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Tuning Dirac states at grain boundaries in the topological insulator Bi2Se3[1]

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Symmetry protected Dirac states have been experimentally observed in topological insulator (TI) bismuth chalcogenides. Recently, we have further demonstrated direct electrical generation and detection of spin accumulation induced by spin-momentum locking of Dirac surface states in Bi2Se3, a critical step forward towards future electronic and spintronic applications. In this talk, I will give an overview of the opportunities and challenges in the epitaxial growth of these layered TIs that exhibit a strong (covalent) intra-layer bonding and weak (van der Waals) inter-layer bonding. Using Bi2Se3 as an example, I will show that this characteristic anisotropic bonding facilitates a spiral growth mode on virtually any substrates by molecular beam epitaxy [2]. The coalescence of these spirals results in a high density of grain boundaries (GBs) [3,4]. Using scanning tunneling and transmission electron microscopies, and density functional theory calculations, I will further show that near the zero-angle GBs (i.e., anti-phase domain boundaries), caused by vertical shifts of a fraction of a Bi2Se3 quintuple layer, the Dirac states are robust against scattering by these extended structural defects. However, electrostatic fields on the order of 108 V/m are found, which locally charge the Dirac state, shifting the Dirac point by up to 120 meV [3]. On the other hand, low-angle (<15o) GBs are found to be of the tilt variant, consisting of alternating edge dislocation pairs [4], resulting in periodic in-plane stretching and compression. Scanning tunneling spectroscopy reveals that in-plane stretching reduces the van der Waals gap, enhancing the Dirac states; while in-plane compression expands the inter-quintuple separation, therefore destroying the Dirac states and opens a gap in the local density of states. These findings demonstrate the tunability of Dirac states by electric field and strain at the atomic scale, and also highlight the inherent formation of GBs during vapor phase epitaxy of layered TIs. Finally, I will discuss methods to possibly control the density and types of GBs to minimize their impact on carrier transport. [1] C. H. Li, O. M. J. van't Erve, J. T. Robinson, Y. Liu, L. Li, and B. T. Jonker, Nat. Nanotechnol. 9, 218 (2014). [2] Y. Liu, M. Weinert, and L. Li, Phys. Rev. Lett. 108, 115501 (2012). [3] Y. Liu, Y. Y. Li, D. Gilks, V. K. Lazarov, M. Weinert, and L. Li, Phys. Rev. Lett. 110, 186804 (2013). [4] Y. Liu, Y. Y. Li, S. Rajput, D. Gilks, L. Lari, P. L. Galindo, M. Weinert, V. K. Lazarov, and L. Li, Nat. Phys. 10, 294 (2014).

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