Abstract Submitted
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Effects of Intrinsic Defects on Topological Insulator Behavior: Theory and Experiments on Ternary Tetradymite Compounds[1] DUANE D. JOHNSON, LIN-LIN WANG, AFTAB ALAM, MIANLIANG HUANG, SRINIVASA THIMMAIAH, TOM LOGRASSO, ADAM KAMINSKI, None, PAUL C. CANFIELD, Division of Materials Science and Engineering, Ames Laboratory and Iowa State University — Ternary tetradymites $Bi_2Te_xSe_{(3-x)}$ are predicted to be topological insulators via density functional theory (DFT) surface band structure calculations. Experimentally, we find that Bi_2Se_3 and Bi_2Te_3 form a continuous solid solution at the two non-equivalent group VI sites with different site preferences for Se and Te. The DFT formation energies for ordered and partially ordered compounds agree well with experimental data. Importantly, we calculated the intrinsic defect formation energies of binary and ternary tetradymites, and find they correlate well with the bulk conductivity measurement. Angle resolved photoemission spectroscopy confirms the existence of the Dirac cone in the surface band of Bi_2Te_2Se.

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