Nucleation and growth dynamics of thin film topological insulator Bi_2Te_3 grown on Si (111) substrates by molecular beam epitaxy

S. Borisova, L. Plucinski, J. Krumrain, M. Luysberg, G. Mussler, and D. Grützmacher
Peter Grünberg Institute, FZ-Jülich and *Jülich Aachen Research Alliance, Jülich, Germany*

The ability to grow thin films of three-dimensional topological insulators [1] will provide insights into fundamental physical phenomena as well as a variety of technological applications. Until now, the preparation of ultrathin films by exfoliation of different layered materials from bulk crystals has dominated due to its availability and possibility to place the film at any substrate. However, the development of a sustainable technology suitable for mass production with required high reproducibility of the structural and electronic characteristics will rely on more advanced thin film technology. In this respect, epitaxial growth is a very promising approach.

Here, we report on ultrathin films of a topological insulator Bi_2Te_3 grown on Si (111) substrates grown by molecular beam epitaxy. Three-dimensional topological insulators like Bi_2Te_3 or Bi_2Se_3 support Fermi-Dirac surface states, which are additionally spin polarized due to strong spin-orbit coupling. The latter may thus enable spin-polarized quasi dissipation-less transport. These states have been experimentally studied by angle-resolved photoemission spectroscopy (ARPES) on cleaved surfaces of bulk crystals [2]. However, due to the large bulk electron concentration it is extremely difficult to unravel their transport properties. To this end, the preparation of ultra-thin Bi_2Te_3 or Bi_2Se_3 films potentially makes it possible to eliminate bulk states and to focus on surface state transport. The preparation of thin films of high structural perfection requires detailed investigation of nucleation and initial growth dynamics, which is provided by *in-situ* STM and scanning TEM in our study. Additionally, spin-resolved ARPES has been performed to study the presence of Fermi-Dirac states on ultra-thin films.

Successful growth of high quality films on non-native substrates with a large lattice mismatch via van der Waals epitaxy [3] has been already demonstrated for different material systems. However, mainly films with thickness >100 nm have been investigated, whereas devices based on advanced materials like topological insulators require ultra-thin films of only a few monolayers. Our results can be viewed as an example of more general phenomena occurring during van der Waals epitaxy of complex crystalline materials. The analysis of Bi_2Te_3 on Si(111) at the initial stage of growth reveals coalescence of islands of two different twin domains, occurring in a sub-quintuple-layer (QL) growth mode followed by a subsequent layer-by-layer growth with a QL growth unit accompanied by the formation of stacking faults and dislocations. We show that in van der Waals epitaxy the non-native substrate determines the crystal orientation in the x-y direction, whereas no information on the stacking sequence is transferred from the substrate to the film.

ARPES clearly reveals the complex hexagram shape of the Bi_2Te_3 Dirac-cone Fermi surface dispersion, as seen before [2] on cleaved surfaces. In the Fermi surface image there is no significant spectral weight related to the bulk conduction band at the zone centre, indicating a suppression of free carriers in the bulk states. Moreover, investigations by ARPES reveal a Fermi-Dirac cone at a film thickness of 3 QLs, for thinner films it vanishes.

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