Atomic Structure Study of 3D Topological Insulators: Bi_2Se_3

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Bi_2Se_3 is a 3D topological insulator (TI) that has attracted a lot of research due to exotic properties associated with topologically protected helical two-dimensional surface states and one-dimensional states associated with bulk line defects such as dislocations [1-3]. While the 2D surface states have been experimentally verified using angle resolved photoelectron spectroscopy and scanning tunnelling spectroscopy (STS), the bulk 1D modes, which also depend on the type of the dislocations and the class of the TIs, are yet to be verified experimentally. In this work we use MBE to control the synthesis of the Bi_2Se_3 and understand the growth, film structure and defects formation on atomic scale by using STM, STS, (S)TEM and DFT. Based on in-situ STM and STEM-HAADF we show that Bi_2Se_3 growth initiates with two-dimensional nucleation, and that spiral growth ensues with pinning of the 2D growth fronts at jagged steps of the substrate or domain boundaries created during coalescence of the 2D islands (Fig.1a). The spiral coalescence produces low and high angle grain boundaries. STEM-HAADF show that Bi_2Se_3 film is epitaxially grown with the following crystallographic orientation: Bi_2Se_3(11-20)||SiC(1-100) and Bi_2Se_3(0001||SiC(0001) (Fig. 1b). The STS show that the TI states (i.e Dirac point) are drastically modified by either the strain (quantified from high resolution HAADF and STM images) as well as the nature of the defects i.e. dislocations at grain boundaries or antiphase domain boundaries. Fig. 2. shows an antiphase domain boundary which is Bi rich, ultimately resulting of the shift of the Dirac states towards deeper electronic states compared to defects free surface regions [4]. Finally we present the strain maps around edge and screw dislocations present in these films, and show that 1D helical mode of line defects is not allowed for Bi_2Se_3.

References

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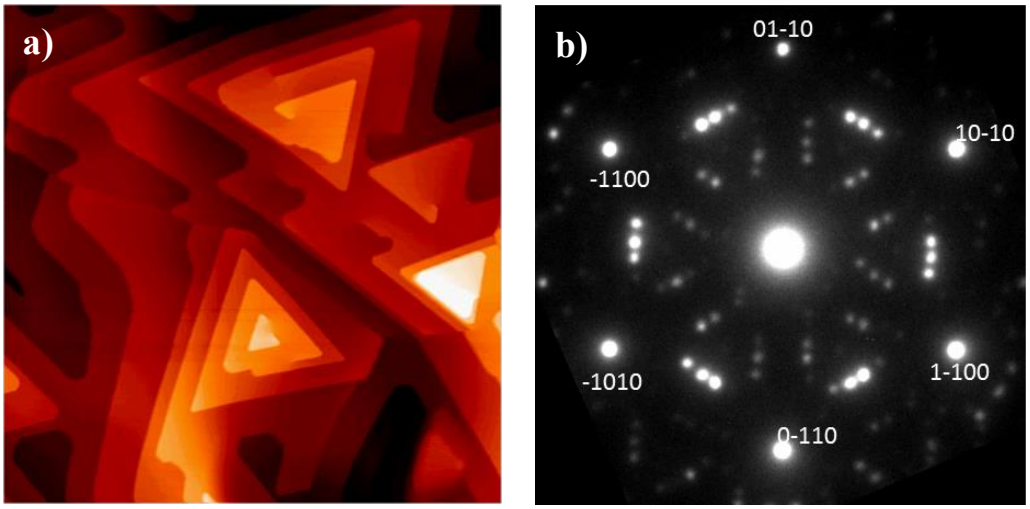

FIG. 1. a) STM image from the spiral growth of Bi_2Se_3. B) plan view selected area diffraction of region showing the epitaxy between the SiC substrate and the Bi_2Se_3 film. The substrate SiC(0001) diffraction spots are indexed.

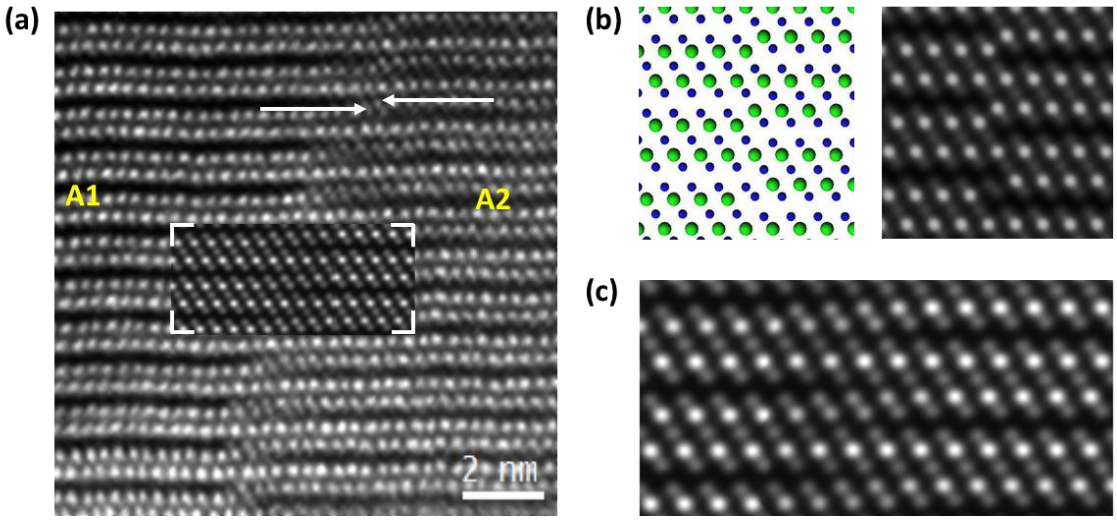

FIG. 2 a) Cross-sectional HAADF image from a region that contain antiphase domain boundary. b) Atomic model of the edge on antiphase boundary and corresponding calculated HAADF map. c) HAADF calculated map for tilt boundary of five degree.