PCSI

Room Redondo - Session PCSI-WeM1

Topological and Magnetic Materials

Moderator: Joan Redwing, The Pennsylvania State University

8:30am **PCSI-WeM1-1 Development of Thin Film Platforms for Tunable Topological Materials***, **Anthony Rice**,* NREL **INVITED**

Cd_3As_2 is a prototypical Dirac semi-metal, a class of materials with gapless topologically protected electronic states. These materials could play a role in a large number of applications, including transistors, spintronics, photodetectors, and thermoelectrics. To be used in these technologies, however, significant progress needs to be made in developing routes to tune their properties as well as combining them with materials that are already technologically relevant. Here, a II-VI/III-V platform is first developed which allows for growth of Cd_3As_2 on GaAs(111) with high electron mobility. This platform is extended for both (110) and (001) film orientations, ultimately allowing for growth of heterostructures relevant for photodetectors. Analogous approaches also allow for integration of Cd_3As_2 with Si(001). Ways to alter the electronic properties of Cd_3As_2 will also be discussed. This work demonstrates routes toward developing quantum materials for a variety of applications and may be extended to a variety of other materials system.

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9:10am **PCSI-WeM1-9 Electrical Transport of Zn-doped Dirac Semimetal Cd_3As_2 Films***, **Ian Leahy**, J. Nelson, A. Rice, K. Alberi,* National Renewable Energy Laboratory

Topological semimetals (TSMs) are emerging as materials with potential use in low powered electronics and spintronic devices [1-4]. In order to translate the useful properties of TSMs to device applications, studies focusing on reliable epitaxial growth, disorder, and the control of electronic states in TSM films are needed. Here, wefocus on the use of alloying with Zn to modify the electronic structure and electrical transport of $(Cd_{1-x}Zn_x)_3As_2$ with x = 0-0.23.

Zn doping of Cd_3As_2 has been used to lower the carrier concentration and move the Fermi energy closer to the Dirac point. However, the addition of Zn is also expected to modify the band structure, causing a change in the electronic structure from Dirac semimetal to semiconductor [5]. By tuning the growth conditions to suppress native defects in our films [6] we are able to produce $(Cd_{1-x}Zn_x)_3As_2$ films with carrier concentrations a full order of magnitude smaller (as shown in Fig. 1b, ~10^{17} cm^{-3}) than other literature reports (>10^{18} cm^{-3}) [7]. Lowering the starting carrier concentration enables us to tune the Fermi energy with smaller amounts of Zn doping.

Figure 1 shows the Zn doping dependence of the low-field mobility and the carrier density for our films. For x < 0.1, we observe a slight reduction in mobility with increasing x paired with an order of magnitude reduction in the carrier density. By x = 0.23, the dominant carrier switches from n-type to p-type accompanied by a 100x reduction of the carrier mobility, consistent with the transition from TSM Cd_3As_2 to semiconducting Zn_3As_2 behavior. We will present a careful analysis of the electrical transport properties to explore the low Zn doping regime where the n-type carrier densities reach their lowest values before the electronic structure is significantly altered.

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[4] B. Zhao, et. al., Advanced Materials, 32:38, 200818 (2020).

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[7] S. Nishihaya, et. al., Physical Review B 87, 245103 (2018).

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9:15am **PCSI-WeM1-10 Epitaxial Growth of Weyl Semimetal TaAs on GaAs(001)***, **Jocienne Nelson**, A. Rice, I. Leahy,* NREL*; R. Kurleto,* University of Colorado at Boulder*; J. Mangum,* NREL*; A. Shackelford,* University of Colorado at Boulder*; M. van Schlifgaarde,* NREL*; M. Holtz,* Colorado School of Mines*; D. Dessau,* University of Colorado at Boulder*; K. Alberi,* NREL

Three dimensional topological semimetals (TSMs) were experimentally discovered in the past decade and exhibit extraordinary properties such as extremely high mobility [1], conductivity [2] and magnetoresistance [3] stemming from their protected bandstructure. They are now emerging as excellent candidates for a wide variety of applications including photovoltaics [4], spintronics [5], thermoelectrics [6], and catalysts [7]. Weyl semimetals in particular have unique bandstructures with a singly degenerate linear band crossings. While there has been a great deal of success studying novel bulk single crystal TSMs, they are not suitable for device applications. Instead, epitaxial thin films are needed to access unique behaviors such as the Chiral anomaly and also insert them into more conventional device structures. Thus, there is a need to develop thin film TSMs compatible with semiconductor manufacturing to accelerate the adoption of TSMs into device applications.

We report epitaxial growth of the Weyl semimetal TaAs on GaAs(001) substrates using molecular beam epitaxy. TaAs has been widely studied in bulk crystal form but has not previously been synthesized as a single crystal film, likely due to the challenge posed by a lack of lattice matched substrates. In this presentation we discuss growth strategies to realize single crystal films and eliminate secondary phases. Fig. 1 shows x-ray diffraction and reflection high energy electron diffraction (RHEED) measurements demonstrating that the TaAs is single crystal. We will also discuss the impact of epitaxial growth on intrinsic doping and magnetoresistance.

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[2] Kumar et. al. *Nat. Comm.***10**, 2475 (2019).

[3] Kumar et. al. *Nat. Comm.* **10,** 2475(2019)

[4] Osterhoudt et. al, *Sci. Adv.***18,** 471-475 (2019)

[5] Sun et. al, *PRL***117,** 146403 (2016)

[6] Wang et. al, *Sci. Bull.* **63,** 411-418 (2018)

[7] Rajamanthi et. al, *Adv. Mater.* **29,** 1606202 (2017)

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9:20am **PCSI-WeM1-11 Quasi Van Der Waals Epitaxy of Magnetic Topological Insulator on GaAs (111) Substrate***, **Yuxing Ren**, L. Tai, S. Chong, G. Qiu, K. Wang,* University of California, Los Angeles

Magnetic topological insulator could achieve quantum anomalous Hall (QAH) effect and spin-orbit torque (SOT) switching in the same structure. This is promising for its future applications in memory or switching applications with its robust surface properties by topological protection. In this work we have grown $Cr:(Bi_xSb_{1-x})_2Te_3$ and $MnBi_2Te_4$ on GaAs (111) substrate through modulation doping by MBE (Molecular Beam Epitaxy). The doping level and the thickness of each layer is examined to tune the bandgap and the Fermi level of the whole sample. In this way, we can tune the Fermi level into the bandgap and optimize the total resistivity to achieve quantization.

Considering the van der Waals nature of the epitaxial layers, it has very weak van der Waals bonding with the substrate. This gives rise to a quasi Van der Waals epitaxial growth mode at the interface of GaAs (111) and epitaxial layers. In this growth mode strain relaxes quickly within the 1st epitaxial layer. Growth mechanism and the influence on its transport properties are also discussed.

9:25am **PCSI-WeM1-12 UPGRADED: Asymmetric Magnetic Proximity Interactions in Ferromagnet/Semiconductor van der Waals Heterostructures***, **Scott Crooker**,* Los Alamos National Laboratory

Magnetic proximity interactions (MPIs) between atomically-thin semiconductors and two-dimensional magnets provide a means to manipulate spin and valley degrees of freedom in nonmagnetic monolayers, without the use of applied magnetic fields.In such van der Waals (vdW) heterostructures, MPIs originate in the nanometer-scale coupling between the spin-dependent electronic wavefunctions in the two materials, and typically their overall effect is regarded as an effective magnetic field acting on the semiconductor monolayer. Here we demonstrate that this picture, while appealing, is incomplete: The effects of MPIs in vdW heterostructures can be *markedly asymmetric*, in contrast to that from an applied magnetic field [1].Valley-resolved optical reflection spectroscopy of $MoSe_2/CrBr_3$ vdW structures reveals strikingly different energy shifts in the *K* and *K'* valleys of the $MoSe_2$, due to ferromagnetism in the $CrBr_3$ layer. Strong asymmetry is observed at both the A- and B-exciton resonances. Density-functional calculations indicate that valley-asymmetric MPIs depend sensitively on the spin-dependent hybridization of overlapping bands, and as such are likely a general feature of such hybrid vdW structures. These studies suggest routes to selectively control *specific* spin and valley states in monolayer semiconductors.

9:45am **PCSI-WeM1-16 Atomic Layer Epitaxial Growth of Kagome Magnet Fe_3Sn_2 Thin Films**, ***Shuyu Cheng***, *B. Wang, I. Lyalin, N. Bagués, A. Bishop, D. McComb, R. Kawakami,* Ohio State University

Kagome magnets are attractive family of materials due to complex spin textures and topological band structures [1]. As a typical example of kagome magnet, Fe_3Sn_2 has been shown to exhibit spin frustration [2] and magnetic skyrmions [3] in real space, and massive Dirac fermions [4] in momentum space. However, most of these studies were done on bulk crystals. The development of epitaxially grown Fe_3Sn_2 thin films will be an exciting future direction, as the thin films of kagome magnets enable potential applications in devices as well as the discovery of new phenomena.

In this presentation, we report our progress in atomic layer molecular beam epitaxy (AL-MBE) growth of kagome magnet Fe_3Sn_2 thin films on Pt(111) buffer layer on Al_2O_3(0001) substrates. During the growth, the RHEED intensity shows oscillatory behavior, indicating layer-by-layer growth mode (Fig. 1(a)). AL-MBE allows us to grow Fe_3Sn_2 at much lower temperatures and therefore produces a sharp interface. The high quality of the sample is confirmed by various methods (Fig. 1(b)). The magnetic properties of Fe_3Sn_2 thin films are also presented here (Fig. 1(c)) [5]. We further show that the anomalous Hall effect (AHE) only has intrinsic contribution, suggesting the magnetic Weyl semimetal nature of Fe_3Sn_2 (Fig 1(d)).

[1] Kuroda, K., et al. *Nature Materials***16**.11 (2017): 1090-1095.

[2]Fenner, L. A., et al. *Journal of Physics: Condensed Matter***21**.45 (2009): 452202.

[3]Hou, Zhipeng, et al. *Advanced Materials***29**.29 (2017): 1701144.

[4] Ye, Linda, et al. *Nature***555**.7698 (2018): 638-642.

[5] Cheng, Shuyu, et al. *APL Materials***10**, 061112 (2022)

9:50am **PCSI-WeM1-17 Selectively Oriented Crystalline Growth of Mn_3Sn on Al_2O_3(0001) using Molecular Beam Epitaxy**, ***Sneha Upadhyay***, *T. Erickson , H. Hall, A. Shrestha,* Ohio University*; J. Moreno,* Universidad Autónoma de Puebla, Instituto de Física, Apartado , Mexico*; D. Ingram ,* Ohio University*; K. Sun,* The University of Michigan*; A. Smith ,* Ohio University

Kagome antiferromagnet Mn_3Sn has garnered attention due to the presence of interesting properties such as anomalous Hall effect below 420K[1], Nernst effects and presence of exchange bias[2]. Until now most thin film growths have been conducted by using sputter deposition or by cleaving. Recently, Higo *et al* reported the finding of the 100% perpendicular full switching of the (01$\underline{1}$0) oriented Mn_3Sn which was grown using molecular beam epitaxy on a MgO (110) substrate having a thin W buffer layer [3]. This result indicated that the orientation and possible strain of the film can be key for film transport properties and therefore its of great interest to explore how one can achieve different crystalline film orientation of Mn_3Sn.

In this talk, we demonstrate the synthesis of crystalline Mn_3Sn on Al_2O_3(0001) without a buffer layer using molecular beam epitaxy. The samples were deposited at two different temperatures T_h (500 ± 9 °C) and T_l (416 ± 9 °C) with Mn: Sn flux ratio of 3.2:1 for 90 minutes. Our analysis indicates that for the two temperatures, the resulting orientations of the films are different, with the T_h sample being predominantly *c*-oriented and T_l sample being 43% *a*-oriented but in our recent template growth method at room temperature we achieved 82% *a*-oriented film. In both cases the reflection high energy electron diffraction (RHEED) patterns were streaky indicating a crystalline film and the cross-sectional scanning tunneling electron microscopy (STEM) gave an insight into the morphology of the samples. In both cases the sample are discontiguous with presence of 3D morphology for sample grown at T_h and quasi-2D morphology for the T_l grown sample. Template grown sample are contiguous and show streaky RHEED patterns throughout the growth. Orientation relationships between the Mn_3Sn films and the sapphire substrate are determined from *in-plane* and *out-of-plane* measurements. The composition of the samples, the strain effects as well as the pseudomorphic overlay will be discussed in detail. Furthermore, we are in the process of doing STM measurements of the samples and performing theoretical calculations.

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[3]T. Higo, K. Kondou, T. Nomoto, M. Shiga, S. Sakamoto, X. Chen, D.N.-Hamane, R. Arita, Y. Otani, S.Miwa and S. Nakatsuji, *Nature* **607**, 474-479 (2022).

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