PCSI

Room Ballroom South - Session PCSI-TuM

Complex Oxides I/Topological Materials II/Semiconductor Growth I-Extended

Moderators: Andrew Millis, Columbia University, Joanna Millunchick, University of Michigan, Ann Arbor, Can-Li Song, Tsinghua University

8:30am **PCSI-TuM-1 Polar Metals by Geometric Design**, ***Chang-Beom Eom,*** University of Wisconsin-Madison **INVITED**

Polar Metals by Geometric Design

Chang-Beom Eom

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Gauss's law dictates that the net electric field inside a conductor in electrostatic equilibrium is zero by effective charge screening; free carriers within a metal eliminate internal dipoles that may arise owing to asymmetric charge distributions. Quantum physics supports this view, demonstrating that delocalized electrons make a static macroscopic polarization, an ill-defined quantity in metals—it is exceedingly unusual to find a polar metal that exhibits long-range ordered dipoles owing to cooperative atomic displacements aligned from dipolar interactions as in insulating phases. Here we describe the quantum mechanical design and experimental realization of room-temperature polar metals in thinfilm *A*NiO_3 perovskite nickelates using a strategy based on atomicscale control of inversion-preserving (centric) displacements. We predict with *ab initio* calculations that cooperative polar *A* cation displacements are geometrically stabilized with a nonequilibrium amplitude and tilt pattern of the corner-connected NiO6 octahedra—the structural signatures of perovskites—owing to geometric constraints imposed by the underlying substrate. Heteroepitaxial thin-films grown on $LaAlO_3$ (111) substrates. Heteroepitaxial thin-films grown on $LaAlO_3$ (111) substrates fulfil the design principles. We achieve both a conducting polar monoclinic oxide that is inaccessible in compositionally identical films grown on (001) substrates, and observe a hidden, previously unreported, non-equilibrium structure in thin-film geometries [1]. We expect that the geometric stabilization approach will provide novel avenues for realizing new multifunctional materials with unusual coexisting properties.

This work has been done in collaboration with T. H. Kim, D. Puggioni, Y. Yuan, L. Xie, H. Zhou, N. Campbell, P. J. Ryan, Y. Choi, J.-W. Kim, J. R. Patzner, S. Ryu, J. P. Podkaminer, J. Irwin, Y. Ma, C. J. Fennie, M. S. Rzchowski, X. Q. Pan, V. Gopalan, J. M. Rondinelli.

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[1] T. H. Kim, et al., *Nature.***533**, 68 (2016)

9:00am **PCSI-TuM-7 Scavenging of Oxygen from $SrTiO_3$ during Oxide Thin Film Deposition and 2DEG at Oxide Interfaces**, *A Posadas, K Kormondy, W Guo, P Ponath, J Geler Kremer,* ***Alexander Demkov,*** The University of Texas

The discovery of a 2DEG at the interface between epitaxial $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) over a decade ago has led to a flurry of research activity exploring the nature and origin of this conductive interface. This 2DEG has sufficient mobility to exhibit SdH oscillationsand much work on developing device applications of this system has been published. Experiment and theory show that the 2DEG at the oxide/oxide interface has many exotic features. It can be paramagnetic, ferromagnetic or even superconducting, with strong Rashba splitting leading to a controllable magnetic moment One explanation involving oxygen vacancies is used for 2DEGs arising in several related interfaces such as amorphous LAO on STO and g -Al_2O_3 on STO. In the vast majority of 2DEGs reported to form at oxide interfaces, the substrate has been TiO_2-terminated STO with only a handful of exceptions.Potential chemical reactions between the arriving metal species during oxide thin film deposition and the substrate have been largely ignored in these explanations for the 2DEG formation although this has recently begun to change. There is growing evidence that many metals steal oxygen from STO even in the presence of relatively high oxygen pressures.

To better understand the effect of metal oxide deposition on a STO surface, we examine the effect of depositing various metals layer by layer on STO in terms of the evolution of the electronic structure and oxidation state of the metal overlayer. We show that the deposition of metals that have a high oxygen affinity on STO, even under an oxygen-rich atmosphere such as in oxide thin film deposition, typically leads to an interfacial layer of oxygen-deficient STO. We analyze the electronic and chemical evolution of metals deposited on STO using in situ XPS and classify metals into three regimes depending on their oxide formation energy and work function. We demonstrate how redox reactions with STO of metals belonging to one of these regimes can be used to produce interfacial 2DEGs that are quite similar to the crystalline LAO on STO system, and that an oxygen-deficient STO layer could even explain the 2DEG in that system.

9:15am **PCSI-TuM-10 Realization of a Vertical Topological p-n Junction in Sb_2Te_3/Bi_2Te_3 Heterostructures**, ***Gregor Mussler,*** *M Eschbach, M Lanius, N Demarina, M Luysberg, L Plucinski, D Grützmacher,* Forschungzentrum Jülich, Germany **INVITED**

I will present results on molecular-beam epitaxy (MBE) of the three-dimensional TI materials Bi_2Te_3 and Sb_2Te_3 grown in Si(111). Due to naturally occurring defects, Bi_2Te_3 and Sb_2Te_3 exhibit a high unintentional carrier concentration in the order of ~ 10^{19} cm^{-3}. It turns out that Bi_2Te_3 and Sb_2Te_3 is intrinsically n-type doped, whereas Sb_2Te_3 show p-type behavior. Consequently, a stack of Sb_2Te_3/Bi_2Te_3 poses a p-n junction, where a built-in voltage drags away carriers from its interface, allowing to tune the carrier concentration by varying the thickness of the topmost Sb_2Te_3 layer.

9:45am **PCSI-TuM-16 Surface Structure and Electronic Properties of Epitaxial Topological Crystalline Insulator Films**, ***Omur Dagdeviren,*** *C Zhou, K Zou, G Simon, S Albright, S Mandal, M Acosta, X Zhu, S Beigi, F Walker, C Ahn, U Schwarz, E Altman,* Yale University

Topological crystalline insulators (TCI) feature surface electronic states are protected by crystal symmetry. As a representative TCI, the structural and electronic properties of SnTe films grown on $SrTiO_3$(001) were investigated using scanning tunneling microscopy (STM), noncontact atomic force microscopy (NC-AFM), electron and x-ray diffraction, and density functional theory. Initially, SnTe (111) and (001) surfaces formed; however, the (001) surface dominated with increasing film thickness. The film grows domain-by-domain with the [011] direction of SnTe (001) islands rotated up to 7.5° with respect to $SrTiO_3$ [010]. Analysis of the diffraction data reveals a mosaic distribution of SnTe (001) domains. Complementary STM and NC-AFM experiments address the properties of the thicker films in real space. It is found that the growth mechanism induces a variety of defects on different length scales that affect the electronic properties, including: domain boundaries; dislocations at the domain boundaries that serve as periodic nucleation sites for pit growth; screw dislocations; and point defects. These features give rise to variations in the electronic structure of the surface states as evidenced in STM images by standing wave patterns and a non-uniform nanometer scale background superimposed on atomic scale images. Simultaneous force versus and tunneling current versus distance curves indicate that the tip is unusually close to the surface during STM imaging making the surface susceptible to tip-induced modification. The results indicate that both the growth process and the scanning probe tip are candidates to induce symmetry breaking defects in a controlled way to pattern the topological surface states which then eventually enable fabrication of devices.

11:00am **PCSI-TuM-31 Epitaxial Semiconductor – Superconductor Hybrid Materials for Topological Superconductivity**, ***Peter Krogstrup,*** Niels Bohr Institute, Denmark **INVITED**

Semiconductor-metal interfaces are key elements in nanostructured electronics and device architectures. This is in particular true in the field of low dimensional topological superconductivity, where semiconductor nanowires with high spin orbit coupling coupled to a superconducting phase constitute some of the most promising candidates in the search for materials suitable for quantum information technology[1] . I will discuss the synthesis, structural and compositional properties hybrid semiconductor-superconductor nanowire and hybrid materials grown in-situ by Molecular Beam Epitaxy [2] . Because these materials give a hard superconducting gap proximitized in the semiconductor, they serve as excellent platform for studying Andreev bound states and Majorana bound states, which opens for new application possibilities in the field. I will present on the synthesis of various types of hybrid semi-super materials and discuss the challenges and material requirements needed for realizing and eventually manipulating topological protected quantum states.

[1] Nayak et al. *Rev. Mod. Phys.***80**, 1083 (2008)

[2] Krogstrup et al. *Nature Mater.* **14**, 400-406 (2015)

11:30am **PCSI-TuM-37 One-dimensional Electronic Transport in Epitaxial-Al/InAs Quantum Well Heterostructures**, ***JoonSue Lee***, *B Shojaei, M Pendharkar, A McFadden, C Palmstrom, Y Kim,* University of California, Santa Barbara*; M Kjaergaard, C Marcus,* Niels Bohr Institute, Denmark

One-dimensional (1D) electronic transport as well as induced superconductivity in a semiconductor is a crucial ingredient to realize topological superconductivity. Our approach employs two-dimensional (2D) semiconductors (InAs quantum wells), which are advantageous for fabricating complex nano-structures consisting of electrically confined 1D channels and superconductors. To achieve transparent superconductor/semiconductor contacts, the InAs quantum wells are cleanly interfaced with epitaxial Al by molecular beam epitaxy. Gate-tunable supercurrent is observed in an S-N-S geometry with a top gate, and it persists in the presence of in-plane magnetic field up to ~800 mT.

We study 1D electronic transport in shallow InAs quantum wells with a thin top potential barrier (10 nm $In_{0.75}Ga_{0.25}As$), after removing Al layer on top, using quantum point contacts and gate-defined quasi-1D channels. Conductance through a quantum point contact is quantized in units of the conductance quantum ($2e^2/h$), and half-integer values of the conductance quantum, due to Zeeman spin splitting, appear as perpendicular magnetic field is applied. We also observe an evolution of 0.5 conductance quantum as the lateral potential confinement of a quantum point contact becomes highly asymmetric. Conductance through gate-defined quasi-1D channel shows quantization only in the quantum Hall regime with large perpendicular magnetic field. Weak localization from magneto-conductance measurements at various gate-voltages, reveals a systematic change of the coherence length of the InAs channel. Our studies of the 1D electronic transport as well as the induced superconductivity in epitaxial superconductor/2D semiconductor systems could realize large-scale nano-structures utilizing multiple Marjorana fermiones for quantum computing applications

11:35am **PCSI-TuM-38 Theoretical Investigations for the Stability and Electronic Structures of Two-dimensional Group-IV Ternary Alloy Monolayers**, ***Toru Akiyama***, *G Yoshimura, K Nakamura, T Ito,* Mie University, Japan

Two-dimensional (2D) nanostructures in the honeycomb lattice have currently been paid much attentions due to their peculiar electronic properties. Furthermore, Si, Ge, and Sn monolayers (silicene, germanene, and stanene, respectively) are expected to be potential alternatives to graphene for electronic devices [1-3]. In contrast to flat 2D monolayers consisting of sp^2 hybridization such as graphene, silicene, germanene, and stanene form a mixture of sp^2 and sp^3 hybridization, resulting in the buckled hexagonal configuration. Recent theoretical calculations within density functional theory (DFT) have suggested that these materials possess a linear band dispersion with Dirac cone at the *K* point regardless of the buckled atomic configuration [4]. Moreover, it has been suggested that monolayer SiGe with buckled configuration also has a linear band dispersion similar to graphene [5]. However, there are few systematic studies for the atomic structure and electronic properties of group-IV alloy monolayers from theoretical viewpoints. In our previous study, we have systematically investigated the structural stability and electronic properties of group-IV binary alloy monolayers, such as monolayer Si_xGe_{1-x}, Ge_xSn_{1-x}, and Si_xSn_{1-x} on the basis of electronic structure calculations within the DFT [6]. In this study, we extend our study to ternary alloy semiconductor monolayers.

Our DFT calculations for $Si_xGe_ySn_{1-x-y}$ monolayers demonstrate that the buckled configuration is stabilized over the entire composition range. The calculated excess energy of $Si_xGe_ySn_{1-x-y}$ monolayers (~0.11 eV/atom) is found to be comparable to that of bulk phase of ~0.16 eV/atom, indicating that the miscibility of ternary alloy monolayers is similar to that of bulk phase. The analysis of band structures reveals that an almost linear band dispersion with Dirac cone at the *K* point similar to graphene appears in $Si_xGe_ySn_{1-x-y}$ over the wide range of Si and Ge compostions, while a small energy gap within 0.17 eV is formed at the *K* point for $Si_{0.5}Ge_{0.125}Sn_{0.375}$. These results thus suggest that the composition control is of importance in tailoring the electronic properties of group-IV ternary alloy monolayers. Furthermore, effects of carbon incorporation on the atomic structures and electronic properties of group-IV monolayers are clarified.

[1] B. Aufray *et al.*, Appl. Phys. Lett. **96**, 183102 (2010).

[2] M. E. Dávila *et al.*, New J. Phys. **16**, 095002 (2014).

[3] F. Zhu *et al.*, Nature Mater. **14**, 1020 (2015).

[4] J. C. Garcia *et al.*, J. Phys. Chem. C **115**, 13242 (2011).

[5] P. Jamdagni *et al.*, Mater. Res. Express **2**, 016301 (2015).

[6] T. Akiyama *et al.*, Jpn. J. Appl. Phys. **55**, 04EP01 (2016).

11:40am **PCSI-TuM-39 A Simple Interpretation for Heteroepitaxial Growth Mode in Terms of Surface and Interface**, ***Tomonori Ito***, *T Akiyama, K Nakamura,* Mie University, Japan

It is well known that hetero-epitaxial systems exhibit various growth behaviors depending on the lattice mismatch including three dimensional island growth (3D-coherent) and two dimensional growth with misfit dislocation formation (2D-MD). Despite a constant lattice mismatch of InAs on GaAs, the 3D-coherent is found on (001) while the 2D-MD appears on (110) and (111)A. Moreover, it is found that insertion of buffer-layer in the InAs/GaAs(110) changes its growth mode from the 2D-MD to the 3D-coherent. Although many studies have been done to investigate the 3D-coherent on the InAs/GaAs(001) [1], there have been very few studies for systematic interpretation for the growth mode depending on orientations. In this study, the growth mode of the InAs/GaAs system is simply interpreted by using our phenomenological macroscopic theory in terms of surface and interface with the aid of microscopic theory such as ab initio and empirical interatomic potential calculations.

In our macroscopic theory, free energy F (eV/Å^2) for the 2D-coherent, the 3D-coherent and the 2D-MD is described as a function of layer thickness h as follows [2].

$$F=\gamma(1+\beta)+1/2M(1-\alpha)\varepsilon^2(1-l_0/l)h+E_d/l,$$

where γ, β, M, α, ε, l_0, l, and E_d denote the surface energy, the effective increase in surface energy of the epitaxial layer due to 3D island formation, the effective elastic constant, the effective decrease in strain energy due to 3D island formation, the intrinsic strain of the system, the average MD spacing, the MD spacing at which strain is completely relaxed, and the formation energy of the MD, respectively. Using eq. (1), the boundary between the 2D-MD and the 3D-coherent is described as $\beta/\alpha=1/(2\gamma)(E_d/l_0)$. Using E_d obtained by ab initio and empirical potential calculations, the growth mode boundaries for the InAs/GaAs is shown in Fig. 1 as functions of β/α and γ. Employing β/α~0.2 and γ~0.05(eV/Å^2), the 2D-MD is favourable in the (110) and the (111)A, while the (001) exhibits the 3D-coherent. This depends on the values of E_d, i.e., the smaller the E_d, the more favourable the 2D-MD. Moreover, decrease in γdue to lattice relaxation with the buffer-layer insertion tends to favour the 3D-coherent found in the (110). Consequently, the growth mode on the InAs/GaAs can be qualitatively interpreted by considering $\gamma$and E_d.

[1] L. G. Wang et al., Phys. Rev. B **62**, 1897 (2000).

[2] K. Shiraishi et al., J. Cryst. Growth **237-239**, 206 (2002).

11:45am **PCSI-TuM-40 Surface Mediated Formation of Horizontal ErSb Nanowires**, ***Nathaniel Wilson***, *S Kraemer, C Palmstrøm,* University of California, Santa Barbara

ErSb, and related Rare Earth-Group V materials, are semi-metallic in nature and compatible with III-V semiconductors structures, forming sharp stable epitaxial interfaces. Unfortunately overgrowth of III-V material is hampered due to the difference in symmetry between ErSb [001] (4-fold) and GaSb [001] (2-fold) resulting in symmetry defects preventing the use of ErSb as a buried contact. One proposed method of circumventing this problem is to use ErSb horizontal nanowires as a buried contact while allowing percolative GaSb growth to occur between the nanowires to maintain crystal orientation. ErSb is known to form a variety of nanostructures in GaSb depending on the ratio of Ga to Er flux during deposition. [1] Understanding the growth mechanisms behind the formation of these different nanoparticles is an important step towards their use as buried contacts, and to achieve nanowire formation in other material systems.

We investigate the growth of horizontal nanowires in the ErSb/GaSb material system, and observe a growth process involving large GaSb macrosteps as the mechanism behind the transition from vertical nanowires to horizontal nanowires.

We also observe a previously unseen low temperature growth mode resulting in horizontal nanowire formation under a much wider range of flux conditions. This new growth mode does not use the embedded growth observed at higher temperatures and may allow for horizontal nanowire formation without the presence of macrosteps, as well as the formation of significantly smaller nanoparticles which may be useful for accessing nanoparticle dimensions that result in electron confinement.

12:00pm **PCSI-TuM-43 Effect of Ga-Dangling Bonds at the GaSb/GaAs Interface of GaSb TPV Cells Grown on GaAs Substrates by IMF Technique**, ***Emma Renteria**, A Mansoori, S Addamane, A Soudachanh, G Balakrishnan,* University of New Mexico

The growth of metamorphic GaSb epitaxial layers on GaAs substrates has become of significant interest in the areas of mid to long wave infra-red (IR) optoelectronic devices. In the case of thermophotovoltaics (TPVs), GaAs substrates are an attractive alternative to GaSb substrates on account of their semi-insulating nature, relatively lower cost, and ability to scale up to large wafer sizes. Unfortunately, the mismatched growth of GaSb epitaxial layers on GaAs substrates results in significant threading dislocations in the GaSb epitaxial layer due to the 7.78% lattice mismatch between the two binary semiconductors. However, the threading dislocation density (TDD) on the GaSb epitaxial layer can be reduced by inducing arrays of 90° interfacial misfit dislocations (IMF) at the GaSb/GaAs interface [1]. This technique reduces the TDD in the GaSb epitaxial layer to the low 10^8 defects/cm^2, which has been sufficient to demonstrate a wide range of devices. However, for TPVs, the residual threading dislocations on the GaSb epitaxial layer severely affects the performance of the GaSb diodes under illumination. Although we are continuously working on optimizing the growth technique to further reduce the TDD, the 90° IMF are made of Ga-dangling bonds localized along the GaSb/GaAs interface which also affect the electronic properties of the devices [2]. These Ga-dangling bonds can act as trap carriers and further affect the performance of metamorphic GaSb TPVs. We have grown and processed a p-n GaSb TPV cell on GaAs substrates. To study the effect of the Ga-dangling bonds on the performance of the cell, we placed the n-type contacts above the IMF interface for some cells and below the IMF for other cells. The presentation will provide extensive characterization data including J-V characteristics of solar cells under dark and illumination.

12:05pm **PCSI-TuM-44 Surface Recombination in Sb-based Infrared Detectors Obtained by Release and Transfer of Membranes**, ***Marziyeh Zamiri,*** University of New Mexico*; B Klein,* Sandia National Laboratory*; V Dahiya, F Cavallo, S Krishna,* University of New Mexico

We have recently isolated Sb-based type II superlattice (T2SL) in the form of free-standing membranes. The tremendous potential of these new structural elements has been demonstrated through fabrication and characterization of infrared (IR) detectors on T2SLs transferred to Si substrates. Here we investigate the effect of surface recombination on the dark current density of IR detectors obtained by release and transfer of membranes. Specifically, we perform a theoretical and experimental study to isolate the contribution of rough sidewalls on the device characteristics.

For this purpose we fabricate and characterize IR detectors on InAs/GaSb T2SLs transferred to bulk Si using two different techniques. Briefly, a 1.6 µm p-i-n T2SL is epitaxially grown onto a 60 nm $Al_{0.4}Ga_{0.6}Sb$ sacrificial layers on a GaSb substrate. Upon selective removal of the $Al_{0.4}Ga_{0.6}Sb$ layer *via* chemical etching, the 25 × 25 µm^2 membrane becomes freestanding, and it can be transferred to the alternative host. In one case, both the top surface and the sidewalls of the membrane are coated with a hard-baked polymer film (*i.e.*, photoresist), and therefore they are unexposed to the chemical etchant. Scanning electron microscopy of the membrane bonded to bulk Si shows that the structure of the T2SL is not altered during release. In the other case, the photoresist is isolating only the top surface of the T2SL, thereby resulting in a significant roughening of the sidewalls. The poor selectivity of the etching solution between GaSb and the $Al_{0.4}Ga_{0.6}Sb$ sacrificial layer is responsible of this structural change in the transferred membrane. Rough sidewalls are expected to enhance surface recombination in the T2SL and therefore increase the dark current density of an IR detector. We quantify this effect by characterizing IR detectors fabricated on the two mesas. A comparative analysis of the dark current density measured for the two devices signify the effect of having exposed sidewalls during membrane release. These experimental results are consistent with theoretical calculations which show a relative enhancement of surface recombination at increasing roughness of the membrane sidewalls.

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