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Twin Boundary Structure in Bi_2Te_3: Experiment and Theory
D.L. MEDLIN, Sandia National Laboratories, Q.M. RAMASSE, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, C.D. SPATARU, N.Y. YANG, Sandia National Laboratories — Establishing the atomic structure and composition of interfaces in thermoelectric materials is important to understanding how these defects mediate thermal and electronic transport. Here, we discuss our experimental observations and theoretical calculations of the Bi_2Te_3 (0001) basal twin in nanocrystalline Bi_2Te_3. This interface is important both because it is common in tetradymite-structured thermoelectric compounds and because it serves as a useful model system for more complex interfaces. Macroscopically, the (0001) twin corresponds to a 180° rotation of the crystal about the [0001] axis, which reverses the stacking of the basal planes. The basal planes of Bi_2Te_3 are arranged in 5-plane groupings of alternating Bi and Te layers. Microscopically, one envisions three possible interface terminations: at the Te layer in the middle of the 5-layer packet, at a Bi layer, or at the Te-double layer at the junction of the 5-layer packet. Using aberration-corrected HAADF-STEM imaging, we have established that the twin boundary terminates at the Te-double layer. This result is consistent with *ab initio* calculations, which predict that the lowest energy for the three candidate structures is for this termination.

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