

Absorption and photoconductivity spectra of Ag_2GeS_3 crystal: Experiment and theory

Abstract

Spectral features of polycrystalline Ag_2GeS_3 samples synthesized from high-purity elements (at least 99.99 wt.% purity) in quartz ampoules evacuated to 0.1 Pa were explored. The band energy gap of Ag_2GeS_3 crystals estimated from the fundamental absorption edge and photoconductivity spectra were found to be equal to 1.98 eV and 2.16 eV, respectively. Simultaneously we have performed calculations of the band structure, total and partial density of states and the electron charge density using the ab initio FP-LAPW method. All the calculations were performed with four different exchange-correlation (xc) potentials. It was found that the effect of using different xc is very marginal on the valence band maximum (VBM) while it is dramatically shifted the conduction band minimum (CBM) towards higher energies with respect to the Fermi energy position. Our theoretical results have given a band energy gap equal to 0.40 eV (for LDA), 0.42 eV (GGA), 1.03 eV (EVGGA) and 1.30 eV (mBJ) xc potentials. Thus the underestimation of the energy gap in LDA and GGA was partially corrected in EVGGA and mBJ model. As a remarkable fact mBJ did not bring the energy band gap very close to the experimental one. We have discovered that the Ag-s states have only a small effect on the conduction bands shifts whereas Ge-s states have a strong effect in extending of the gap, while remaining the valence bands unchanged.