Materials Science in Semiconductor Processing 26 (2014) 477–490

Contents lists available at ScienceDirect

Materials Science in Semiconductor Processing

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

First principle study of the physical properties of semiconducting binary antimonide compounds under hydrostatic pressures

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ARTICLE INFO

Available online 5 June 2014

Keywords:
III–V compounds
FP-LAPW
mBJ-GGA
Elastic constants
Hydrostatic pressure
Optical properties

ABSTRACT

First-principle calculations have been performed to investigate the structural phase transition, electronic, elastic, thermodynamical and optical properties of III-Sb compounds under hydrostatic pressure up to their first order transitions pressure (Zinc Blende to Rock Salt). Four different exchange–correlation functionals comprising Perdew–Burke–Ernzerhof generalized parameterization of gradient approximation, Wu-Cohen, local density approximation as well as modified Becke and Johnson were used. The structural properties such as phase transitions, equilibrium lattice parameters, bulk modulus and its first pressure derivative were obtained using an optimization method. Moreover, elastic constants, Young's modulus, shear modulus, Poisson's ratio, sound velocities for longitudinal and shear waves, Debye average velocity, Debye temperature and Grüneisen parameters were calculated up to the first order phase transition pressure. The obtained structural and elastic parameters are consistent with the available experimental data. The static calculations predict that Zinc Blende to Rock Salt phase transitions occur at 48.5, 9.5, 5.87 and 3.15 GPa for BSb, AlSb, GaSb and InSb respectively. The optical properties of these compounds, such as dielectric function, refractive index and the optical band gap were also calculated for the radiation up to 14 eV. In addition, the influence of the hydrostatic pressure on the elastic parameters, energy band structures and the refractive index of these compounds were investigated. The linear and quadratic pressure coefficients of the compounds were also calculated. Results have been discussed and compared with available experimental and theoretical data, which show an overall good agreement with the other studies.

1. Introduction

During the last century, III–V semiconductors have been extensively served as substances for electronic and optoelectronic devices. These applications make them as vital elements in an advanced information society [1]. Among III–V compounds, the narrow band gap antimonide based compound semiconductors (ABCS) are broadly regarded as the first nominee materials for the manufacturing of the third generation infrared photon detectors and ICs with ultra-high speed and ultra-low power consumption. Their distinctive physical aspects and band gap structures provide a large space to design varied unique devices [2]. At ambient pressure, III-Sb compounds crystallize in the zinc blende (ZB) structure. Boron antimonide and aluminum antimonide have indirect band gap, while gallium antimonide and indium antimonide have direct ones. Even though a few investigations on some of the physical properties for this group are available, a comprehensive study is needed. In recent years, III-Sb compounds have

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http://dx.doi.org/10.1016/j.mssp.2014.05.020
1369-8001/

drawn more attention owing to their possible application in rechargeable lithium batteries. Boron antimonide shows a strong covalent nature and a rare behavior due to the small core and absence of "*p*" electrons in boron atom compared to other III–V substances. They make BSb as a possible material for high temperature optical and electronic uses [3]. Likewise, GaSb is a noble nominee for thermo-photovoltaic cells for the structures with low radiator temperature, as its cell technology is fairly simple resulting in higher effectiveness than Si thermo-photovoltaic cells. III-Sb compounds, owing to their high mobility, are henceforth known as forward-thinking device applications [4].

Recently, first-principle computations based on density-functional theory have developed the vital part of materials investigations. The DFT (Density Functional Theory) Full-Potential linear augmented plane wave (FP-LAPW) method has been broadly recognized as the approach of choice for computational solid-state researches. The calculation of various properties such as the structural, elastic, thermodynamical, optical and electronic properties for several compounds has been done by the DFT method. The calculations supply the full recognition of materials' properties and the chance to scheme new compounds for special uses [5].

III–V semiconductors have been broadly investigated theoretically and experimentally in recent decades. Even though III-Sb compounds have been widely studied in theory [6–16], there is no complete study comprising all III-Sb compounds about the effects of pressure on their electronic structure, elastic and optical properties. This study aims to investigate the consequence of pressure on the structural, electronic, elastic, and the optical properties of the III-Sb compounds. The calculation method is FP-LAPW with various approximations. Exchange–correlation functionals and corresponding potential have a prominent role in DFT based total energy calculations. The calculations using local density approximation (LDA) or generalized gradient approximation (GGA) for exchange correlation functionals and corresponding potential yield lower values of band gap energy. Thus, we used modified Becke and Johnson (mBJ)-GGA which is another new exchange correlation functional. This functional yields better results for the electronic properties of semiconductors [17].

2. Computational approach

FP-LAPW approach within the DFT framework, was applied to obtain the structural, phase transition, elastic, thermodynamical, optical and electronic properties of XSb (X=B, Al, Ga and In) compounds under hydrostatic pressure up to their first order phase transition pressure by using WIEN2k package [18]. LDA, GGA (PBE: Perdew–

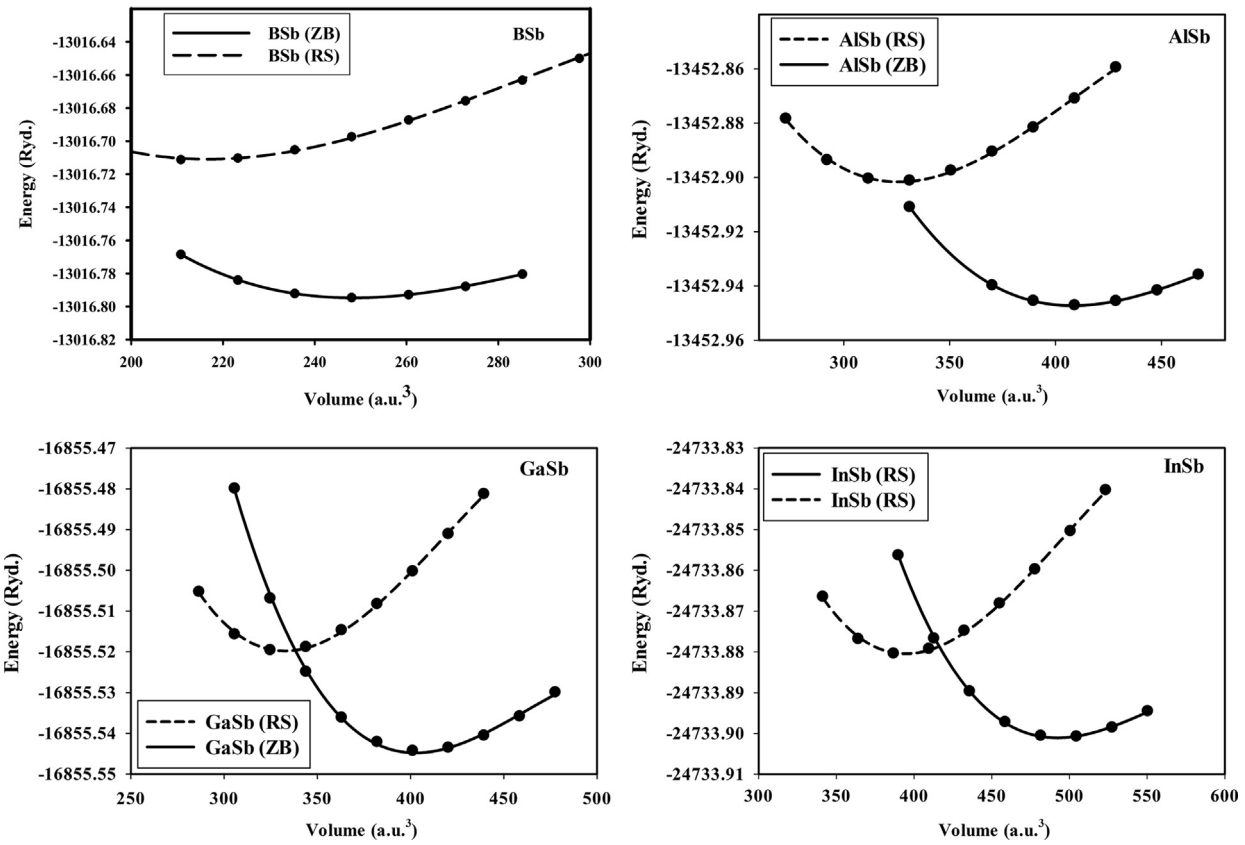

Fig. 1. Energy versus volume curves of ZB and RS phases for III-Sb compounds with PBE-GGA approximation.