Simulation of Electronic Structure and Properties for Amorphous $GeSe_2$ - X_2Se_3 (X= As, Sb) Films

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One of the top problems in the development of novel electronic devices is the prediction of the electronic properties of functional materials. Wide spectrum of chalcogenide compounds find application in nano- and opto-electronics, infrared optics, information recording et al. The main purpose of the present work was to explain the peculiarities of concentration dependences of the optical band gap, conduction activation energy and trapping centres in ternary chalcogenide thin films based on the studies of electronic structure - properties relationship.

Amorphous thin films thermally deposited in vacuum from ternary glassy chalcogenides of $(GeSe_2)_x(As_2Se_3)_{1-x}$ (x=0-0.8) and $(GeSe_2)_x(Sb_2Se_3)_{1-x}$ (x=0.4-0.9) families have been the subject of the investigation. For the materials under investigation the results of the calculation of the top of the valence band, the bottom of the conduction band, the optical band gap, the Fermi level, the position of the levels formed gap by the homopolar bonds and clusters have been presented. The calculation procedure has been based on the linear combination of the atomic orbitals and pseudo-potential methods [1]. The energy values have been determined in the Γ-point - the centre of the Brillouin zone. The atomic terms taken from the generalized periodic table [2] have been used in the calculations, as well as the available experimental data on the photoemission [3] and average interatomic distances [4]. For the films the experimental data on the absorption edge, temperature dependence of d. c. conduction, photoconduction and thermally activated depolarization currents have been given.

The quantitative agreement between calculated energy band diagram and experimental data for the studied materials has been shown. The peculiarities of the composition dependences for the properties of the films under investigation have been discussed.

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