MgO(001) substrates while MgO tunnel barriers and CoFe top electrodes were grown at room temperature and annealed post-growth. MTJ's with areas varying from 2.5x5μm^2 to 12.5x25μm^2 were fabricated using optical lithography. The MTJ structures were determined to be epitaxial and single crystalline before annealing as assessed by *in-situ* reflection high energy electron diffraction (RHEED). While they crystal quality of the top CoFe layer was observed by RHEED to improve somewhat upon annealing, we find that the transport properties of fabricated devices are altered dramatically. Samples annealed above 250°C show an expected monotonic increase in tunneling magnetoresistance (TMR) with decreasing temperature while the omission of the annealing step results in devices with an unexpected maximum TMR at temperature near 30K while TMR declines for lower temperatures. Differential conductance vs. voltage measurements performed at 2K show the presence of electronic structure near zero bias which vanishes upon annealing and which suppresses conductance when the magenetic layers are in a parallel orientation while enhancing conductance when in the antiparallel configuration. The anomalous decline of TMR with decreasing temperature in unannealed MTJ's is explained by the presence of this interfacial electronic structure combined with the thermal distribution of tunneling electrons about the Fermi energy

9:15am **PCSI-WeM-10 Valley Excitons in van der Waals Heterostructures**, ***Kyle Seyler,*** *P Rivera, D Zhong,* University of Washington*; J Schaibley,* University of Arizona*; X Linpeng, B Huang, E Schmidgall,* University of Washington*; R Cheng,* Carnegie Mellon University*; H Yu,* University of Hong Kong*; M McGuire, J Yan, D Mandrus,* Oak Ridge National Laboratory*; W Yao,* University of Hong Kong*; D Xiao,* Carnegie Mellon University*; K Fu, X Xu,* University of Washington **INVITED**

Two-dimensional materials have recently developed into a powerful platform from which to explore the science of surfaces and interfaces. Of particular excitement is their use as versatile building blocks for more advanced van der Waals heterostructures. Here we present our latest experimental progress in understanding the interfacial effects on excitons in two types of van der Waals heterostructures. We first discuss the interlayer excitons formed at the interface between two different monolayer semiconductors, $MoSe_2$ and WSe_2. Through photoluminescence measurements, we reveal that these excitons possess valley pseudospin properties like their intralayer counterparts, but with enhanced lifetime and intriguing relaxation dynamics. We then introduce a new van der Waals heterostructure between monolayer WSe_2 and an ultrathin ferromagnetic semiconductor, CrI_3. Strong interfacial magnetic interactions have a dramatic effect on the WSe_2 exciton valley properties. We also

demonstrate that basic optical studies on this type of heterostructure can provide rich information on the spin interactions in layered magnets.

9:45am **PCSI-WeM-16 Influence of the Dielectric Environment on Exciton Properties in 2D Semiconductors: Insights from High Magnetic Fields**, ***Andreas Stier,*** Los Alamos National Laboratory*; N Wilson, G Clark, X Xu,* University of Washington*; S Crooker,* Los Alamos National Laboratory

Excitons in atomically thin 2D semiconductors such as monolayer MoS_2 or WSe_2 necessarily lie close to a surface, and therefore their properties such as size and binding energy (E_B) are expected to be strongly influenced by the surrounding dielectric environment.

However, studies exploring this role are both scarce and challenging, in part because the most readily accessible exciton property, its optical transition energy, is largely unaffected by the surrounding dielectric medium. This is because any reduction in E_B is accompanied by an equal reduction of the free-particle bandgap, resulting in a nearly unchanged exciton transition energy. Therefore, it is desirable to identify alternative optical probes of some other exciton parameter that is directly impacted by the surrounding dielectric medium.

Here we show that the exciton size can be directly measured via the small diamagnetic shift of the exciton transition energy in pulsed magnetic fields to 65 Tesla [1]. Utilizing a new measurement technique (Fig. 1(a)), in which we transfer exfoliated WSe_2 flakes over the core of a single mode optical fiber, we tune the surrounding dielectric environment by encapsulating the flakes with different materials and perform circularly-polarized low-temperature magneto-absorption studies [2]. As determined from the systematic increase of the diamagnetic shift of the exciton with increasing dielectric screening of the environment (Fig. 1(b)), we find a systematic increase of the A exciton size in monolayer WSe_2 from 1.2 nm to 1.6 nm.

The increase in exciton size and concurrent reduction in the binding energy are compared with the leading theoretical (Keldysh) model. Within this model, we find E_B systematically varying from 200 - 450 meV for our examined samples and extrapolate to freestanding WSe_2 where we find $E_B \approx$ 500 meV.

9:50am **PCSI-WeM-17 Electronic Properties and Defects in Germanane**, ***Thaddeus Asel,*** *E Yanchenko, S Jiang, K Krymowski, W Windl, J Goldberger, L Brillson,* The Ohio State University

We have used a combination of surface science techniques to study the electronic properties and defects in germanane, a chemically functionalized two dimensional (2D) material. With the advent of graphene there has been a focus on 2D materials due to their unique properties, and the ability to further manipulate them both chemically and mechanically. Similar to graphene and MoS_2, germanane is a 2D material with a direct band gap that can be manipulated by terminating with different ligands, making it an exciting candidate for optoelectronic applications. Germanane is synthesized by deintercalating $CaGe_2$ in an acid to result in a particular termination [1]. We applied depth-resolved cathodoluminescence spectroscopy (DRCLS)[2] to measure the electronic transitions including the band gap in hydrogen terminated germanane (GeH), methyl-terminated germanane ($GeCH_3$), dimethylether terminated germanane ($GeCH_2OCH_3$), and allyl-terminated germanane ($GeCH_2CH{=}CH_2$). Using surface photovoltage spectroscopy (SPS) and DRCLS we have directly observed defects in "bulk" germanane.

A key feature of germanane is that terminating the germanium lattice with different ligands can affect the size of the direct band gap. The combination of the effects due to ligand size and electronegativity. The electronegativity of the ligand is believed to determine the extent of electron density withdrawal from the germanium scaffold, which weakens Ge-Ge bonding and reduces the band gap. Large ligand size can introduce strain and as a result also reduce the band gap energy. We used DRCLS to examine this relationship. The electronegativity of each ligand decreases from $-CH_2OCH_3$ > -H > $-CH_3$ > $-CH_2CH{=}CH_2$. DRCLS finds the band gap energies increase from CH_2OCH_3 (1.47 eV) > $-CH_2CH{=}CH_2$ (1.50 eV) > -H (1.52 eV) > $-CH_3$ (1.62 eV). These values follow the trend in electronegativity with the exception of the allyl termination, which can be explained using strain as it is the largest ligand.

We used SPS and DRCLS to observe sub band gap optical states in $GeCH_3$. SPS shows E_C - 0.85 eV and E_V+1.05 eV. DRCLS shows complementary transtions due to gap states at 0.82, 0.96, 1.02, and 1.35 eV. Investigating $GeCH_3$ samples that have been deintercalated for one week and three weeks the 1.02 eV feature disappears in the sample that had been deintercalated for three weeks. This can be tentatively attributed to the removal of residual CaI_2 from interlayer spacing of the $GeCH_3$ layers. This demonstrates that defects can be identified and eliminated. through systematic chemical processing. This work supported by NSF MRSEC under award number DMR-1420451.

9:55am **PCSI-WeM-18 Electrostatic Doping and Hybrid Carriers in Graphene on a Polar $SrTiO_3$ (111) Surface: Theoretical Investigation**, *D Shin,* ***Alexander Demkov,*** The University of Texas

Figure 1. (a) Band structure of graphene on STO (111). A dashed line represents the Fermi level which is set to zero. Probability distribution calculated within the energy window (± 0.03 eV) corresponding to the band crossing point (b) and charge density corresponding to the Fermi level ©. It shows the charge density of graphene sheet and the surface of STO (111).

Graphene is a two-dimensional carbon sheet with a honeycomb lattice structure. It is a zero-gap-semiconductor that has a linear energy dispersion near the Fermi level [[file:///C:/Users/Alexander/Documents/ALEX/Papers/Abstracts/2016/PCSI-44_Abstract_grphene.doc#_ENREF_1], [file:///C:/Users/Alexander/Documents/ALEX/Papers/Abstracts/2016/PCSI-44_Abstract_grphene.doc#_ENREF_2]].Doping graphene layers presents a difficult practical and fundamental problem. We consider theoretically, the possibility of electrostatic doping of graphene by the intrinsic field of a polar substrate. Density functional theory calculations are carried out for a graphene sheet placed on the (111)-oriented perovskite $SrTiO_3$ surface. We find that the Fermi surface moves well below the Dirac point of graphene, resulting simultaneously in a fast conducting channel in graphene, and a slow, large effective mass channel in the oxide surface. Electrostatic gating may allow one to explore peculiar states that, through the "no-crossing" reminiscent of polaritons, would represent a hybrid carrier that exists simultaneously in both materials. In Fig. 1 we show the near edge electronic structure and corresponding charge distribution of the system. Importantly, in addition to the field doping, we identify a more "obvious" mechanism of doping through the contact potential difference, which may have wider applications in the doping of two-dimensional materials.

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11:00am **PCSI-WeM-31 Dielectric Related Issues in GaN Based MIS HEMTs**, ***Gaudenzio Meneghesso,*** University of Padova, DEI, Italy*; D Bisi, I Rossetto, M Ruzzarin, C De Santi, M Meneghini, E Zanoni,* University of Padova - DEI, Italy **INVITED**

Over the last few years GaN has emerged as an excellent material for the fabrication of high-voltage devices (high electron mobility transistors, HEMTs) for application in the power conversion systems. Thanks to the low on-state resistance (<100 mW for a 20 A transistor [1]) and the low leakage (<1-10 μA at 650 V [2]) these devices are currently targeting the 650 V market segment. One of the most promising solutions for normally-off operation is the combined use of a normally-on GaN HEMT and a low-voltage silicon MOSFET in cascode configuration [3], [4]. A metal-insulator-semiconductor (MIS) HEMT can be used to this aim. This approach guarantees low gate leakage current levels and a high intrinsic robustness. However, in a MIS-HEMT the dielectric represents a critical element, that is subject to a relevant electric field: under off-state conditions, the field peaks at the edge of the gate (or field plate) on the drain side, while under positive gate bias conditions the field on the dielectric is more uniform, since the 2-dimensional electron gas (2DEG) is formed under the gate.

Several dielectrics can be used for the fabrication of MIS-HEMTs including SiN[5], Al_2O_3[6], SiO_2[7], HfO_2[8], and TiO_2[9]. In most of the cases these dielectrics are deposited by chemical vapor deposition (CVD, as in the case of SiN) or by atomic layer deposition (ALD, as in the case of Al_2O_3).

This paper reviews the most relevant dielectric-related trapping mechanisms in GaN-based transistors. Metal-insulator-semiconductor (MIS) devices with partially-recessed gate have been submitted to pulsed and constant voltage stress, with the aim of evaluating the impact of charge trapping processes on the dynamic properties of the devices and on the negative-bias threshold instabilities (NBTI) induced by negative gate bias. Three different dielectrics were considered for this investigation: SiN deposited by rapid thermal chemical vapour deposition (RTCVD), SiN deposited by plasma enhanced atomic layer deposition (PE-ALD), and Al2O3 deposited by atomic layer deposition (ALD). The results obtained within this paper are critically compared to previous literature reports, to provide a more complete view of the state-of-the-art.

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11:30am **PCSI-WeM-37 Device Physics Modeling of Metal-Semiconductor Interfaces from an Induced Gap State Perspective**, ***John Wager***, *K Kuhn,* Oregon State University

Induced gap state (IGS) modeling attempts to explain the electronic properties of metal, semiconductor, or insulator surfaces or interfaces in terms of intrinsic behavior associated with quantum mechanically induced evanescent states arising from the abrupt termination of a bulk material at a surface or interface [1]. Although IGS modeling pertains to a wide variety of surfaces and interfaces, this presentation will focus primarily on one specific case – the metal-semiconductor (MS) interface – in order to provide a tutorial introduction to the topic of IGS modeling.

Figure 1. Equivalent circuit of a MS interface for (a) an ideal (ignoring interface states) macroscopic dipole, (b) a non-ideal (including interface states) microscopic dipole, and © a non-ideal (including interface states) macroscopic dipole.

A very unusual but powerful aspect of IGS modeling is its persistent use of equivalent circuits to elucidate surface and interface electronic behavior. For example, Figure 1 shows three equivalent circuits that are useful for assessing an MS interface. For an ideal situation in which interface states are ignored, Figure 1a reveals that the surface potential, ψ_{Sm}, is simply equal to the MS work function difference, $\Phi_S - \Phi_M$. This idealized case is described as involving a macroscopic dipole since charge separation between the sheet of charge at the MS interface and the charge centroid associated with the semiconductor space charge region is of macroscopic (rather than atomic) dimensions. In contrast, Figure 1c shows that when interface states are accounted for, the true surface potential, ψ_S, is degraded from what it would be in the absense of interface states, i.e., ψ_{Sm}, by a microscopic (atomic dimensions) dipole voltage due to interface states, i.e., Δ_{MS}. Evaluation of Δ_{MS} requires using Figure 1b to determine how much the charge neutrality level misalignment voltage, $\Phi_{CNLS} - \Phi_M$, drops across the microscopic dipole interface capacitance, C_i.

The origin of the eqivalent circuits shown in Figure 1 will be clarified in the presentation via a discussion of the electrostatics of MS interface formation.

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[1] J. F. Wager and K. Kuhn, Crit. Rev. Solid State Mater. Sci. (in press).

11:35am **PCSI-WeM-38 Investigation of ZnO/PbS Nanocrystal Interfaces for Photonic Device Applications**, ***Diogenes Placencia***, Naval Research Laboratory*; I Sellers,* University of Oklahoma*; J Boercker, J Tischler,* Naval Research Laboratory

Research into lead sulfide (PbS) nanocrystal devices has garnered much attention recently due to their notable performance as photovoltaic devices and short wave infrared photodetectors, among other applications.[1,2] Common within such devices is the use of metal oxide thin-films (e.g., ZnO, ITO, NiO, etc.) that act as charge-selective contacts. Therefore, characterization of the interfacial properties between metal oxides and PbS nanocrystals is crucial to the overall development of these technologies. In this contribution, we present our investigations into the properties that dominate operational efficiency of the ZnO/PbS heterojunction. Through a series of varying oxide pre-treatments (e.g., plasma cleaning, small-molecule surface modifications, and wet-chemical etching), we investigate how the state of the surface affects band-edge offsets (via Ultraviolet Photoemission Spectroscopy), changes in the surface chemistry at the interface (through X-ray Photoemission Spectroscopy), and overall structural changes (utilizing Scanning Probe Microscopy). Additionally, we provide insight into how these pre-treatments affect overall device performance in the standard inverted device geometry.

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[2] R. J. Curry, Nat. Photonics **10**, 81(2016).

11:40am **PCSI-WeM-39 Defect Density Reduction in Core layer of ZnTe Electro-Optical Waveguide by Low Lattice Mismatched Interfaces**, ***Wei-Che Sun***, Waseda University, Japan*; T Nakasu, K Odaka,* Waseda University*; M Kobayashi,* Waseda University, Japan*; T Asahi,* JX Nippon Mining & Metals Corp.

ZnMgTe(Cladding)/ZnTe(Core) thin film waveguide has been proposed to form a practical Electro-optical (EO) device due to the high EO coefficient of ZnTe (r_{41}= 4.5 pm/V) [1]. For low loss ZnMgTe/ZnTe waveguide, large refractive index difference between layers can be achieved by adding Mg content (Mg %). However, high Mg% results in lattice mismatch enlargement (lattice mismatch between ZnTe and MgTe is 4.1%), and misfit dislocations at interfaces would befall and degrade the crystal quality. In previous study, waveguide with Mg 20%, 0.6 μm cladding layer was found to have high-performance [2]. However, large in-plane lattice mismatch (0.8%) between ZnMgTe and core layers, and high defect density in core layer at the interface region was observed (4×10^9 /cm^2). Therefore, low Mg % interlayers were introduced to create a series of low lattice mismatch interfaces and circumvent the effect of the large lattice mismatch (two-step index waveguide). In this study, two kinds of structures were considered to realize a low loss two-step index waveguide. One structure was designed to insert 0.1 μm low Mg% interlayers, and cladding layer thickness and Mg % were kept about 0.6 μm and 20%, respectively (sample 1). The other structure was designed to have the cladding layer 0.3 μm with Mg 20% and Mg 10% 0.45-μm-thick interlayer (sample 2).

By cross-sectional transmission electron microscope observation, both samples had lower defect densities (2×10^8 /cm^2 for sample 1; 2×10^9 /cm^2 for sample 2) than the single-step index waveguide in core layer at the interface region. It indicates that extra interfaces with lower lattice mismatches were successfully helped to improve crystallographic properties. The interlayer worked efficiently even if thickness was only about 0.1 μm thick. With the reduction in defect density of the ZnTe layer, the EO property of the device is expected to be improved. However, the propagation loss was not improved by the introduction of the low Mg % interlayers when the average Mg % of ZnMgTe layers was in sufficient. By carefully control of the average Mg %, ZnTe waveguide with a series of low lattice mismatches interfaces could have better crystal quality without dropping the optical confinement.

11:45am **PCSI-WeM-40 Charge Transfer and Lattice Strain at Oxide Interfaces: Emergent Mottness, Multiferroicity and Antisite Defects**, ***Andrew Millis***, Columbia University **INVITED**

Interfaces separating transition metal oxide materials of different functionalities have the potential to host novel and potentially behavior. Understanding how to design interfaces that optimize desired properties while minimizing the potential for undersireable effects is an important research goal. In this talk I highlight the important roles of substrate-induced strain and across-interface charge transfer in controlling the properties of transition metal oxide-based superlattices. Charge transfer is controlled by the relative electronegatives of the transition metal ions while strain is controlled by the substrate. I give examples of how charge transfer and strain may lead to desirable properties including emergent Mott insulating behavior [1] and multiferroicity [2] as well as undesirable properties including antisite defects [3]. Strengths and weaknesses of calculational methods are outlined [4]. This work was performed in collaboration with Hanghui Chen and supported by DOE ER-046160 and NSF-DMR-1120296.

12:15pm **PCSI-WeM-46 Large Piezoelectric Characteristics of $KNbO_3$ Nanorods**, ***SeolHee Oh***, Ewha Womans University, Republic of Korea*; B Yun, J Jung,* Inha University, Republic of Korea*; W Jo,* Ewha Womans University, Republic of Korea

Piezoelectric nanomaterials have been receiving a great deal of attention because its applicable features to an energy conversion devices using mechanical-electrical-thermal coupling. $KNbO_3$ (KNO), potassium niobate, is one of the promising lead-free piezoelectric materials due to its high Curie temperature and large piezoelectric constants for nanoscale energy harvesting devices [1,2]. In this study, the piezoelectric properties of KNO nanorods (NRs) with respect to their intrinsic structural properties were studied via piezoresponse force microscopy. High-quality KNO NRs with orthorhombic as well as monoclinic structures were synthesized by using a hydrothermal method. It is notable that the stable monoclinic phase is only observed in nanoscale structure. The effective value of piezoelectric constant, d_{eff}, is 83.5(1) pm/V for monoclinic KNO NRs, which is 1.6 times larger than that of the orthorhombic KNO NRs (54.2(1) pm/V). It is caused by unconstrained rotational polarization of monoclinic KNO NRs, whereas

polarizations of orthorhombic KNO NRs are constrained along the direction which is differ from maximum piezoresponse axis. In addition to, approximately 6% piezoelectric enhancement compared to as-grown KNO NRs was observed as a result of the alignment of the polarization of KNO NRs by applying bias on monoclinic and orthorhombic KNO NRs.

12:20pm **PCSI-WeM-47 Strain Engineering and Interfacial Effects on the Photovoltaic Response in Epitaxial Complex Oxides***, **Adrian Podpirka**, A Bennett-Jackson, D Imbrenda, Z Gu,* Drexel University*; V Fridkin,* Drexel University/Shubnikov Inst. for Crystallography

Ferroelectric oxide perovskites are promising for use in photovoltaic solar energy conversion because carrier separation can occur even in the absence of a *p-n* junction, photovoltage can exceed the band gap, and power conversion efficiencies greater than the band gap-specific limit can be attained.[1] While ferroelectric devices exhibit efficiencies as high as ≈8%,[2] the influences of strain and of space charge near the ferroelectric-metal interface on photovoltaic properties are only beginning to be understood. [3] Using epitaxial $BaTiO_3$ films produced by pulsed laser deposition as a model system, we report here on investigation of the effects of strain profiles and interfacial band offsets on the photovoltaic response. Work supported by the US Army Research Office under W911NF-14-1-0500 and the SunShot Program of the US Department of Energy under DE-SC000144664.

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12:25pm **PCSI-WeM-48 Symmetry Breaking in Abnormally Elongated $PbVO_3$ Thin Films Epitaxially Grown by Pulsed Laser Ablation***, **SeolHee Oh**,* Ewha Womans University, Republic of Korea*; C Roh, J Lee,* Gwangju Institute of Science and Technology (GIST), Republic of Korea*; W Jo,* Ewha Womans University, Republic of Korea

An intriguing polar magnetic $PbVO_3$ (PVO) has a VO_5 square-pyramidal structure rather than VO_6 octahedron due to extreme tetragonal distortion, which leads the 2-dimensional antiferromagnetic ordering and large pyroelectric polarization by 152 $\mu C/cm^2$. In this study, we fabricated epitaxial PVO thin films on $LaAlO_3$ (LAO) (001) and $SrTiO_3$ (STO) (001) substrates by pulsed laser deposition with off-stoichiometric condition [1]. Structural properties of the epitaxial PVO thin films with respect to mechanical strain induced by lattice mismatch with substrates were investigated by X-ray diffraction, high-resolution transmission electron microscopy, Raman scattering spectroscopy. As a result, abnormal lattice elongation of the PVO thin films along c-axis and consequent octahedral distortion were observed. In addition, the experimental characterizations of linear and nonlinear optical properties for the PVO thin films were performed through spectroscopic ellipsometry and second harmonic generation (SHG), respectively. Symmetry breaking along c-axis in PVO thin films were demonstrated by using SHG signal with nonlinear susceptibility and Fresnel's formula fitting.

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