Tuning Dirac States in Topological Insulator Thin Films

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3D topological insulators (TIs) are a class of materials that host novel spin-momentum locked electronic phases on their surfaces which are topologically protected from disorder.[1] This property makes them very attractive for future spin/electron applications in devices for quantum computing and alike. The correlation between atomic structure and functionality in thin films, surfaces, and heterostructures of TIs is a key for their exploitation. Hence, the understanding of the growth mechanism, grain structure and interfaces role on the topologically protected states is fundamental.

In this work, on the case of Bi_2Se_3, we show how defects, such as antiphase domain boundaries and misfit edge dislocations, modify Dirac surface states. Based on *in-situ* scanning tunneling microscopy and scanning-transmission electron microscopy we show that MBE grown Bi_2Se_3 initiates with two-dimensional nucleation, and that spiral growth ensues with pinning of the 2D growth fronts at jagged steps on the substrate.[2] Coalescence of the film grains results in grain boundaries with modified atomic surface structure. At antiphase domain boundaries we show that internal electric filed is responsible for the shift of the Dirac point towards lower/higher energy level depending of their atomic structure.[3] In addition, at low-angle tilt grain boundaries, consisting of arrays of alternating edge dislocation pairs, these dislocations introduce periodic in-plane compressive and tensile strains. From tunneling spectroscopy experiments and first-principles calculations, we find that whereas the energy of the Dirac state shifts in regions under tensile strain, a gap opens in regions under compressive strain, indicative of the destruction of the Dirac states at the surface.[4] These results demonstrate that Dirac states can be tuned by strain at the atomic scale.

References

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