Journal of Materials Science, vol. 49(22), 2014, pages 7809-7818

Structural, electronic, and optical properties of orthorhombic and triclinic BiNbO4 determined via DFT calculations

Abstract

We performed ab initio calculations using the FPLAW method with the local density approximation (LDA) implemented in the WIEN2 k code for the orthorhombic (α) and triclinic (β) phases of BiNbO4. The modified Becke-Johnson exchange potential (mBJ)-LDA approach was also used to improve the electronic properties. The lattice constants calculated for both structures using the LDA are in good agreement with the experimental values. For the band structure calculations, the mBJ-LDA approach provides reasonable agreement for the band gap value compared with the LDA. The estimated (mBJ)-LDA band gap values are 2.89 eV (3.73 eV) and 2.62 eV (3.15 eV) for the α and β phases of BiNbO4, respectively. Significant optical anisotropy is clearly observed in the visible-light region. We also calculated and evaluated the electron energy loss spectrum for BiNbO4. This work provides the first quantitative theoretical prediction of optical properties and electron energy loss spectra for both the orthorhombic and triclinic phases of BiNbO 4.

Keywords

Electron energy loss spectroscopy; Band-gap values; DFT calculation; Optical properties