



Structural phase transition, elastic and thermal properties of boron arsenide: Pressure-induced effects



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ABSTRACT

The phase transition of boron arsenide (BAs) has been studied by means of a density-functional theory calculation. Features such as structural phase stability, elastic properties, sound velocity, Debye temperature and melting temperature have been obtained at zero and high pressures. The transition pressure (P_t) of the material of interest from zinc-blende to NaCl phase has been determined and found to agree well with experiment. At pressures lower than P_t the zinc-blende phase is found to be thermodynamically and mechanically more stable than the NaCl phase. The mechanical behavior has been studied in terms of ductility and brittleness by means of different methods and found to differ only on the exact border between the two types of mechanical behaviors. The behavior of the longitudinal sound velocity under pressure indicated the softening of its corresponding phonons.

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1. Introduction

In view of their important properties for eventual technological applications in the field of linear and nonlinear optics, solar cells, light-emitting diodes, laser diodes and integrated optical devices such as modulators, switches and filters; the binary tetrahedral semiconductors compounds: cadmium, zinc and beryllium chalcogenides and indium, aluminum, gallium and boron pnictides with zinc-blende (ZB) and wurtzite (Wu)-type structures have attracted increasing research interest in the last few years [1].

The investigation of the pressure and temperature dependence of the fundamental properties of semiconductors has been the subject of many studies in the past years [2–4]. As a matter of fact, the development of the diamond anvil cell and its inherent ruby fluorescence manometer

[5,6] has given new impetus to the study of the fundamental properties of semiconductors under high pressure [7,8]. Pressure tuning should also prove a valuable tool in the search for new materials with enhanced or optimized properties. On the theoretical side, efforts have been also made using methods with varying degree of sophistication so as to gain a deeper understanding of the relevant physical parameters [9–13].

Although some papers [14–27] have reported studies on fundamental properties of boron based materials, only a few of them that dealt with theoretical aspect [25,26] have been devoted to the study of the effect of hydrostatic pressure on the mechanical properties of boron arsenide (BAs).

In order to fully take advantage of the properties of boron arsenide (BAs) for eventual technological applications, an accurate investigation of the fundamental properties such as structural, elastic and thermal properties under pressure, is needed. In the present work, we report on first-principles calculations of the hydrostatic pressure effect on the independent elastic stiffness constants, mechanical behavior

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(ductile and brittle nature), sound velocities, Debye temperature and melting temperature of BAs compound in the zinc-blende structure (B3) using the pseudopotential plane wave method in the framework of density functional theory (DFT) [28], and the density functional perturbation theory (DFPT) [29], within the local density approximation (LDA). Besides, the structural phase transition and the mechanical stability criteria are also examined and presented.

2. Computational methods

There are different methods to obtain the elastic constants through the first principle calculations. Currently, these elastic constants can be obtained with the help of the Nielsen and Martin [30] method, which uses the strain–stress relation. Hamann et al. [31] developed a reduced coordinate metric tensor method for the linear response formulation of strain type perturbations which could be calculated by the DFPT. Using this approach, the elastic constants are obtained with a total energy method by calculating the second derivatives of the total energy with respect to all the perturbation. This can be realized by computing the energy of the system with respect to the strain perturbation. The DFPT was widely applied to the direct calculation of phonon spectra, interatomic force constants, Born effective charges and a variety of other properties. In this respect, the inter-atomic force constants are obtained with the Fourier transform of the dynamical matrix on a discrete mesh of spacing. The calculations in the present study were carried out using the ABINIT code [32] based on the pseudopotential plane wave approach in the framework of the DFT and the DFPT. ABINIT code is a package whose main program allows one to find the total energy and several others properties of systems made of electrons and nuclei. It is a common project of the University Catholique de Louvain, Corning Incorporated, the University de Liège, and other contributors.

The norm-conserving nonlocal pseudopotentials of Trouiller–Martins [33] in the context of the LDA are employed in the computation. The electron–electron interaction was considered within the LDA by Goedecker–Teter–Hutter parameterization [34], which reproduces the correlation scheme of Perdew and Wang [35].

The two parameters that affect the accuracy of calculations are the kinetic energy cutoff which determines the number of plane-waves in the expansion and the number of special k -points used for the Brillouin zone (BZ) integration. The BZ integrations were replaced by discrete summations over a special set of k -points, using the standard k -point technique of Monkhorst and Pack [36]. In this work, the used k -point meshes are $6 \times 6 \times 6$. The plane-wave energy cut-off to expand the wave functions is set to be 70 Hartree. Careful convergence tests show that with these parameters, the relative energy is converged to better than 10^{-5} Hartree. The tolerances for the geometry optimization were: difference in total energy within 5×10^{-6} eV/atom, maximum ionic Hellmann–Feynman force within 0.01 eV/Å, maximum ionic displacement within 5×10^{-4} Å and maximum stress within 0.02 eV/Å³.

3. Results and discussions

3.1. Pressure phase transition

Thermodynamically, a phase transition occurs when a change in the structure appears, which is caused by the variation of the free energy. The stability of any particular structure corresponds to the lowest Gibbs free energy, which is given by [3]

$$G = U + PV - TS \quad (1)$$

where U is the total internal energy, P the pressure, T the temperature, S the entropy and V is the volume.

To investigate the pressure-induced structural transition, we have optimized (at $T=0$ K) both the cell parameters and atomic positions for zinc-blende (B3) and NaCl (B1) phases. At $T=0$ K, the Gibbs free energy becomes equal to the enthalpy i.e. $H=U+PV$. The computed enthalpies versus hydrostatic pressure curves for both phases of interest are shown in Fig. 1(a). From Fig. 1(a), we can see that the Gibbs' free energy for zinc-blende phase is more negative and hence B3 is thermodynamically and mechanically more stable than B1 phase. The two H's versus pressure curves corresponding to the B3 and B1 phases cross at a pressure of 110.82 GPa suggesting therefore that the transition pressure (P_t) from B3 to B1 is 110.82 GPa. As pressure increases,

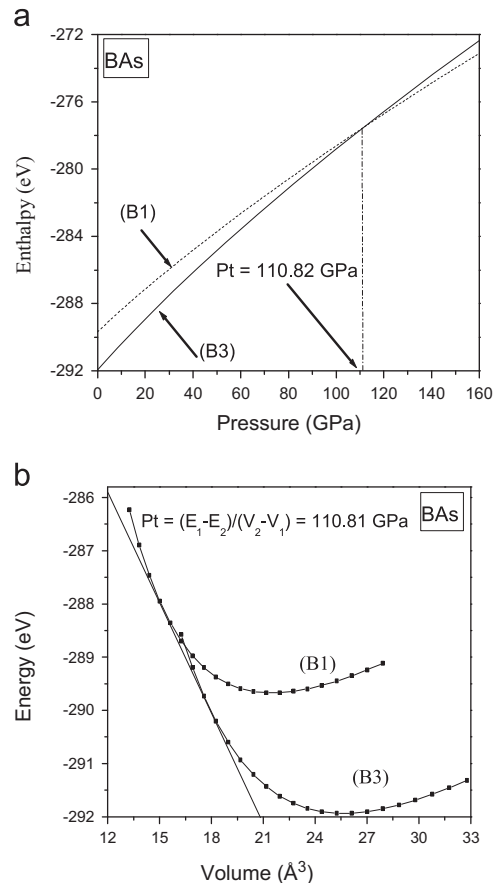


Fig. 1. (a) Enthalpies versus pressure for B1 and B3 phases of BAs. (b) Total energy versus volume for B1 and B3 phases of BAs.

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