PCSI

Room Ballroom South - Session PCSI-MoE

Topological Materials & Interfaces II

Moderator: Joshua Goldberger, The Ohio State University

7:30pm **PCSI-MoE-1 Large Magnetotransport Responses and Spintronic Functionalities of Topological van der Waals Ferromagnets*, Jun Sung Kim,*** Pohang University of Science and Technology (POSTECH), Republic of Korea **INVITED**

Topological van der Waals (vdW) ferromagnets has emerged as a promising material platform for investigating novel magentotransport responses and spintronic functionalities. Their unique topological electronic structures in combination of magnetism, spin-orbit interaction, and orbital-driven topological band degeneracy gives rise to large magnetotransport responses and magnetic tunability. In addition, their unique vdW structure allows for the isolation of atomically thin layers as well as the creation of atomically sharp and clean interfaces in heterostructures. In this talk, I will discuss our recent demonstrations of these magnetotransport and spintronic properties on various topological vdW ferromagnets and their heterostructures, highlighting large anomalous Hall effect [1], large angular magnetoresistance [2], highly-tunable spin-valve operations [3], and highly efficient magnetic switching [4]. These findings demonstrate that topological vdW ferromagnets have great potential for realizing novel spin-dependent electronic functionalities, which may be suitable for all-vdW-material-based spintronic applications.

[1] K.Kim, et al. Nat. Mater. 17. 794 (2018)

[2] J. Seo et al. Nature 599, 576–581 (2021).

[3] K.-H. Min, et al. Nat. Mater. 21, 1144 (2022)

[4] G. S. Choi *et al.* submitted

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8:10pm **PCSI-MoE-9 Tuning the Curie Temperature of a 2D Magnet/Topological Insulator Heterostructure to Above Room Temperature by Epitaxial Growth*, Wenyi Zhou,*** *A. Bishop,* The Ohio State University*; X. Zhang,* Cornell University*; K. Robinson, I. Lyalin, Z. Li, R. Bailey-Crandell,* The Ohio State University*; T. Cham,* Cornell University*; S. Cheng,* The Ohio State University*; Y. Luo,* University of Southern California*; D. Ralph, D. Muller,* Cornell University*; R. Kawakami,* The Ohio State University

Heterostructures of two-dimensional (2D) van der Waals (vdW) magnets and topological insulators (TI) are of substantial interest as candidate materials for efficient spin-torque switching, quantum anomalous Hall effect, and chiral spin textures. However, since many of the vdW magnets have Curie temperatures below room temperature, we want to understand how materials can be modified to stabilize their magnetic ordering to higher temperatures. In this work, we utilize molecular beam epitaxy to systematically tune the Curie temperature (T_C) in thin film Fe_3GeTe_2/Bi_2Te_3 from bulk-like values (~220 K) to above room temperature by increasing the growth temperature from 300 °C to 375 °C (Figure 1). For samples grown at 375 °C, cross-sectional scanning transmission electron microscopy (STEM) reveals the spontaneous formation of different $Fe_mGe_nTe_2$ compositions (e.g. $Fe_5Ge_2Te_2$ and $Fe_7Ge_6Te_2$) as well as intercalation in the vdW gaps, which are possible origins of the enhanced Curie temperature. This observation paves the way for developing various $Fe_mGe_nTe_2$/TI heterostructures with novel properties.

8:15pm **PCSI-MoE-10 Kagome Antiferromagnetic Mn_3GaN grown on MgO(001) using Molecular Beam Epitaxy*, A. Abbas, A. Smith, Ashok Shrestha,*** *S. Upadhyay, T. Erickson,* Ohio University*; K. Sun,* University of Michigan*; D. Ingram,* Ohio University

Antiperovskite materials are intermetallic compounds with perovskite crystal structure (space group Pm3m) but with anion and cation positions interchanged in the unit cell [1]. Similar to oxide-perovskite structure, antiperovskite materials have a variety of physical properties including antiferromagnetism, superconductivity and giant magnetoresistance [2]. There have been very few studies of antiperovskite structure Mn_3GaN in general although it was seen in molecular beam epitaxial growth as a second-phase precipitate when growing MnGaN [3]. Here we discuss the molecular beam epitaxial growth and surface study of Mn_3GaN. In our work, Mn_3GaN is deposited at 250 ± 10 °C onto magnesium oxide (001) substrates with a Mn: Ga: N flux ratio of 3:1:1. The sample surface is continuously monitored throughout the growth using reflection high energy electron diffraction. During the growth, the RHEED pattern was observed to be highly streaky, indicating an atomically smooth surface. The calculated *in-plane* lattice constant based on RHEED is 3.89 ± 0.06 Å. This value is close to the theoretical lattice constant *a* of Mn_3GaN (3.898 Å) [3]. X-ray diffraction confirms the majority 002 peak, and the value calculated is 3.84 ± 0.06 Å which also agrees well with the theoretical value (3.898 Å) [3] and with the experimental reported *c* value (3.881 Å) [2]. Since we did not observe significant second-phase peaks, the phase purity of the sample is quite high. Furthermore, cross-sectional STEM was done to understand the interface and the surface of the film. The plan is to also present *in-situ* scanning tunneling microscopy results for the surfaces of these MBE-grown Mn_3GaN layers.

This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-06ER46317.

[1] S. V. Krivovichev, Minerals with antiperovskite structure: A review. Z. Kristallogr. 223, 109–113 (2008).

[2] KH. Kim, KJ. Lee, HS. Kang, FC. Yu, JA. Kim, DJ. Kim, KH. Baik, SH. Yoo, CG. Kim, YS. Kim, "Molecular beam epitaxial growth of GaN and GaMnN using a single precursor," Physica Status Solidi (b) 241(7), 1458 (2004).

[3] E. F. Bertaut, D. Fruchart, J. P. Bouchaud, and R. Fruchart, (1968). Diffraction Neutronique de Mn3GaN. Solid State Commun. 6, 251–256 (1968).

8:20pm **PCSI-MoE-11 Investigation of Smooth Epitaxial Growth of Mn_3Sn Films on *C*-Plane GaN Using Molecular Beam Epitaxy*, Sneha Upadhyay,*** *H. Hall, C. D'Mello,* Ohio University*; J. Hernandez,* Universidad Autonoma de Puebla, Mexico*; T. Erickson,* Ohio University*; K. Sun,* The University of Michigan, Ann Arbor*; G. Cocoletzi,* Universidad Autonoma de Puebla, Mexico*; N. Takeuchi,* Universidad Nacional Autónoma de México*; A. Smith,* Ohio University

Recently, Chen *et al.* studied the all-antiferromagnetic tunnel junction consisting of Mn_3Sn / MgO/ Mn_3Sn (011$\underline{1}$), where they observed a tunnel magnetoresistance (TMR) effect at a ratio of 2% at room temperature. [1] Furthermore, Bangar *et al.* reported the epitaxial growth of *c*-plane Mn_3Sn on the Al_2O_3 substrate using a Ru seed layer. They demonstrated a technique of engineering intrinsic spin Hall conductivity in Mn_3Sn by adjusting the Mn composition slightly for functional spintronic devices.[2] These works indicate great potential for kagome antiferromagnetic material, and it is essential to investigate the growth of Mn_3Sn on various substrates. In our previous work, we demonstrated the deposition of Mn_3Sn (0001) on Al_2O_3 (0001) at 524 ± 5°C, which resulted in a 3D island growth. We observed dome-like structures, which may be related to the significant lattice mismatch with sapphire (19%).[3] Subsequently, we began to explore new substrates, and recently, we tried the growth on the MBE-grown N-polar GaN (000$\underline{1}$). The growth was monitored *in-situ*using reflection high energy electron diffraction and measured *ex-situ* using X-ray diffraction, Rutherford backscattering, and atomic force microscopy. The sample grew at 524 ± 5°C for 71 mins, resulting in an epitaxially smooth growth of Mn_3Sn on GaN (000$\underline{1}$). The *in-plane* lattice constants indicate a strain of -2.13 %, while the XRD indicates a 0001 orientation with a strain of -0.53% and an 11$\underline{2}$0 orientation with a strain of + 2.73%. Furthermore, the effect of varying growth temperature and Mn: Sn flux ratio on film orientation and crystallinity will be discussed in detail. We are also planning to begin scanning tunneling microscope experiments.

The authors acknowledge support from the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-06ER46317. We acknowledge the financial support of the Nanoscale & Quantum Phenomena Institute.

[1] X. Chen *et al.*, "Octupole–driven magnetoresistance in an antiferromagnetic tunnel junction." Nature **613**, 490 (2023).

[2] H. Bangar *et al.*, "Large Spin Hall Conductivity in Epitaxial thin films of Kagome Antiferromagnet Mn_3Sn at room temperature", Adv. Quantum Technol. **6**, 2200115 (2023).

[3]S. Upadhyay *et al.*, "Exploring the interfacial structure and Crystallinity for Direct Growth of Mn_3Sn (0001) on Sapphire (0001) by Molecular Beam Epitaxy", *Surfaces and Interfaces (accepted).*

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8:25pm **PCSI-MoE-12 Symmetry Constraints on Topological Invariants*, Jing Zhang,*** Imperial College London, UK

Classification of topologically trivial/non-trivial crystalline insulators are based on the homology of Berry connection on the Bloch (vector) bundle

with the BZ as the base manifold. Specifically, the trivial phase correspond to zero Berry phase defined in terms of Wilson loop operator integrated along closed path in the BZ. (Eq.1).The transformation properties of eigenstate in the Berry connection are well defined for a given k but it is generally a function of k. This makes the analysis of symmetry properties of Berry phase difficult (path integrals in BZ do not form a representation). There are symmetry analysis such as symmetry indicator method but they lack the group theoretical justification like Wigner-Eckart theorem. In this contribution, it is shown that ϕ_B can be evaluated using the band representation basis (EBRs) under the tight binding model and Stokes theorem. (Eq.2). The transformation properties of these EBRs contains no explicit k dependence and RHS of Eq.2 form a representation of the space group (Symmetry operation takes the closed path to others in the BZ belonging to a closed set. These set of Berry phases along different paths within the set form the representation). As a closed path in the BZ is frequently not contained in the representation domain, full group method is used.

The BZ are 2-torus or 3-torus. It is not simply connected and one needs to consider inquivalent un-contractable closed path, as in homotopy analysis involving the fundamental group. The symmetry operation naturally permute closed path between such set. Symmetry analysis shows the ϕ_B is generally not forbidden by symmetry of layer/space group. However, presence of some symmetry (e.g. inversion) may leads to specific selection rules that forces the Berry phase to be zero.

For a set of physically connected bands with symmetry at high symmetry points identical to direct sum of the EBRs, they have the same transformation properties as the set of EBRs and may be represented as such with appropriate interactions. The same symmetry analysis then may be applied. For close path containing the Γ point, what forms a representation of the group is not necessarily restricted to the whole close path, but half of a close path given that Γ point is invariant. Graphene is used as an example to illustrate both the trivial (sp2 bands) and non-trivial (pz band with spin).

The general conclusions are that not all ocuppied EBRs are symmetry forbidden from having non-zero Berry phase and occurrence of trivial phase are the exceptions. The symmetry indicator method at identifying trivial phase may include non-trivial phases.

8:30pm **PCSI-MoE-13 UPGRADED: Epitaxial Kagome Thin Films as a Platform for Topological Flat Bands and Dirac Cones**, *S. Cheng, M. Nrisimhamurty,* Ohio State University*; T. Zhou,* University at Buffalo*; N. Bagues, W. Zhou, A. Bishop, I. Lyalin,* Ohio State University*; C. Jozwiak, A. Bostwick, E. Rotenberg,* Advanced Light Source, Lawrence Berkeley National Laboratory*; D. McComb,* Ohio State University*; I. Zutic,* University at Buffalo*;* ***Roland Kawakami****,* Ohio State University

Metals consisting of kagome lattices have interesting band structures consisting of topological flat bands and Dirac cones. Systems with flat bands are ideal for studying strongly correlated electronic states and related phenomena due to the smaller bandwidth *W* compared to the Coulomb repulsion *U*. Kagome metals such as CoSn have been recognized as promising candidates due to the proximity between the flat bands and the Fermi level. A key next step will be to realize epitaxial kagome thin films with flat bands to enable tuning of the flat bands across the Fermi level via electrostatic gating or strain. Here we report the band structures of epitaxial CoSn thin films grown directly on insulating substrates [1]. Flat bands are observed using synchrotron-based angle-resolved photoemission spectroscopy (ARPES). The band structure is consistent with density functional theory (DFT) calculations, and the transport properties are quantitatively explained by the band structure and semiclassical transport theory. We are also developing kagome metals that have the Dirac cones near the Fermi level, which are interesting for investigating the intrinsic anomalous Hall effect and to potentially realize the quantum anomalous Hall effect at elevated temperatures.

[1] Cheng *et al.,* Nano Letters, 23(15), 7107-7113 (2023).

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