Computational Materials Science 87 (2014) 202–208

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

First principles calculations of structural, electronic and optical properties of $Zn_{1-x}Be_xSe_yTe_{1-y}$ quaternary alloys

A. Boumaza [a], O. Nemiri [a], K. Boubendira [a], S. Ghemid [a], H. Meradji [a,*], F. El Haj Hassan [b]

[a] Laboratoire LPR, Département de Physique, Faculté des Sciences, Université Badji Mokhtar, Annaba, Algeria
[b] Laboratoire de physique et d'électronique, Faculté des Sciences I, Université Libanaise, Elhadath, Beirut, Lebanon

ARTICLE INFO

Article history:
Received 14 October 2013
Received in revised form 2 January 2014
Accepted 16 February 2014

Keywords:
Alloys
Ab initio calculations
Electronic structure
Optical properties

ABSTRACT

The structural, electronic and optical properties of $Zn_{1-x}Be_xSe_yTe_{1-y}$ quaternary alloys are investigated using the full potential-linearized augmented plane wave (FP-LAPW) method within density functional theory (DFT). We used both the Wu–Cohen and the Engel–Vosko generalized gradient approximations of the exchange-correlation energy that are based on the optimization of the total energy and the corresponding potential, respectively. Some basic physical properties, such as lattice constant, bulk modulus, electronic band structures, and optical properties (dielectric constant and refractive index) are calculated, nonlinear dependence on the compositions x and y are found. In addition, the energy band gap of zinc-blende $Zn_{1-x}Be_xSe_yTe_{1-y}$ quaternary alloys lattice matched to GaAs substrate is investigated. To our knowledge this is the first quantitative theoretical investigation on $Zn_{1-x}Be_xSe_yTe_{1-y}$ quaternary alloys and still awaits experimental confirmations.

1. Introduction

The quaternary II–VI semiconductor alloys with two disordered sublattices whose chemical formulas have the general form $A_{1-x}B_xC_yD_{1-y}$ have important technological device applications where x and y are the compositions and AC, AD, BC and BD are the constituents binary compounds. Tailoring of these compounds could lead to new semiconductor materials with desired band gaps over a continuous broad spectrum of energies [1,2]. The semiconductors play more and more important role in electronic and optoelectronic devices. A major requirement for optoelectronic applications of materials is the ability to tune independently the band gap to realize the desired optical properties and the lattice parameter for a given substrate. The quaternary II–VI alloys are promising candidates to satisfy such requirements [3,4].

Mixing of binary semiconductor II–VI provides new semiconductor alloys and diversifies the physical properties such as band gap, lattice matching, and dielectric constant. Such procedure replays to the requirement of new generation device applications [5,6] in the field of nonlinear optics, electronics, photovoltaic detectors, light-emitting diodes, solar cells, photo-detectors, transistors, and pulsed laser diodes.

Be-chalcogenides provide interesting aspects for fundamental physics investigation exhibiting covalent bonding and reduced band polarity. The incorporation of Be element in ZnTe and ZnSe compounds will strongly affect the physical properties of these materials; the advantages of this incorporation is to strengthen latter highly ionic lattices, with concomitant impact on defect generation and propagation, and thereby device lifetime [7–10]. However, the beryllium incorporated $Zn_{1-x}Be_xSe_yTe_{1-y}$ quaternary alloys are very attractive for middle visible range, i.e., yellow-to-green laser diodes (LDs) and light emitting diodes (LEDs) [11–13]. This system is very effective for strengthening the lattice bonds due to the high cohesive energies of BeSe and BeTe compounds [14]. To the best of our knowledge, no extensive theoretical and experimental works on the physical properties of the quaternary $Zn_{1-x}Be_xSe_yTe_{1-y}$ lattice matched to GaAs substrate have been reported so far. Therefore, our main goal of this work is to study the structural, electronic and optical properties of $Zn_{1-x}Be_xSe_yTe_{1-y}$ alloys by using first-principles calculations to gain better insight into these technologically promising materials.

The organization of this article is as follows. In Section 2 we briefly describe the computational method used in this work. Results will be presented and discussed in Section 3. A summary of the work will be given in Section 4.

2. Computational details and theoretical background

All the calculations presented in this work have been carried out using the full-potential linear augmented plane wave method

* Corresponding author. Tel.: +213 779278221; fax: +213 38875399.
E-mail address: hmeradji@yahoo.fr (H. Meradji).

http://dx.doi.org/10.1016/j.commatsci.2014.02.028
0927-0256/