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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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Introduction

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, and the lattice parameter of these Bi_2Te_3 structures were measured by X-ray diffraction (XRD). 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, 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[2].

Sample growth

Molecular Beam epitaxy

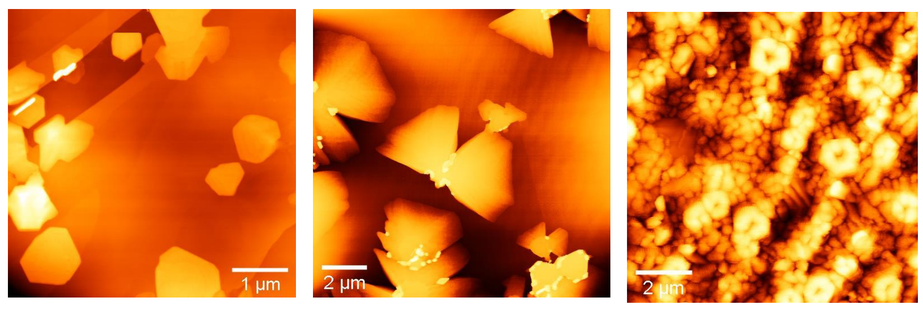
- Growth temperature $\mathbf{T_{HOPG}= 170°C}$
- One effusion cell was filled with nominal Bi_2Te_3, while two other cells charged with pure tellurium were used to keep the desired Te_2/Bi_2Te_3 beam equivalente pressure ratio of 2.
- Deposition rate of 0.14 QLs/min
- The set o sample used here had deposition times of 10,20,40,60, 100 and 180 min that led to nominal coverages of 1.4, 2.8, 5.6, 8.4, 14 and 25.2 QLs, respectively

Characterization

- **Atomic Force microscopy**
  tapping mode
- **Raman spectroscopy**
  Backscattering geometry
  excitation source: 632.8 nm HeNe laser
- **X-ray diffraction**
  Coplanar 2-theta-theta geometry
  Transmission 2-theta-theta geometry
  Energy 10 KeV (λ = 1.2399 Å)
- **DFT calculation**

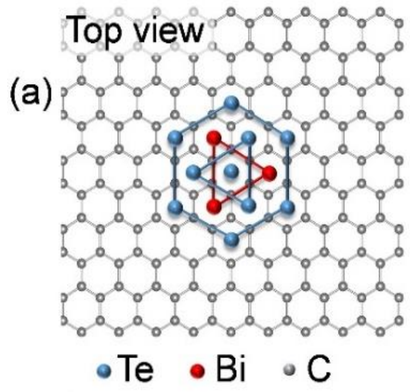
Results

- Typical AFM imagens showing the change in Bi_2Te_3 morphology with growth time



20 min 40 min 100 min

- Expected epitaxial relation between HOPG graphite and Bi_2Te_3

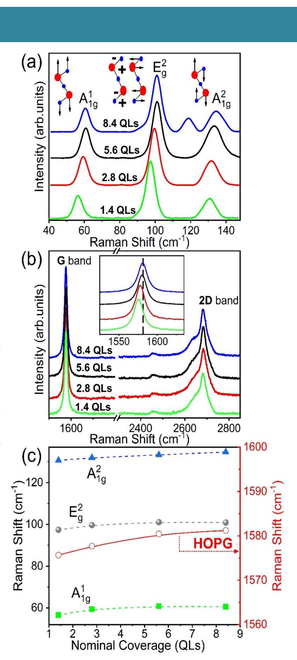


In-plane Lattice parameters:

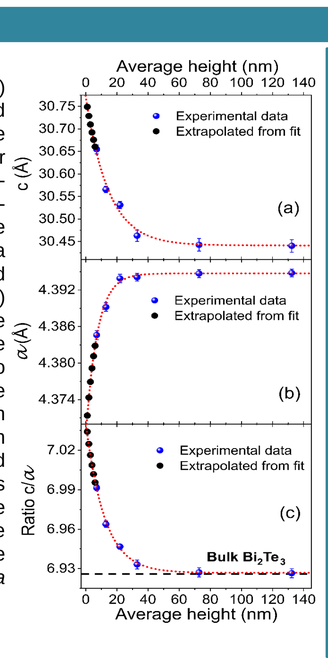
a Bi_2Te_3 = 4.39 Å
a HOPG = 2.46 Å

Lattice mismatch ~ 40%

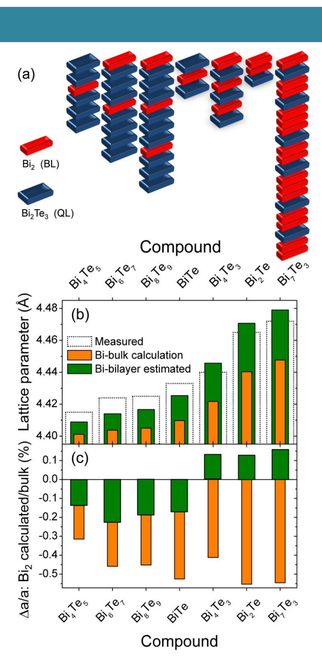
Raman spectra measured for the Bi_2Te_3 / HOPG samples set with coverage ranging from 1.4 to 8.4 QLs: (a) in the energy interval of Bi_2Te_3 A^1_{1g}, E^2_g and A^2_{1g} peaks showing a shift of the Raman modes for the 1.4 QLs and 2.8 QLs samples with respect to other coverages; (b) in the energy interval of graphite G and 2D bands, exhibiting a gradual shift of the G band position to lower energies as the coverage reduces. The inset presents a zoom in the G band, where a maximum shift of 6 cm^{-1} can be observed for our sample with lowest coverage; (c) Energy shifts of the Raman peak positions as a function of nominal coverage for the Bi_2Te_3 / HOPG samples, extracted from the Raman spectra displayed in figs. 6(a) and 6(b).



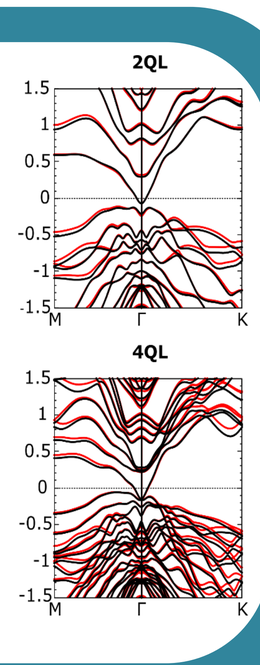
Measured (blue dots) and extrapolated (black dots) lattice parameters from our XRD results. (a) Out-of-plane and (b) In-plane lattice parameter as a function of island average height. (c) The behavior of the *c*/*a* ratio showing the complete relaxation to the bulk Bi_2Te_3 lattice parameters for high coverage samples. In all panels, the red short dotted lines represent the exponential fit. The bottom dashed line shows the bulk *c*/*a* ratio.



(a) Schematic representation of the stacked layers that form the crystal structures of the Bi_xTe_y series of compounds, made from Bi_2Te_3 QLs (blue) and Bi_2 BLs (red) building blocks. (b) Comparison of in-plane lattice parameter for the Bi_xTe_y series for measured values (white/dashed bars), values calculated from elastically strained Bi_2 and Bi_2Te_3 layers using the bulk Bi elastic constants (narrow orange bars) and the stack of Bi_2/Bi_2Te_3 layers with the optimized E_{11} and ν_{21} elastic constants for Bi_2 layers that minimize strain and elastic energy for the compound layer stack. (c) Lattice parameter difference of Bi_2 layers with respect to the measured values using the Bi bulk parameters (orange bars) and the retrieved Bi_2 BL elastic constants E_{11} and ν_{21} (green bars).



Calculated band structure of Bi_2Te_3 for different values of thickness in quintuple layers. Red lines represent the band dispersion obtained using the lattice constants found by our XRD measurements whereas black lines denote the ones obtained considering bulk values for *a* and *c*.



Conclusions

We have shown here that Bi_2Te_3 flat islands change the morphology with increase in the growth time. The islands exhibit a large in-plane compressive strain at the Bi_2Te_3/HOPG interface accompanied by a consequential out-of-plane pseudomorphic expansion. We also have estimated the elastic constants of Bi_2 bilayers. Finally, from DFT calculations such strain do not affect the eletronic structure at the center of Brillouin zone, they can play a major role at the M and K edges.

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REFERENCES

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[2] Rodrigues-Junior *et al.,*Phys. Rev. Materials, 4 (2020),023602

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