3034
doi:10.1017/S1431927620023600
Microsc. Microanal. 26 (Suppl 2), 2020

Relating Crystal Symmetry to Topological Phases: Convergent Beam Electron Diffraction Studies of the Dirac Semimetal Cd_3As_2

Tyler Pardue[1], Manik Goyal[1], Honggyu Kim[2] and Susanne Stemmer[1]

[1]University of California, Santa Barbara, Santa Barbara, California, United States, [2]University of Florida, Gainesville, Florida, United States

Crystal symmetry plays a pivotal role in protecting topological phases. Thin film strain, which breaks these symmetries, can therefore completely alter the properties of these materials. Cd_3As_2(space group $I4_1/acd$) has surface states and a pair of bulk Dirac nodes, which classifies it as a three-dimensional Dirac semimetal. Four-fold rotational and inversion symmetries protect the four-fold degenerate bulk Dirac nodes. Breaking the four-fold rotational symmetry may induce a topological insulator phase by generating a gap in the bulk band structure but leaving the surface states unperturbed. Previous studies have accessed the topological insulator phase through quantum confinement of a thin Cd_3As_2film [1], but strain engineering of epitaxially-grown films to break rotational symmetry offers additional degrees of freedom. Strain-engineered Cd_3As_2 films require structure characterization to determine symmetry elements broken. Convergent beam electron diffraction (CBED) was previously utilized to confirm the presence of an inversion center in epitaxially grown, relaxed Cd_3As_2, definitively classifying it as a Dirac rather than a Weyl semimetal [2]. Epitaxially strained Cd_3As_2 films must be very thin – routinely less than 40 nm in thickness – to avoid strain relaxation. CBED allows for determination of point group symmetry in films of this thickness. Here, we employ CBED for point group identification of coherently strained films of Cd_3As_2 with different orientations. We establish the connection between the thin film symmetry and the transport properties of the topological material.

Films were grown by molecular beam epitaxy (MBE) with two different surface orientations: parallel to the $(112)_T$ plane and the $(001)_T$ plane, respectively (the subscript refers to the tetragonal unit cell of Cd_3As_2). Cross-sectional TEM specimens were prepared along zone axes $[-201]_T$, $[02-1]_T$, and $[1-10]_T$ in the compressive $(112)_T$ film for direct comparison with a previous study of relaxed $(112)_T$ films [2]; Only $[1-10]_T$ was prepared in the compressive $(001)_T$ film, as this is sufficient for examination of rotational symmetry and the and the other zone axes are not orthogonal to the growth direction.

Figure 1 shows the zero-order Laue zone (ZOLZ) and whole pattern (WP), which includes the first-order Laue zone (FOLZ), from the three zone axes prepared in the compressive $(112)_T$ film. The CBED patterns from all three zone axes display a single mirror plane *m* in both the ZOLZ and WP. For the $[1-10]_T$ zone axis, this differs from the same direction in relaxed $(112)_T$ films, which had 2*mm* symmetry. Using tabulated diffraction groups [3], this combination of symmetries in the three CBED patterns of the compressive $(112)_T$ film indicate it has adopted the orthorhombic *mmm* point group. The ZOLZ and WP from CBED of the $[1-10]_T$ zone axis in the compressive $(001)_T$ film, shown in Figure 2, exhibit 2*mm* symmetry, indicating no loss of symmetry from the nominal 4/*mmm* point group. These results imply a loss of four-fold rotational symmetry and gapping of the bulk Dirac points in compressively strained $(112)_T$ Cd_3As_2 films, but not for compressively strained $(001)_T$ films. Transport measurements of the compressive $(112)_T$ film show two-dimensional transport, namely the quantum Hall effect, suggesting surface states are preserved [4]. The transport and CBED data show it is possible to produce a topological insulator from a Dirac semimetal by removing discrete rotational symmetry with appropriate epitaxial strain. This work experimentally connects the crystal symmetry of a topological material to its transport properties and the CBED method could be applied for structural characterization in future topological tuning studies modifying growth conditions and applying different materials.

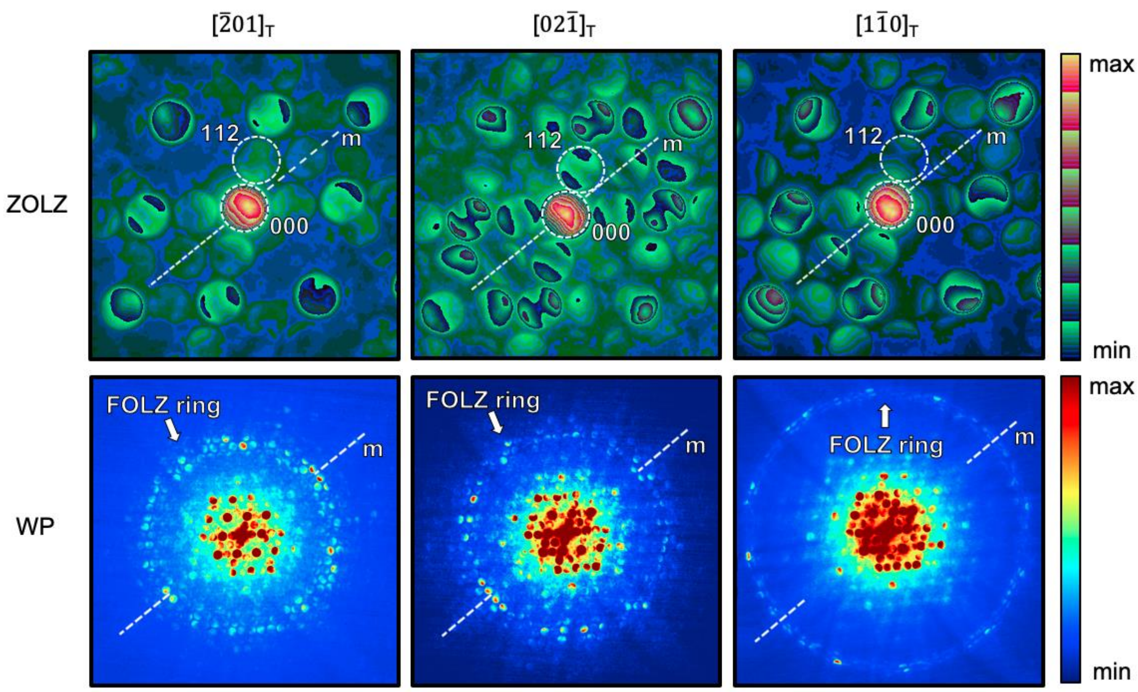

Figure 1. Experimental CBED patterns along zone axes [-201]T, [02-1]T, and [1-10]T for a compressive Cd3As2 film, each showing the ZOLZ pattern (top) and WP (bottom). Note that different color scales are used for WP and ZOLZ patterns to more easily distinguish the symmetry elements.

https://doi.org/10.1017/S1431927620023600 Published online by Cambridge University Press

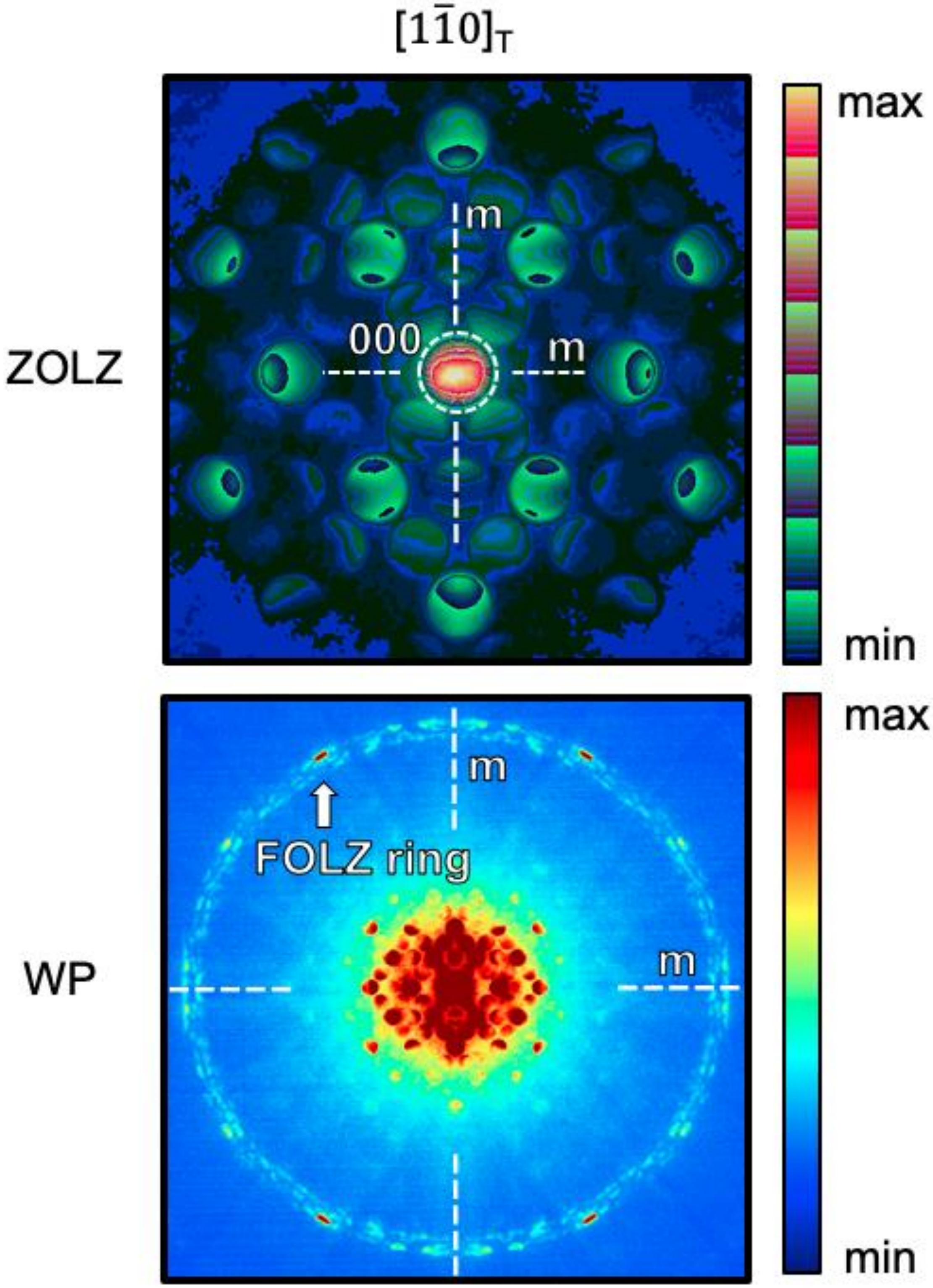

Figure 2. Experimental CBED pattern along the [1-10]T zone axis for a compressive (001)T Cd3As2 film, showing the ZOLZ pattern (top) and WP (bottom).

https://doi.org/10.1017/S1431927620023600 Published online by Cambridge University Press

References
[1] T. Schumann, L. Galletti, D. A. Kealhofer, H. Kim, M. Goyal, and S. Stemmer, Phys. Rev. Lett. **120**, 16801 (2018).
[2] H. Kim, M. Goyal, S. Salmani-Rezaie, T. Schumann, T. N. Pardue, J.-M. Zuo, and S. Stemmer, Phys. Rev. Mater. **3**, 084202 (2019).
[3] B. F. Buxton, J. A. Eades, J. W. Steeds, and G. M. Rackham, Philos. Trans. R. Soc. London. Ser. A **281**, 171 (1976).
[4] M. Goyal, H. Kim, T. Schumann, L. Galletti, A. A. Burkov, and S. Stemmer, Phys. Rev. Mater. **3**, 064204 (2019).