Bull. Mater. Sci., Vol. 38, No. 2, April 2015, pp. 365–372. © Indian Academy of Sciences.

First-principle calculations of the structural, electronic, thermodynamic and thermal properties of ZnS_xSe_{1-x} ternary alloys

S BENDAIF[1], A BOUMAZA[1], O NEMIRI[1], K BOUBENDIRA[1], H MERADJI[1,*], S GHEMID[1] and F EL HAJ HASSAN[2]

[1]Laboratoire LPR, Département de Physique, Faculté des Sciences, Université Badji Mokhtar, Annaba 23000, Algeria
[2]Laboratoire de Physique et d'électronique, Faculté des Sciences, Université Libanaise, Elhadath, Beirut 6573-14, Lebanon

MS received 20 November 2013; revised 12 May 2014

Abstract. **First-principle calculations were performed to study the structural, electronic, thermodynamic and thermal properties of ZnS_xSe_{1-x} ternary alloys using the full potential-linearized augmented plane wave method (FP-LAPW) within the density functional theory (DFT). In this approach the Wu–Cohen generalized gradient approximation (WC-GGA) and Perdew–Wang local density approximation (LDA) were used for the exchange–correlation potential. For band structure calculations, in addition to WC-GGA approximation, both Engel–Vosko (EV-GGA) generalized gradient approximation and recently proposed modified Becke–Johnson (mBJ) potential approximation have been used. Our investigation on the effect of composition on lattice constant, bulk modulus and band gap for ternary alloys shows a linear dependence on alloy composition with a small deviation. The microscopic origins of the gap bowing were explained using the approach of Zunger and co-workers. Besides, a regular-solution model was used to investigate the thermodynamic stability of the alloys which mainly indicates a phase miscibility gap. Finally, the quasi-harmonic Debye model was applied to see how the thermal properties vary with temperature at different pressures.**

Keywords. **FP-LAPW; DFT; energy band structure; thermal properties; Debye model; critical temperature.**

1. Introduction

Zinc-based semiconductor compounds have attracted considerable theoretical and experimental interest in the last decades since they have a potential to be employed as base materials for light-emitting and laser diodes, infrared detectors, photovoltaic devices and quantum dots applications.[1] ZnS and ZnSe semiconductor compounds have attracted significant interest for their potential applications in opto-electronics and electronics.[2–5] ZnS and ZnSe crystallize in the zinc-blende structure and are characterized by a large and direct gap of 3.68 eV for ZnS[6] and 2.69 eV for ZnSe.[6] Therefore, the application of band gap engineering to ZnSSe ternary alloys, which can be obtained as a result of the band gap engineering of ZnSe and ZnS, would be of great interest to researchers aiming to develop optoelectronic or photonic devices with high performance. Several studies have examined the tunability of the energy band gap of ZnSe by adding sulphur as an alloying element to ZnSe.[7–10] The ternary alloy ZnS_xSe_{1-x}, has been extensively used for designing opto-electronic devices.[11–15] Although a number of experimental[9,16–20] and theoretical studies[6,21–26] of ZnS_xSe_{1-x} semiconductor alloys have been published, to the best of our knowledge there are no available data for their thermal properties. Usually, the thermodynamic properties of materials are the basis of solid-state science and industrial applications. Furthermore, thermodynamic properties for crystalline materials are very important in many applications involving high pressure and high temperature. Although *ab-initio* calculations have successively predicted the electronic and structural properties of various materials, these calculations are very often restricted to the 0 K temperatures. In this work, thermal properties are considered by the use of the quasi-harmonic Debye model,[27] and in order to provide another reference data for completing the existing theoretical and experimental works on these alloys, we have performed the present work using the full-potential augmented plane-wave method (FP-LAPW) based on the density functional theory (DFT) combined with the quasi-harmonic Debye model. The paper is organized as follows: computational details are described in section 2. The obtained results are presented in section 3. Finally, we present the main conclusions of the present work in section 4.

2. Method of calculations

The calculations presented in this work were performed using the FP-LAPW method[28] within the framework of the

*Author for correspondence (hmeradji@yahoo.fr)