Observation of an anomalous termination of Bi_2Te_3 by scanning tunneling microscopy and x-ray crystal truncation rod scattering

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Bi_2Te_3 is part of a very specific group of materials known as topological insulators. The motivation of the study of these materials comes from their conductivity: they are insulators in the bulk and conductors at the surface [1], features that are very important for electronic applications. The atomic structure of Bi_2Te_3 is similar to graphene, since van der Waals interactions keep the layers of the material connected. Its stable configuration also includes five monolayers connected by covalent bonds at the following order: Te-Bi-Te-Bi-Te. Since their electronic properties are related to the surface termination, the surface atomic structure is very important and has not been completely determined yet. In this experimental study we have prepared the Bi_2Te_3 (0001) surface by Argon sputtering and annealing under vacuum. We have observed different terraces at the atomic level of the sample surface using Scanning Tunneling Microscopy (see figure 1). We concluded that after being cleaved, Bi_2Te_3 does not break only into five monolayers, corresponding to a 1nm step in figure 1, but also in smaller atomic steps. The sample was also characterized using X-ray diffraction (XRD). XRD data were analysed and compared to a surface termination model (see figure 2). The final fit reveals the presence of a Bismuth rich conduction termination layer on top of the 5 monolayer terraces [2]. A theoretical study was carried out to explain the sample electronic structure and simulate stable atomic terminations. We conclude that this Bi termination has a significant impact on the transport properties of the Bi_2Te_3 surface.

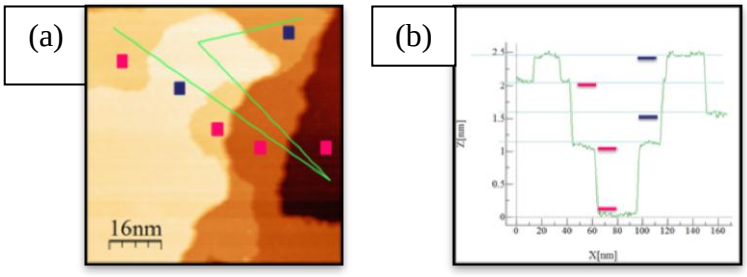

Figure 1: STM image (a) and profile (b) showing different terraces height on the surface of Bi2Te3

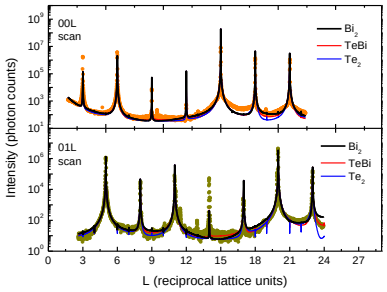

Figure 2: XRD data comparison with three different termination models.

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[1] D. Hsieh, M. Z. Hasan, *et. al*, A topological Dirac insulator in a quantum spin Hall phase, Nature. Vol 452, 24 (2008). [2] X. He, J. A. Yarmoff, *et.al*, Surface Termination of Cleaved Bi2Se3 Investigated by Low Energy Ion Scattering, Physical Review Letters, 110,156101(2013).