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Probing Two-dimensional $(Bi,Sb)_2Te_3$/h-BN Heterostructures Using Complementary S/TEM and Simulation Techniques

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To revolutionize electronics, materials must be developed, characterized, and engineered that can outperform conventional, silicon-based technology. Because of their momentum-locked surface states, topological insulators (TIs) are emerging as materials that could provide important advances for magnetoelectronic technologies. Already, spin-transfer torque [1], current-induced spin polarization [2,3], and room-temperature spin injection [4] have been demonstrated as phenomena of interest in TI-based devices.

To construct high-quality devices, the atomic-scale properties of TIs and their heterostructures must be well characterized. Scanning and conventional transmission electron microscopy (S/TEM) are ideal tools to achieve this. Here, we present a S/TEM-based structural study of TI heterostructures of $(Bi,Sb)_2Te_3$ grown onto hexagonal boron nitride (h-BN) by molecular beam epitaxy (MBE). The heterostructure consists of an insulating h-BN substrate and a TI ($(Bi,Sb)_2Te_3$) that has the Fermi level located in the bulk band gap, which is of particular interest for probing the ambipolar transport in the TI [3].

Complementary experimental microscopy modes, combined with *Multislice* simulation [5] of the sample–electron beam interactions, elucidate such features as the atomic structures of grain boundaries and dislocation arrays, small regions of an impurity phase, and misorientations between the TI and the substrate (Figure 1). Here, high-angle annular dark-field STEM (HAADF-STEM) is used to image atomic features, electron energy-loss spectroscopy (EELS) and energy-dispersive X-ray spectroscopy (EDX) are used to understand global and local compositions, and the combination of conventional TEM experiment and *Multislice* simulation is used to understand the relative orientations of the sample and substrate.

The heterostructures studied here were prepared by MBE growth of $(Bi,Sb)_2Te_3$ onto h-BN that had been exfoliated onto a Si wafer support. Then, samples were prepared for TEM analysis in two ways. First, cross-sectional samples were created using a focused ion beam system (FEI Quanta 3D FIB). Second, plan-view samples were exfoliated from the Si substrate and deposited onto a TEM grid. For S/TEM studies, an FEI Titan G2 60-300 S/TEM was used, which was equipped with a Schottky X-FEG gun and operated at 200 kV [6].

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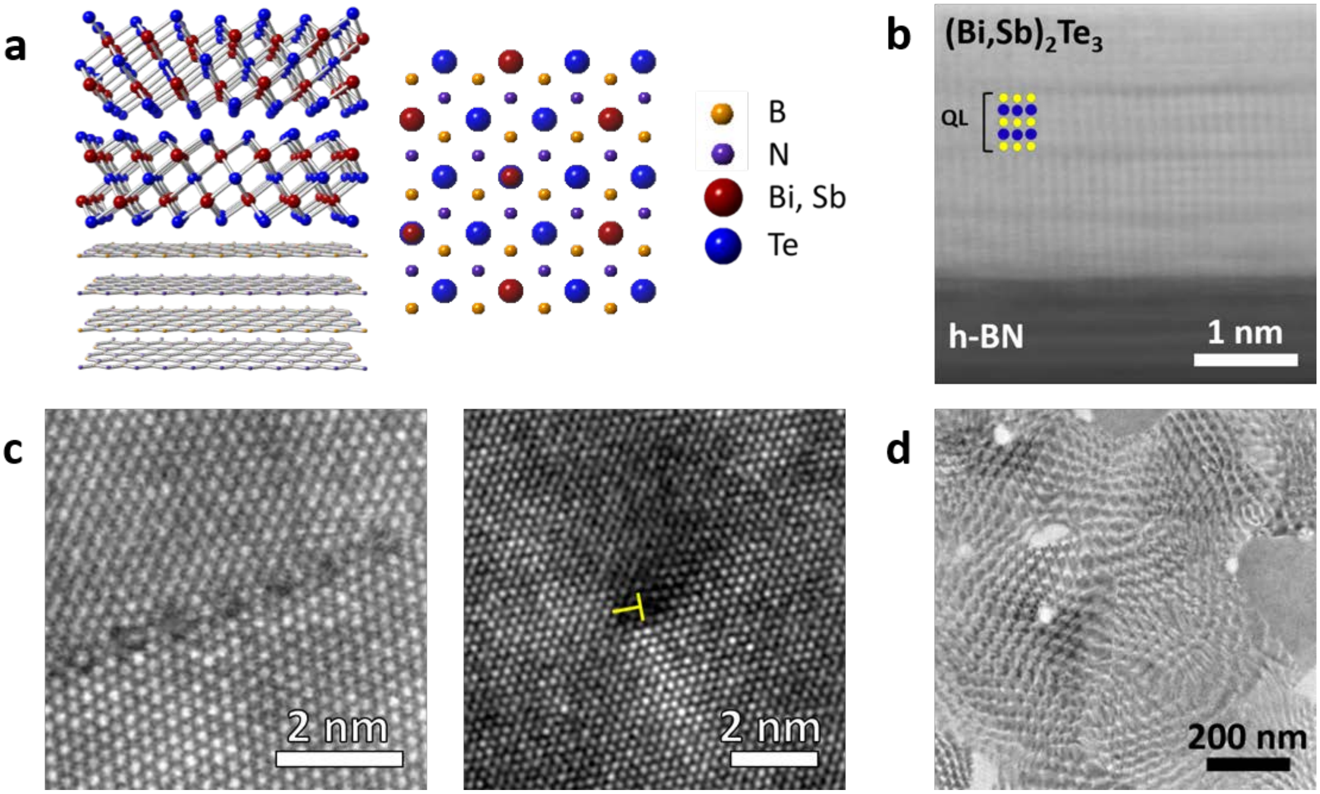

Figure 1. (Bi,Sb)$_2$Te$_3$ on h-BN: (a) crystal structure model, (b) cross-sectional HAADF-STEM image (QL represents the characteristic five-atom quintuple layer), (c) plan-view atomic-resolution HAADF-STEM images of grain boundary and dislocation in the (Bi,Sb)$_2$Te$_3$ film, and (d) bright-field TEM image showing Moiré fringes.

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