Elastic, mechanical and thermodynamic properties of zinc blende III-X (X= As, Sb): ab-initio calculations

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Abstract – In this work, density functional theory plane-wave full potential method, with local density approximation (LDA) are used to investigate the structural, mechanical and thermodynamic properties of of zincblende III-X ( X= As, Sb) componds. Comparison of the calculated equilibrium lattice constants and experimental data shows very good agreement. The elastic constants were determined from a linear fit of the calculated stress-strain function according to Hooke’s law. From the elastic constants, the bulk modulus B, shear modulus G, Young’s modulus E, Poisson’s ratio σ, anisotropy factor A, the ratio B/G and the hardness parameter H for zincblende III-X ( X= As, Sb) compound are obtained. Our calculated elastic constants indicate that the ground state structure of III-X ( X= As, Sb) is mechanically stable. The sound velocities and Debye temperature are also predicted from elastic constants.

Keywords: Mechanics, Mechanics, energy, DFT, LDA

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I. Introduction

The method developed by Charpin (modified by Ferenc Karsai) and integrated in WIEN2k code [1] has been used to obtain elastic constants of considered binary compounds. The knowledge of elastic parameters of solids is very important because they provide important information about the stability and mechanical properties of solids such as sound velocities, load deflection, fracture toughness, thermoelastic stress and internal strain etc.

II. Elastic and mechanical properties

The elastic constants Cklmn (where the letter k, l, m, n refer to Cartesian components) are defined by the help of a Taylor expansion of the total energy of the system, E(V, ϵ), in accordance with a small strain ϵ of the lattice (V is the volume of the system). The energy E(V, δ) fit curve versus strain, δ, for the three different types of strains, namely the volume conserved, tetragonal and rhombohedral shear strains, are plotted in Figure 1 (a)-(c), respectively, for the studied binary compounds. The total energy has been calculated for five to seven different distortions for each of the three different deformations of the lattice. There are 21 independent elastic constants Cij, but symmetry of the cubic lattice reduces this number to only 3 independent constants (C_{11}, C_{12}, and C_{44}) for cubic lattices. The calculated values of elastic constants are summarized in Table 1. The calculated elastic constant values of studied binary compounds are in good agreement with the results of other calculations [2, 4] and the available experimental data [3, 5].The obtained values for the elastic tensor constants satisfy the mechanical stability restrictions for cubic unit cells C_{11} - C_{12} > 0, C_{11} + 2C_{12} > 0 and C_{12} < B < C_{11} [6]. Resistance to shear distortions of a cubic crystal is best characterized by the two moduli the tetragonal shear constant C’ = (C_{11} - C_{12})/2 and C_{44}. The elastic constant C_{44} is related to an orthorhombic deformation whereas C’ is related to a tetragonal deformation. At any volume V, the bulk modulus B for a cubic crystal is related to elastic constants by B_0 = (C_{11} + 2C_{12})/3 [7]. The C_{11} and C_{12} can be obtained from the calculated bulk modulus and C’.
The Kleinmann parameter \( \zeta \), is an important parameter describing the piezoelectric effect of solids [9]. It is given by the following relation:

\[
\zeta = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}}
\]

The obtained values of \( \zeta \) for the materials are between 0.575 and 0.716 as shown Table 1. The obtained results for studied binary compounds fairly coincide with previous first-principles calculations [2, 10]. We have also found the anisotropy factor \( A = 2C_{44}/(C_{11} - C_{12}) \). For an isotropic crystal, \( A \) is equal to 1, while any value smaller or larger than 1 indicates anisotropy. From Table 1, it is clearly seen that the calculated anisotropy factor for these compounds deviate from 1. The magnitude of the deviation from 1 is a measure of the degree of elastic anisotropy possessed by the crystal.

The isotropic bulk modulus \( B_0 \), which is related to \( C_{11} \) and \( C_{12} \), and shear modulus \( G \) are determined by the calculated elastic constants [11]. However, there is no distinct expression for the polycrystal-averaged shear modulus with respect to the \( C_{ij} \), but one can evaluate approximate averages of the lower and upper bounds given by various theories [12]. Voight [13] found upper bounds, while Reuss [14] discovered lower bounds for all lattice.

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The B₀/G ratio of studied materials is presented in Table 1. It is clearly seen from this table that B₀/G ratio of considered structures should be classified as brittle character. The calculated H values are 9.40GPa, 11.09GPa, 5.87GPa, 7.50GPa, 8.10GPa and 5.12 GPa for AlAs, GaAs, InAs, AlSb, GaSb and InSb at zero pressure, respectively. The positive value of Cauchy pressure is responsible for a ionic bonding while a negative Cauchy pressure, however, requires an angular or directional character in the bonding (covalent bonding). The more negative the Cauchy pressure, the more directional and of lower mobility the bonding. Moreover, a material with more negative value of Cauchy pressure will have more brittle nature. The calculated values of C’ are summarized in Table 2, which indicate that the sign of the Cauchy pressure is negative for all studied materials. The kind of bonds can be also determined by means of the value of Poisson’s ratio (ν). The value of Poisson’s ratio is nearly 0.25 or more for a typical ionic material, while it is much less than 0.25 (around 0.1) for a typical covalent bond.
velocity in the polycrystalline material is approximately

\[ V \approx \frac{\Theta_D}{k} \frac{C''}{C'' + \mu} \]

where \( V \) is the wave velocity, \( \Theta_D \) the Debye temperature, \( k \) the Boltzmann constant, and \( C'' \) and \( \mu \) the elastic constants. For an isotropic system, \( \lambda = \mu \), and \( \mu \) is related to a fraction of Young's modulus. For an isotropic media, \( \lambda \) is known as Lame's first constant and \( \mu \) as the second constant. Therefore, our obtained results do not satisfy the later relations, which are valid only for the isotropic systems, which is in agreement with the obtained results.

### III. Thermodynamic properties

The Debye temperature \( (\Theta_D) \) which is a significant fundamental parameter closely related to many physical properties such as elastic constants, specific heat and melting point can be obtained from the average sound velocity \( (v_m) \) by the following classical relation [26]:

\[ \Theta_D = \frac{h}{k_B} \left( \frac{6\pi^2 n}{V_0} \right)^{1/3} v_m \]

where \( V_0 \) is atomic volume and \( v_m \) is the average wave velocity in the polycrystalline material. The Debye temperatures \( (\Theta_D) \) by the following classical relation [26]:

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where \( V_0 \) is atomic volume and \( v_m \) the average wave velocity in the polycrystalline material is approximately calculated from the following equation [26]:

\[ v_m = \left[ \frac{1}{3} \left( \frac{2}{v_t} + \frac{1}{v_l} \right) \right]^{1/3} \]

constant. The scatter of all the different points falls within plus or minus 300 K of the following equation for \( T_m \) in units of K [28]:

\[ T_m = 553 K + (591/Mbar) C_{11} \pm 300 K \]

The calculated wave velocities \( (v_t, v_l, v_m) \), Debye temperature \( (\Theta_D) \) and melting point \( (T_m) \) of studied binary compounds and ternary alloys estimated from elastic constants are listed in Table 2. It is clearly seen from Table 2, the Debye temperature of the considered compounds decrease with increasing atomic number. The high value of the Debye temperature for AlAs implies that its thermal conductivity is to be higher than other studied compounds. The sound velocities are related to the elastic moduli. Therefore, for a material having larger elastic moduli means higher sound velocity. Thermal conductivity, \( \kappa \), is the property of a material that indicates its ability to conduct heat. So, in order to know if material is a potential candidate for thermal barrier coating application, its thermal conductivity need to be investigated.

Based on the Debye model, Clarke [29] suggested that the theoretical minimum thermal conductivity can be calculated after replacing different atoms by an equivalent atom with a mean atomic mass \( M/n \):

\[ \kappa_{\text{min}} = \frac{0.87 k_B N_A^{2/3} \rho^{2/3} \Theta_D^{1/2} \Theta_D^{1/2}}{M^{2/3}} \]

where \( k_B \) is the Boltzmann’s constant, \( M \) is the molecular mass and \( n \) is the number of atoms per molecule, \( N_A \) the Avogadro’s number, \( \rho \) the density. The calculated minimum thermal conductivity of studied materials is summarized in Table 2. Table 2 indicates that the value of minimum thermal conductivity decreases when one moves from Al to In in the compound XAs (Sb) (X=Al, Ga and In). The reduction can be attributed mainly to the difference in Young’s modulus, which is a measure of the second derivative of the bonding energy at the
equilibrium interatomic distance $x_0$, between the studied binary compounds.

Where $v_1$ and $v_l$ are the transverse and longitudinal elastic wave velocities, respectively, obtained using the shear modulus $G$ and the bulk modulus $B$ from Navier’s equations [27]:

$$v_1 = \sqrt{\frac{G}{\rho}}$$

$$v_l = \sqrt{\frac{3B+4G}{3\rho}}$$

where $\rho$ is the density.

Fine et al. [28] have studied many cubic metals and compounds and have obtained an approximate empirical.

**IV. Conclusion**

In this study, the structural, mechanical and thermodynamic properties of III-X (X= As, Sb) compounds have been investigated by means of the DFT within Wien2k code. Our results for the optimized lattice parameters (a) and (c) are in good within Wien2k code. Our results for the compounds have been obtained an approximate empirical.

The III-X (X= As, Sb) compound is mechanically stable according to the elastic stability criteria, while no experimental results of elastic moduli for comparison. The calculated Zener factor indicates that III-X (X= As, Sb) compound is elastically anisotropic. The values of the ratio B/G and Cauchy pressure (C12–C44) show a ductile manner for the III-X (X= As, Sb) compound. The polycrystalline III-X (X= As, Sb) turns out to be a low stiff material according to the calculated hardness parameter (H). Finally, from the knowledge of the elastic constants and the average sound velocities, the Debye temperature has been predicted successfully.

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