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First-principles study of structural and mechanical properties of AgB_2 and AuB_2 compounds under pressure

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ABSTRACT

In this work, density functional theory calculations on the structural, mechanical, and lattice dynamical properties of AgB_2 and AuB_2 compounds in AlB_2, OsB_2, and ReB_2 structures are reported. Generalized gradient approximation has been used for modeling exchange-correlation effects. The detailed information is given for the energetically most stable structure for AgB_2 and AuB_2 compounds. Specifically, the lattice parameters, bulk modulus, cohesive energies, elastic constants, shear modulus, Young's modulus, Poisson's ratio, Debye temperature, sound velocities, and anisotropic factors are studied. The elastic properties are also studied under pressure. The phonon dispersion curves and corresponding phonon density of states are calculated and discussed. Our structural and some other results are in agreement with the available experimental and theoretical data.

1. Introduction

The transition metal borides are attracting the attention of researchers due to their highly refractory properties and corrosion resisting characteristics [1]. Also, the discovery of superconductivity in MgB_2 at $T_c = 39$ K [2] has revived new interest in finding superconductivity in other diborides. However, superconductivity is observed [3–5] in only some of them, and various studies are currently directed to shed light on other properties of diborides, including their elastic, mechanical, and thermodynamical properties [5–9].

Kwon et al. [10] suggested that AgB_2 and AuB_2 metal diborides, which correspond to effectively hole-doped systems, are potential candidates for high-T_c (BCS) superconductors. Tomita et al. [11] reported the synthesis of a novel silver boron inter-metallic compound. They observed a sharp transition to zero resistance at $T_c = 6.7$ K for AgB_2 compounds. The observed critical temperature of AgB_2 of 6.7 K is significantly lower than the calculated T_c of 59 K [10]. Islam et al. [12] explained the reason for the discrepancy of the observed T_c with the theoretically calculated T_c by invoking the role of enhanced spin fluctuations on the critical temperature of AgB_2. Obrowski [13] investigated lattice parameters of AgB_2 and AuB_2 in C32 phase using X-ray diffraction (XRD). Oguchi [14] studied the systematic trend in lattice constants and heat of formation for these compounds. The electronic properties and superconductivity of AgB_2 and AuB_2 were investigated by Yang et al. [15]. Shein et al. [16] reported electronic structure and cohesive properties of AgB_2 by means of the projected augmented wave method in the framework of the density functional theory. Shein and Ivanovskii [17] studied the structural and elastic properties using the full-potential linearized augmented plane-wave (FP-LAPW) method with the generalized gradient approximation (GGA) for the same compounds. Lal et al. [18] reported the synthesis of AgB_2 compounds and analyzed their resistivity behavior down to 12 K in terms of impurity scattering, electron–phonon scattering, and weak localization. Pelleg et al. [19] studied, experimentally, the films of the Ag–B and Au–B systems using various techniques (magnetron co-sputtering, XRD, secondary electron microscopy (SEM), X-ray photo spectroscopy (XPS), Auger analysis and optical microscope (OM)) for observing superconductivity. Recently, Musa et al. [20] studied the bulk AgB_2 by using reactive Spark Plasma Sintering technique for the same purpose. In fact, the synthesized AgB_2 compounds, up to date, showed some inhomogeneous structures [19–21].

Recent theoretical studies based on electronic structure calculations of AgB_2 and AuB_2 in AlB_2 structure are associated with their superconducting behaviors. Their structural and mechanical properties are still uncompleted and controversial. As far as we know, there is no systematic research on the elastic, mechanical, and vibrational properties of AgB_2 and AuB_2 in AlB_2, ReB_2 and OsB_2

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structures, to date. Therefore, we have aimed to provide some additional information to the existing data on the physical properties of these compounds by using the ab initio total energy calculations. The method of calculation is given in Section 2; the results are discussed in Section 3. Finally, the summary and conclusion are given in Section 4.

2. Method of calculation

In the present paper, all calculations have been carried out using the Vienna ab initio simulation package (VASP) [22–25] based on the density functional theory (DFT). The electron–ion interaction was considered in the form of the projector-augmented-wave (PAW) method with plane wave up to energy of 450 eV [24,26]. This cut-off was found to be adequate for studying the structural, elastic, and lattice dynamical properties. For the exchange and correlation terms in the electron–electron interaction, Perdew–Burke–Ernzerhof (PBE) type functional [27] was used within the generalized gradient approximation (GGA). For k-space summation the $17 \times 17 \times 13$ gamma-centered for AlB_2 and ReB_2-type and $9 \times 17 \times 11$ for OsB_2-type structure Monkhorst and Pack [28] grid of k-points have been used. Structural optimization was performed for each structure for all lattice constants, angles, and internal atomic coordinates until the difference in total energy and the maximum force being within 1.0×10^{-5} eV and 1.0×10^{-4} eV/Å, respectively.

3. Results and discussion

3.1. Structural properties

We have fully relaxed the cell volume and the ionic positions of atoms in reciprocal coordinates which are supported by VASP code [22–25] for all considered compounds. In all calculations, we have used these relaxed parameters. The crystallographic parameters of the considered structures are given in Table 1. The energy–volume values are calculated using the fully relaxed lattice constants and atomic position in each a step. These energy–volume values are fitted using by means of Murnaghan's equation of state (EOS) [29] and are given in Fig. 1. The calculated lattice parameters are given in Tables 2 and 3 along with the other experimental and theoretical values. It can be clearly seen that the AlB_2 for AgB_2 and OsB_2 structure for AuB_2 compounds are the most stable phase among the considered three different crystal structures. The present lattice

Table 1
Crystallographic data for considered structures of AgB_2 and AuB_2 compounds.

Compound	Space group (number)	Structure	Atom	Site
AgB_2	P6/mmm (191) Hexagonal	AlB_2 C32	Ag B	1a (0, 0, 0) 2d (1/3, 2/3, 1/2)
AgB_2	$P6_3/mmc$ (194) Hexagonal	ReB_2 C7	Ag B	2c (1/3, 2/3, 1/4) 4f (1/3, 2/3, Z_B)
AgB_2	Pmmn (59) Orthorhombic	OsB_2	Ag B	2a (1/4, 1/4, Z_X) 4f (X_B, 1/4, Z_B)
AuB_2	P6/mmm (191) Hexagonal	AlB_2 C32	Au B	1a (0, 0, 0) 2d (1/3, 2/3, 1/2)
AuB_2	$P6_3/mmc$ (194) Hexagonal	ReB_2 C7	Au B	2c (1/3, 2/3, 1/4) 4f (1/3, 2/3, Z_B)
AuB_2	Pmmn (59) Othorhombic	OsB_2	Au B	2a (1/4, 1/4, Z_X) 4f (X_B, 1/4, Z_B)

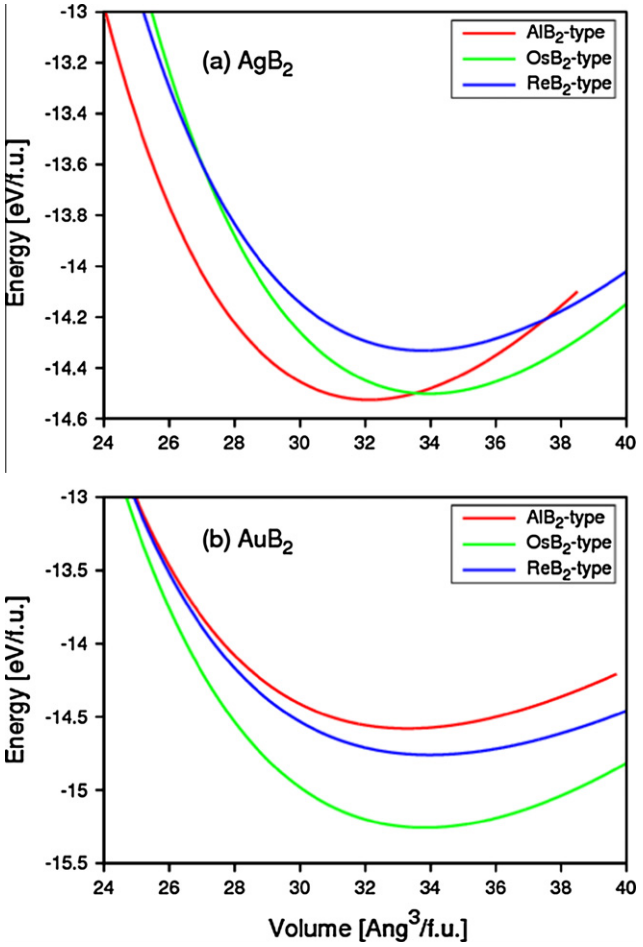

Fig. 1. Energy versus volume curves for (a) AgB_2 and (b) AuB_2 compounds.

parameters are in well agreement (around 1.7%) with theoretical ones except for lattice constant c (3.3%) in Ref. [10] for AgB_2 and (4%) in Ref. [10] for AuB_2 in AlB_2 structures. The observed small differences between our results and the other theoretical studies may stem from the different pseudopotentials used in calculations. The experimental and theoretical values are slightly different, because the calculations have been performed for the perfect crystal at zero temperature and at zero pressure. Also, these discrepancies may be caused by the inhomogeneous structure and the formation of the new phase of the synthesized materials [19–21]. The bulk modulus, and its pressure derivative have also been estimated based on the same Murnaghan's EOS, and the results are given in Tables 2 and 3 along with the other theoretical values. It is seen that the present bulk modulus are in good agreement with the theoretical ones in Refs. [12,16]. In the present case, the largest value of bulk modulus (165.3 GPa) is obtained for AuB_2 in OsB_2 structure.

The cohesive energy (E_{coh}) is known as a measure of the strength of the forces, which binds atoms together in the solid state. In this context, the cohesive energy of the considered compounds are estimated using the relation

$$E_{coh}^{XB_2} = E_{total}^{XB_2} - [E_{atom}^{X} + 2E_{atom}^{B}] \quad (1)$$

where $E_{total}^{XB_2}$ is the total energy (in formul unit) of the compound at equilibrium lattice constant and E_{atom}^{X} and E_{atom}^{B} are the isolated atomic energies of the pure constituents. The energy of the isolated atoms (free atoms) are calculated in the fcc box with a large lattice constant, a = 15 Å, that contains the related atoms. The calculated cohesive energies listed in Tables 2 and 3 are in consistent with the energy–volume curves in Fig. 1.