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Suppressing twin formation in Bi2Se3 thin films

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The goal of the present work was to reveal the origin of the formation of different structural defects in Bi2Se3 thin films. We conducted a detailed comparative study of layers grown on InP(111)A and -B terminated flat and rough substrates using reflection high-energy electron diffraction (RHEED), atomic force microscopy (AFM), X-ray reflectivity (XRR), X-ray diffraction (XRD) and probe-corrected scanning transmission electron microscopy (STEM). This choice of substrate reduces the formation of mosaicity twist sufficiently due to an almost perfect lattice match (0.2%) between InP and Bi2Se3. The use of substrates with different terminations and roughnesses allows the factors that define twin formation to be identified, providing conclusions about how twinning can be controlled and suppressed. In particular we have shown that growth using molecular beam epitaxy on rough Fe-doped InP(111) substrates leads to the formation of high quality thin films, with very low mosaicity twist and with complete suppression of twins in the Bi2Se3 thin films. No extra layer was observed at the interface between the film and the substrate. We also showed that the substrate surface termination (A or B) defines which family of twin domains dominates. The only types of structural defects that remain in the films are antiphase grain boundaries associated with the variation in substrate height. We believe that our study is relevant not only for Bi2Se3 growth but that it also provides essential insight for obtaining monocrystalline A2B3 (A = Bi, Sb; B = Se, Te) chalcogenide thin films and for realizing desirable electrical properties within this class of materials.

Keywords: thin films, topological insulators, defects