

PCSI

Room Ballroom South - Session PCSI-3MoM

Topological Materials

Moderator: Javad Shabani, New York University

11:00am PCSI-3MoM-31 Topological Heterostructures by Molecular Beam Epitaxy, *Susanne Stemmer*, University of California, Santa Barbara INVITED

Topology, both in real space and in reciprocal space, has emerged as a new design principle for materials that can host a wealth of novel properties. Interfaces and heterostructures with topological materials offer opportunities to control and manipulate their electronic states and associated phenomena, for example, via electric field effect, strain, or symmetry breaking. In this presentation, we will discuss recent progress in the growth of thin films of the three-dimensional Dirac semimetal Cd_3As_2 by molecular beam epitaxy. We show that high-mobility, epitaxial Cd_3As_2 films can be grown and discuss some of the phenomena that can be observed, such as an unusually large negative longitudinal magnetoresistance under parallel electric and magnetic fields. The heterostructures allow for experimental tests of theoretically predicted transitions between topological states by manipulating parameters, such as confinement and film strain. For example, as the film thickness is reduced, a band gap opens in the bulk Dirac electronic states and we observe a quantum Hall effect. Using electric field gating and Landau level spectroscopy, we demonstrate the Dirac dispersion of these two-dimensional states.

11:30am PCSI-3MoM-37 Structural Distortions and Surface/Bulk Competition in Quasi-2D SnSe-TiSe_2 Nanolayered Heterostructures, *Sage Bauers*, National Renewable Energy Laboratory; *D Hamann, D Merrill, J Ditto, M Esters*, University of Oregon; *D Roberts*, University of Colorado at Boulder; *A Zakutayev*, National Renewable Energy Laboratory; *D Johnson*, University of Oregon

Low dimensional materials and their heterostructures are becoming increasingly important due to their emergent properties not observed in bulk analogues. As the fraction of surface or interface atoms become comparable to the bulk, so too do their contributions to the free energy. Since the most stable interface structure does not necessarily agree with the most stable bulk structure, competition between structures can cause size-dependent distortions or phase transitions. These structural behaviors can fundamentally alter the electronic environment, significantly affecting the material properties.

I will present on multilayer heterostructures formed by self-assembly of designed precursors. This will focus on a system containing quasi-2D layers of SnSe interleaved with TiSe_2 , which exhibits size-dependent structures and transport properties. When a single bilayer of SnSe is present all atoms reside at a TiSe interface, templating is observed and long-range 3-dimensional order is established in the heterostructure.[1] However, as the number of SnSe layers increases and “bulk” atoms are introduced, distortions, additional structures, and new stacking sequences are observed.[2] These findings are corroborated by DFT calculations. The changing SnSe structure has profound effects on the composite transport properties with a shift in carrier type, as shown by Seebeck coefficient and Hall measurements.

This designed precursor approach has also been used to study thermoelectric enhancement[3] and quantum phase transitions[4] as a function of layer thickness in other selenides. Work extending this approach to sulfides is currently underway at NREL, and I will briefly present our initial results synthesizing similar heterostructures via combinatorial sputter deposition.

[1] D. M. Hamann, *et al*, *Inorg. Chem.* 2017, 56, DOI 10.1021/acs.inorgchem.6b03063.

[2] D. M. Hamann, *et al*, *ACS Nano* 2018, 12, DOI 10.1021/acsnano.7b07506.

11:35am PCSI-3MoM-38 Gold-gold Dimer Buckling and Electronic Structure of Epitaxial LaAuSb Films., *Patrick Strohbeen, D Du, C Zhang, E Shourov*, University of Wisconsin-Madison; *F Rodolakis, J McChesney*, Argonne National Laboratory; *P Voyles, J Kawasaki*, University of Wisconsin-Madison

Recently, a new subset of hexagonal Heuslers with composition LnAuSb ($\text{Ln} = \text{La-Nd, Sm}$) was predicted to exist and shown to be stable in bulk polycrystalline samples¹. These compounds contain 19 electrons per formula unit, typically thought to be unstable through traditional electron counting rules, however these compounds have been predicted to be stabilized through by highly localizing the 19th electron in Au-Au dimer bonds. Of these new phases, LaAuSb was also predicted through bandstructure calculations to be a Topological Dirac Semimetal (TDS). Here, we will (1) investigate this unique crystal structure and (2) study the electronic properties and structure of single phase epitaxial LaAuSb thin films.

In the original study, LaAuSb was grown in a bulk crystal, however it was both polycrystalline and full of impurity phases and thus it did not lend itself well to study. Here we use molecular beam epitaxy (MBE) to grow single crystalline thin films on c-plane sapphire to investigate the proposed “dimerized” structure. Growth was monitored in-situ by reflection high energy electron diffraction (RHEED) in which the resultant film patterns were streaky and well-resolved Kikuchi lines were observed (Fig. 1a,b), indicating the well-ordered and relatively flat surface of the film. Strong RHEED oscillations were observed throughout growth as well as Kiessig fringes (Fig. 1d,e) which is also consistent with a layer-by-layer growth mode resulting in a smooth surface and substrate/film interface. Magnetotransport measurements were conducted and show the expected metallic behavior with a residual resistivity ratio (RRR) of 2.25 (Fig. 1f). Angle-resolved photoemission spectroscopy (ARPES) measurements were conducted at BL-29ID at the Advanced Photon Source, using a vacuum suitcase to protect the film surface. The valence band density of states is compared to DFT calculations assuming both the dimerized and non-dimerized versions of the LaAuSb crystal. The crystal structure, magnetotransport, and electronic structure will be discussed.

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11:40am PCSI-3MoM-39 MBE Growth of Cd_3As_2 on $\text{GaAs}(001)$ Substrates, *Anthony Rice, K Alberi*, National Renewable Energy Laboratory

The Dirac semimetal Cd_3As_2 has become a useful material in the scientific community, as it provides access to a variety of interesting phenomena ranging from topological superconductivity to massless Dirac fermions. It is also potentially useful for energy-related applications due to its high electron mobility and large phonon-phonon scattering. Both single crystal and thin film synthesis has been achieved, however thin film research to date has been confined to non-traditional substrates, such as mica [1], or zinc blende (111) orientations [2,3] due to the preferred (112) growth plane of Cd_3As_2 . To aid integration of Cd_3As_2 into current technological applications, growth on a (001) substrate must be pursued.

Here, we explore the use of a $\text{II-Te/GaAs}(001)$ platform to support Cd_3As_2 . CdTe grown directly onto $\text{GaAs}(001)$ results in a (111) orientation due to the large lattice mismatch (14.6%), as shown by X-ray diffraction (XRD). A high temperature anneal prior to CdTe growth, resulting in a Ga-rich surface reconstruction, further improves the interface and resulting film morphology. Atomic force microscopy reveals film roughness comparable to CdTe structures on $\text{GaAs}(111)$. Growth of Cd_3As_2 on this platform is explored and compared to similar films on $\text{GaAs}(111)$ substrates.

[1] P. Cheng *et al*, *New J. Phys.* 18 083003 (2016)

[2] T. Schumann *et al*, *APL Mater.* 4, 126110 (2016)

[3] M. Goyal *et al*. *APL Mater.* 6, 026105 (2018)

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