Effect of Inversion Asymmetry on Quantum Confinement of Dirac Semimetal Cd_3As_2

Christopher Chou,[1†] Manik Goyal,[2]

[1]Washington High School, 38442 Fremont Blvd., Fremont, CA 94536

[2]Materials Department, University of California, Santa Barbara, CA 93106

[†]Corresponding author: christopherchou03@gmail.com

UC SANTA BARBARA Research Mentorship Program

WASHINGTON HIGH SCHOOL

Overview

Dirac semimetals have been found to possess promising potential to be extremely fast and efficient for electronic transport while dissipating very low energy due to properties such as:

- High magnetoresistance
- High mobility
- Linear dispersion cone
- Dirac fermions in surface states [1]

Cd_3As_2 exhibits various topological states depending on film thickness

- 3D Topological Dirac semimetal in normal conditions
- Similar to 3D Topological Insulator under quantum confinement with insulating bulk and conducting surface states

We use various methods to analyze these properties:

- Effect of structural inversion asymmetry and hybridization by simulating on Kwant
- Reconcile simulation results with experimental data
- Propose new possible topological devices by manipulating inversion asymmetry and hybridization

We observe the following properties due to inversion asymmetry:

- Lifting of spin degeneracy
- Development of spin-polarized states

Dirac Semimetals

Why the Dirac semimetal Cd_3As_2?

- High electron mobility allows for fast reading/writing of data
- Inverted band structure opens possibility for tunable band gap for electrical transport
- Chiral Dirac fermions on surface states allows data to be read in up/down spin of electrons
- Backscattering suppression leads to dissipationless transport

Quantum Confinement

Process and Effect

- Decreasing the thin film thickness at an incredibly low temperature leads to quantum confinement
- This leads to an increase in the bandgap in the bulk state which means most of the transport is done on the surface state
- Dirac Semimetals like Cd_3As_2 can exhibit quantum spin hall state with backscattering suppression during confinement [1]

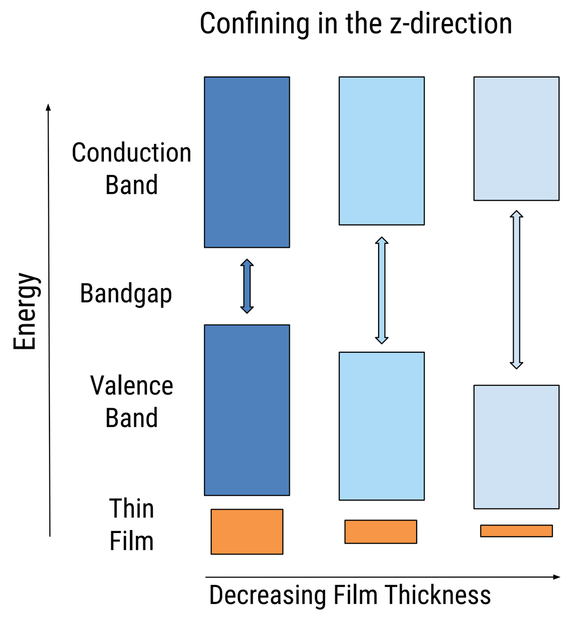

FIG. 1. By decreasing the thin film thickness, the apparent energy difference increases.

The Problem

- Surface states are closer to each other, creating greater interaction which is known as hybridization [3]
- Inversion asymmetry from potential differences on top and bottom surfaces affect transport [3]
- Not much is known about electronic interaction under these effects

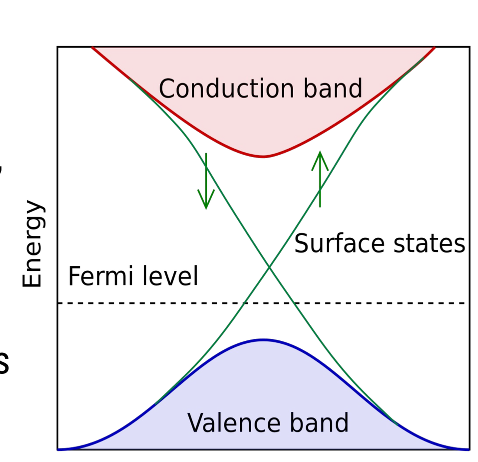

Image Source: Wikipedia

FIG. 2. Quantum confinement opens the band gap of a Dirac Semimetal

Research Objectives

- Simulate electronic transport under quantum confinement
- Compare theoretical predictions of electronic transport with experimental data
- Propose explanations to electronic interactions under quantum confinement in order to open the possibility to new topological applications

Acknowledgements:

The first author would like to express his gratitude towards the second author for his expertise in condensed matter physics and extremely optimistic mindset throughout research. The first author also thanks Dr. Lina Kim and Andrew McGrath for their constant help and support through the program.

References:

[1]J. Hu, S.-Y. Xu, N. Ni, and Z. Mao, "Transport of Topological Semimetals," *Annual Review of Materials Research*, vol. 49, no. 1, pp. 207–252, 2019.

[2]C. Brüne, C. X. Liu, E. G. Novik, E. M. Hankiewicz, H. Buhmann, Y. L. Chen, X. L. Qi, Z. X. Shen, S. C. Zhang, and L. W. Molenkamp, "Quantum Hall Effect from the Topological Surface States of Strained Bulk HgTe," *Physical Review Letters*, vol. 106, no. 12, 2011.

[3]H. Pan, M. Wu, Y. Liu, and S. A. Yang, "Electric control of topological phase transitions in Dirac semimetal thin films," *Scientific Reports*, vol. 5, no. 1, 2015.

Analyzing Electronic Interactions

System Model

Thin Film

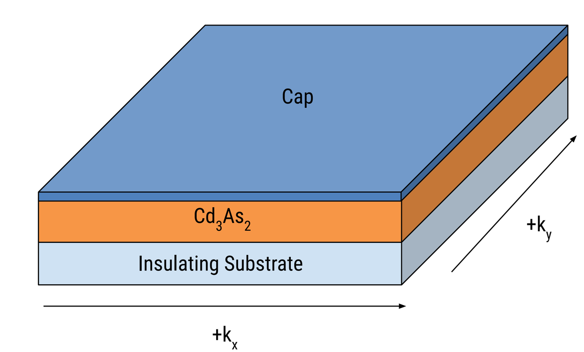

FIG. 3. Physical representation of a thin film of Cd_3As_2 and possible manipulations of inversion symmetry and hybridization

Dirac Hamiltonian

$$\mathcal{H} = \hbar v_f(k_x\sigma_y - k_y\sigma_x)\otimes\tau_z + \Delta_i\mathbf{1}\otimes\tau_z + \Delta_h\mathbf{1}\otimes\tau_x + g^*\mu_B B_0\sigma_z\otimes\mathbf{1}$$

- The Dirac Hamiltonian represents the energy of the two-state system as it evolves with time as a function of the momentum in the x,y direction, inversion symmetry, and hybridization term [2]
- The inversion symmetry Δi term can be varied by using a different material for top and bottom surface that creates a potential difference/asymmetry
- The hybridization term Δh can be varied by manipulating the thickness of the thin film which changes the level of interaction between the top and bottom surface states
- The Zeeman type term $g^*\mu_B B_0\sigma_z$ accounts for the external magnetic field

Quantum Simulation

- Utilized the Python package Kwant
- Generated theoretical model based on Dirac Hamiltonian by manipulating hybridization and inversion symmetry
- Through simulation results, we proposed a possible topological application through manipulation of these terms

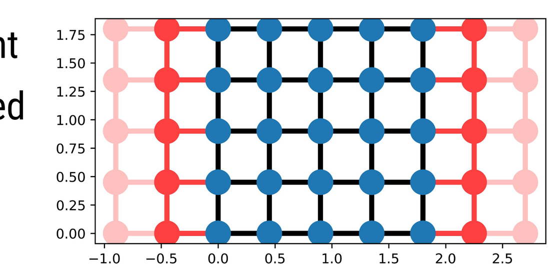

FIG. 4. Example of a surface state with lattice constant a = 0.45 nm^{-1}, length of 2 nm, and width of 2 nm. The site colors are in blue, lead colors in red, and hoppings in black

Comparing Data

After simulating electronic transport under quantum confinement in Kwant, we compared our theoretical model with previous experimental data by analyzing:

- Landau Level Index Diagram describes the type of electrons on the surface states
- Quantum Oscillations allows for experimental detection of spin degeneracy lifting
- Energy-Momentum Dispersion shows the band structure of the surface states

Impact of Breaking Inversion Symmetry and Hybridization

Eigenenergies of Dirac Hamiltonian

$$E_{\alpha t}(n) = t\sqrt{2ne\hbar^2 v_f^2 B + \mu_B^2 g^2 B^2 + \Delta_h^2 + \Delta_i^2 + 2\alpha\sqrt{\mu_B^2 g^2 B^2 \Delta_h^2 + \mu_B^2 g^2 B^2 \Delta_i^2 + 2\Delta_i^2 ne\hbar^2 v_f^2 B}} \qquad n = 1, 2, \ldots$$

$$E_\alpha(0) = \mu_B g^* B_0 + \alpha\sqrt{\Delta_i^2 + \Delta_h^2} \qquad n = 0$$

Energy vs. Magnetic Field

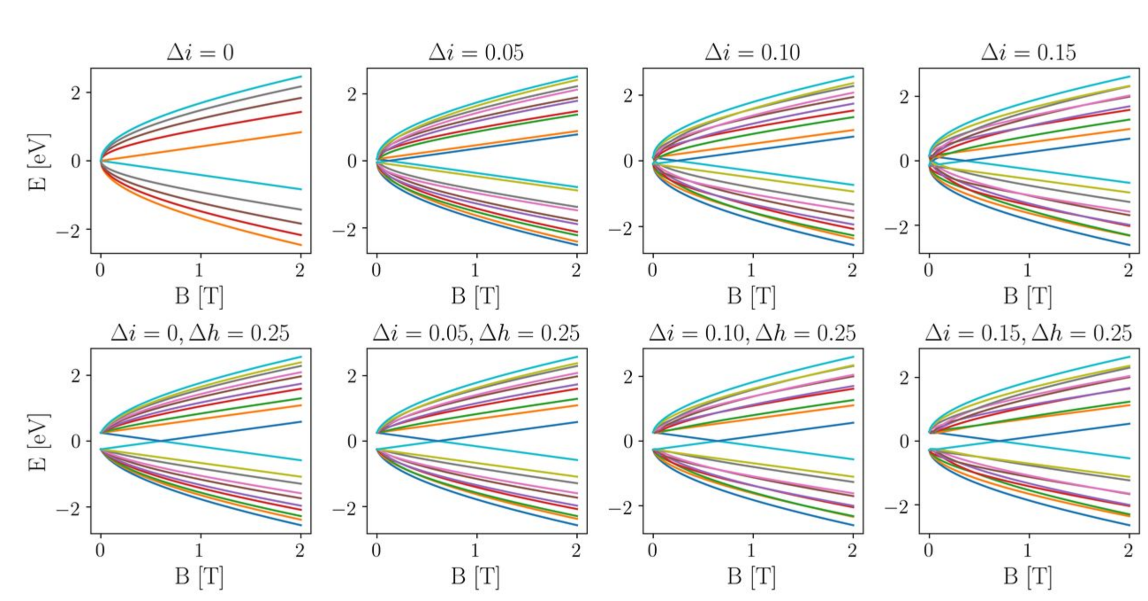

FIG. 5. First row: Energy vs. Magnetic Field with inversion asymmetry but no hybridization
Second row: Energy vs. Magnetic Field with inversion asymmetry and hybridization

- We notice an E ∝ √B relationship when n > 0 which characterizes Dirac semimetals
- Zeroth Landau Level appears because Cd_3As_2 contains Dirac fermions which have a linear dependence to magnetic field
- Broken inversion asymmetry leads to lifted spin degeneracy which can be experimentally tested by analyzing peaks in Shubnikov-de Haas Oscillations

Energy-Momentum Dispersion

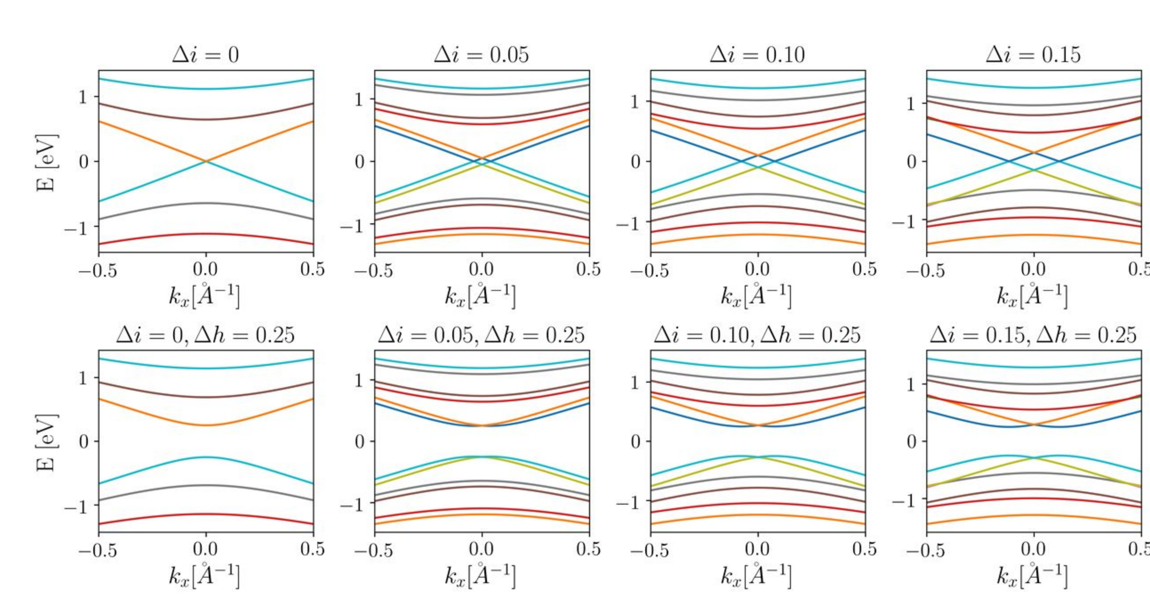

FIG. 6. First row: Energy-Momentum Dispersion with inversion asymmetry but no hybridization
Second row: Energy-Momentum Dispersion with inversion asymmetry and hybridization

- Except for the Dirac point, spin degeneracy is lifted due to broken inversion symmetry which can be seen in the momentum shift
- Spin-polarized states are created as a result of broken inversion symmetry since as the momentum is shifted, the superposed Dirac node splits into two Weyl nodes with opposite chirality
- Hybridization causes a band gap between the conduction and valence band leading to gapped electronic transport and transforming linear band dispersion to a parabolic band dispersion

Device Applications

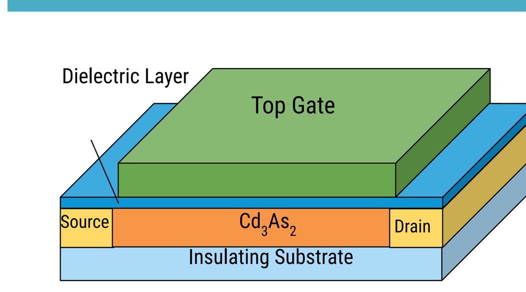

FIG. 7. Topological Field Effect Transistor

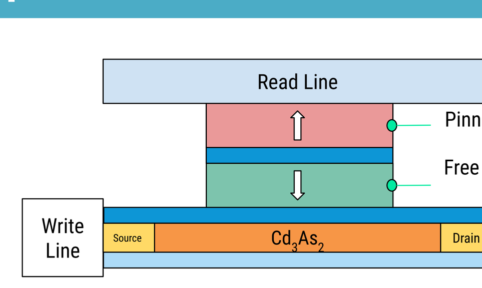

FIG. 8. Spin Orbit Torque MRAM

Transistors

- Bandgap can be induced by increasing hybridization/decreasing film thickness
- With an external electric field tuning the Fermi-level, electronic transport can be turned on or off, giving full electric control of state of transistor as seen in Figure 7

Spintronics

- Because inversion asymmetry creates spin-polarized states, the measurement of the electron spin can lead to reading/writing of data such as the SOT MRAM in Figure 8
- Spin signals can be turned on and off through the tuning of Fermi-level with an external electric field

Conclusions

Analysis of electronic interactions shows that band structure of Cd_3As_2 can be manipulated and optimized for topological devices

Inversion Asymmetry:

- Spin-polarized states can be created by varying chemical potentials through different substrates or an external electric field
- Spin-degeneracy of electrons is lifted, causing a topological phase transition and momentum shift

Hybridization:

- Bandgap can be increased by decreasing thickness of thin film which increases hybridization of surface states

Future Work

- Experiments on measurement of electron spin and storage of memory using Dirac semimetal Cd_3As_2
- Creation of topological device with full electric control of electron spin and manipulation of band gap