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A. Rationale

Cadmium arsenide (Cd_3As_2) is a well-known semiconducting material that has recently been classified as a three-dimensional (3D) Dirac semimetal, a newly discovered category of quantum matter. The electronic band structure of Dirac semimetals is an intermediate state between insulators and metals, in which the valence and conduction bands cross at discrete points in momentum space called Dirac nodes. While these point-like degeneracies have previously been observed in spineless graphene, a two-dimensional (2D) system, it was only recently that a 3D analog was experimentally realized. The four-fold rotational symmetry of the tetragonal crystal structure of Cd_3As_2 protects the Dirac nodes, even at high Fermi energies. The non-trivial topology of Cd_3As_2 along with its unique band structure generates surface states similar to that of 3D topological insulators. This means that when a bandgap opens in the bulk of the material, metallic surface states will arise.

While a variety of other Dirac semimetals have been discovered, Cd_3As_2 is the only one known to be electrochemically stable at room temperature. Because of this, Cd_3As_2 is compatible with the conditions in functional electronic devices. Additionally, the Fermi level of Cd_3As_2 can be adjusted, allowing it to be utilized across a wide range of technological applications. A recent study found that Cd_3As_2 could be tuned to a topological superconducting state when placed under high pressure conditions. Topological superconductors are a known source of Majorana fermions: quasiparticles which can be used in quantum computers. The linear band dispersion and zero bandgap of Cd_3As_2, along with its high carrier mobility, give it a high responsivity to electromagnetic waves. This is a necessary quality for materials used in infrared and photodetectors. Spin polarization of carriers is also possible in Cd_3As_2, making it a possible candidate for use in spintronics devices.

Manipulation of different aspects of Cd_3As_2 heterostructures allows for the properties of the films to be tuned. The buffer on which the Cd_3As_2 films are deposited is known to have effects on the film's properties. One study subjected Cd_3As_2 films to both compressive and tensile strain by varying the lattice parameter of a $Ga_{(1-x)}In_{(x)}Sb$ buffer layer. Another study found that the surface morphology of the films could be improved through the use of an InAs wetting layer. While buffer layers have been used to improve Cd_3As_2 films, they can also have negative impacts on the film's quality. A buffer layer with a mismatched lattice parameter may cause dislocations, which can lower the electron mobilities in thin films.

The orientation of the film growth can also be changed. The presence of Fermi arcs on the surface of Cd_3As_2 films grown in the (112)-orientation has been observed in momentum space. The arcs create a tunnel-like path through the Dirac nodes, allowing conduction through a Fermi loop. While (001)-oriented films have been grown successfully, better established (112) orientations are more widely studied. The (001) orientation differs from that of the (112) direction in that the two Dirac nodes project onto a single point.

While much had been discovered about Cd_3As_2 in recent years, much is still unknown about this material. A model for better understanding the fundamental aspects of this material is necessary in order to realize it's many interesting applications.

B. Research Outcome, Hypothesis, Engineering Goals, Expected Outcomes

Great progress has been made in the understanding and improvement of the electronic properties of Cd_3As_2 in recent years. Despite this development, much is still unknown about this material. This investigation seeks to explore the electrical transport qualities of a (001) Cd_3As_2 film grown epitaxially on an $Al_{(.42)}In_{(.58)}Sb$ lattice matched buffer layer deposited on a GaSb substrate. This is expected to create a novel heterostructure with minimal dislocations in the Cd_3As_2 layer. The goal of this study is to create a film with enhanced electrical transport as compared to films on lattice mismatched buffers, which often have dislocations, and to gain insight into the effect of buffer composition on carrier mobility and carrier density of thin Cd_3As_2 films.

C. 1. Procedures

Thin films will be grown using molecular beam epitaxy (MBE) under ultrahigh vacuum conditions (10^{-10} mTorr). MBE will be used as the growth method because it is a low energy process, allowing for a greater degree of control over film growth as opposed to other methods like laser deposition. A (001) GaSb wafer will first be heated to 510 °C to desorb oxides under Sb flux. Then, a 50 nm thick (001) GaSb layer will be deposited on the substrate to provide a clean interface for the next layer. A 700 nm thick layer of (001) $Al_{(.42)}In_{(.58)}Sb$ will then be grown on the GaSb. Finally, (001) Cd_3As_2 will be grown for 100 sec (40 nm). Reflection high-energy electron diffraction (RHEED) will be used to monitor film growth *in situ*. The finer details of this procedure have been reported elsewhere [17]. The Panalytical MRD PRO Diffractometer will be used to carry out x-ray diffraction (XRD) and x-ray reflectivity (XRR), with Cu Kα (1.5405 Å) radiation. Out-of-plane 2θ-ω XRD scans will be taken in the (004) plane to avoid overlap of the Cd_3As_2 and $Al_{(.42)}In_{(.58)}Sb$ peaks. Bragg's law will be used to determine the lattice parameter of each layer, and Vegard's law will be used to calculate the buffer composition. X-ray reflectivity (XRR) measurements will be used to calculate the thickness of the Cd_3As_2 layer. Atomic force microscopy images will allow for analysis of the surface morphology of both the buffer layer and Cd_3As_2 layer. After film characterization, Hall bar devices will be constructed in the cleanroom and processed via Ar ion milling. Carrier density and carrier mobility measurements will be taken in a Quantum Design Physical Properties Measurements Dynacool system under magnetic fields (-0.5 T to 0.5 T) at low temperatures (2 K to 20 K). Magnetoresistance measurements will be taken at 2K under magnetic fields of -9 T to 9 T.

2. Risk and Safety

All machinery will be operated under the direct supervision of a trained scientist. The molecular beam epitaxy machine, which requires special training to operate, will only be operated by a trained scientist. Nitrile gloves, goggles, and lab coats will be worn in the presence of machinery. Hazardous chemicals will not make direct contact with skin.

3. Data Analysis

RHEED images will be captured during film growth. Python will be used to analyze XRD and XRR data, allowing for the lattice parameter and film thickness to be determined. Python will also be used to analyze transport data. Transport data of a previously reported film from Kealhofer et al. [15] will be used for a comparison between the lattice matched and mismatched film.

D. Bibliography

[**1**] Young, S., Zaheer, S., Teo, J., Kane, C., Mele, E. and Rappe, A. (2012). Dirac Semimetal in Three Dimensions. *Physical Review Letters*, 108(14).

[**2**] Liu, Z., Jiang, J., Zhou, B., Wang, Z., Zhang, Y., Weng, H., Prabhakaran, D., Mo, S., Peng, H., Dudin, P., Kim, T., Hoesch, M., Fang, Z., Dai, X., Shen, Z., Feng, D., Hussain, Z. and Chen, Y. (2014). A stable three- dimensional topological Dirac semimetal Cd3As2. *Nature Materials*, 13(7), pp.677-681.

[**3**] Young, S. and Kane, C. (2015). Dirac Semimetals in Two Dimensions. *Physical Review Letters*, 115(12).

[**4**] Borisenko, S., Gibson, Q., Evtushinsky, D., Zabolotnyy, V., Büchner, B. and Cava, R. (2014). Experimental Realization of a Three-Dimensional Dirac Semimetal. *Physical Review Letters*, 113(2).

[**5**] Wang, C., Sun, H., Lu, H. and Xie, X. (2017). 3D Quantum Hall Effect of Fermi Arcs in Topological Semimetals. *Physical Review Letters*, 119(13).

[**6**] Yang, B. and Nagaosa, N. (2014). Classification of stable three-dimensional Dirac semimetals with nontrivial topology. *Nature Communications*, 5(1).

[**7**] Wang, Z., Weng, H., Wu, Q., Dai, X. and Fang, Z. (2013). Three-dimensional Dirac semimetal and quantum transport in Cd3As2. *Physical Review B*, 88(12).

[**8**] He, L., Jia, Y., Zhang, S., Hong, X., Jin, C. and Li, S. (2016). Pressure-induced superconductivity in the three-dimensional topological Dirac semimetal Cd3As2. *npj Quantum Materials*, 1(1).

[**9**] Wang, Q., Li, C., Ge, S., Li, J., Lu, W., Lai, J., Liu, X., Ma, J., Yu, D., Liao, Z. and Sun, D. (2017). Ultrafast Broadband Photodetectors Based on Three- Dimensional Dirac Semimetal Cd3As2. *Nano Letters*, 17(2), pp.834-841.

[**10**] Yang, S. (2016). Dirac and Weyl Materials: Fundamental Aspects and Some Spintronics Applications. *SPIN*, 06(02), p.1640003.

[**11**] Schumann, T., Goyal, M., Kealhofer, D. and Stemmer, S. (2017). Negative magnetoresistance due to conductivity fluctuations in films of the topological semimetal Cd3As2. *Physical Review B*, 95(24).

[**12**] Schumann, T., Galletti, L., Kealhofer, D., Kim, H., Goyal, M. and Stemmer, S. (2018). Observation of the Quantum Hall Effect in Confined s of the Three- Dimensional Dirac Semimetal Cd3As2. *Physical Review Letters*, 120(1).

[13] Liang, T., Gibson, Q., Ali, M., Liu, M., Cava, R. and Ong, N. (2014). Ultrahigh mobility and giant magnetoresistance in the Dirac semimetal Cd3As2. *Nature Materials*, 14(3), pp. 280-284.

[**14**]Goyal, M., Kim, H., Schumann, T., Galletti, L., Burkov, A. and Stemmer, S. (2019). Surface states of strained thin films of the Dirac semimetal Cd3As2. *Physical Review Materials*, 3(6).

[**15**] Kealhofer, D., Kim, H., Schumann, T., Goyal, M., Galletti, L. and Stemmer, S. (2019). Basal-plane growth of cadmium arsenide by molecular beam epitaxy. *Physical Review Materials*, 3(3).

[16] Lebedev, V., Cimalla, V., Baumann, T. and Ambacher, O. (2019). Effect of dislocations on electrical and electron transport properties of InN thin films. II. Density and mobility of the carriers: *Journal of Applied Physics*: Vol 100, No 9.

[17] Schumann, T., Goyal, M., Kim, H. and Stemmer, S. (2016). Molecular beam epitaxy of Cd3As2 on a III-V substrate. *APL Materials*, 4(12), p.126110.

[18] Straumanis, M. and Kim, C. (2019). Lattice Parameters, Thermal Expansion Coefficients, Phase Width, and Perfection of the Structure of GaSb and InSb.

[19] Jamieson, J. (1963). Crystal Structures at High Pressures of Metallic Modifications of Compounds of Indium, Gallium, and Aluminum. *Science*, 139(3557), pp.845-847

E. Post summary

No changes have been made to this research summary.