Direct observation of large strain through van der Waals gaps on epitaxial Bi_2Te_3/graphite: pseudomorphic relaxation and the role of Bi_2 layers on the Bi_xTe_y topological insulator series

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Layered materials can usually grow without strain on top of distinct substrates if the only interaction between them is due to van der Waals forces [1]. In such scenario it would be expected that the heterointerface made up of weak bounds would not affect the overlayed material significantly for several large lattice-mismatched systems [1]. Here we have studied the first stages of the heteroepitaxial growth of layered bismuth telluride topological insulator on top of highly oriented pyrolitic graphite (HOPG) by molecular beam epitaxy. Atomic Force Microscopy (AFM) images show hexagonal/triangular flat islands with exposed HOPG areas for the low coverage regime (Figure 1**a**), and the lattice parameter of these Bi_2Te_3 structures were measured by X-ray diffraction (XRD) (Figure 1**b**). The existence of pseudomorphic strain at the initial Bi_2Te_3 layers was retrieved by both X-ray diffraction and Raman spectroscopy. We have found out evidence that Bi_2Te_3 layers near the interface are subject to an in-plane compressive strain, leading to a pseudomorphic out-of-plane lattice expansion. Furthermore, the presence of Bi_2Te_3 islands locally distorts the topmost layer of HOPG, resulting in tensile strain which is measured by Raman spectroscopy. The observed relaxation of 0.1 – 0.2 % for each van der Waals gap is used to calculate elastic constants of Bi_2 bilayers (Figure 1**c**), which are crucial building blocks to the formation of other Bi_xTe_y topological insulator compounds. Finally, the impact of such strain in Bi_2Te_3 electronic structure was investigated by DFT calculations. The results show that band structure of this strained material remains unchanged at the center of the Brillouin zone, confirming the robustness of surface states, but it is consistently affected at the M and K zone edges (Figure 1**d**).

REFERENCES

[1] C. Parra *et. al*., Nano Letters, 17 (2017), 97-103

FIGURES

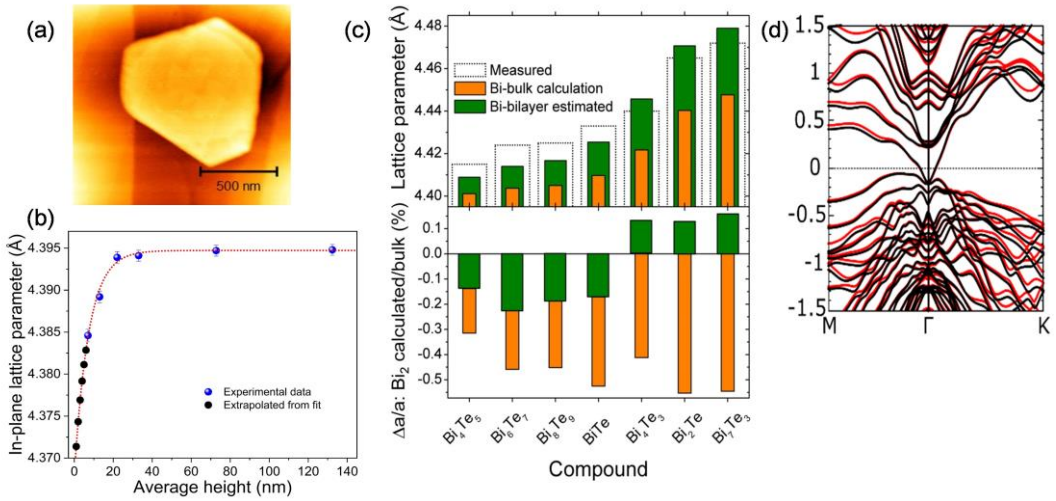

Figure 1: (a) Typical hexagonal Bi_2Te_3 island on HOPG. **(b)** Experimental in-plane lattice parameter as a function of island height (blue dots). **(c)** Comparison of in-plane lattice parameter for the Bi_xTe_y series for measured values (white/dashed bars). **(d)** Calculated band structure of Bi_2Te_3.