Band Gap and Structure of Single Crystal Bii3: Resolving Discrepancies In Literature

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Abstract: Bismuth tri-iodide (Bii3) is an intermediate band gap semiconductor with potential for room temperature gamma-ray detection applications. Remarkably, very different band gap characteristics and values of Bii3 have been reported in literature, which may be attributed to its complicated layered structure with strongly bound BiI6 octahedra held together by weak van der Waals interactions. Here, to resolve this discrepancy, the band gap of Bii3 was characterized through optical and computational methods and differences among previously reported values are discussed. Unpolarized transmittance and reflectance spectra in the visible to near ultraviolet (UV-Vis) range at room temperature yielded an indirect band gap of 1.67 +/- 0.09 eV, while spectroscopic ellipsometry detected a direct band gap at 1.96 +/- 0.05 eV and higher energy critical point features. The discrepancy between the UV-Vis and ellipsometry results originates from the low optical absorption coefficients (alpha similar to 10(2) cm(-1)) of Bii3 that renders reflection-based ellipsometry insensitive to the indirect gap for this material. Further, electronic-structure calculations of the band structure by density functional theory methods are also consistent with the presence of an indirect band gap of 1.55 eV in Bii3. Based on this, an indirect band gap with a value of 1.67 +/- 0.09 eV is considered to best represent the band gap structure and value for single crystal Bii3. (C) 2013 AIP Publishing LLC.