



THEORETICAL STUDY OF ZINC-BLENDE COMPOUND

Ashutosh Kumar Mishra and Dr. Ashok Kumar Jha

Upgraded High School, Darbhanga and Department of Chemistry, C.M.Sc. College,
Darbhanga

ABSTRACT

Applying the first principles method of the full potential linear augmented plane waves (FPLAPW), the structural and the electronic properties of AlBi are investigated. It is found that this compound has a small and direct semiconducting gap at Γ . Through the quasi-harmonic Debye model, in which the phononic effects are considered, the dependences of the volume, the bulk modulus, the variation of the thermal expansion α are successfully obtained.

Keywords :- full potential linear augmented plane waves (FPLAPW), Debye model, the bulk modulus, the quasi-harmonic.

INTRODUCTION:

Zinc blende is the most extensively studied compound as regards the lattice dynamical and thermodynamical properties. Compared to other III-V materials, less is known about bismuth GaBi, AlBi and InBi binaries. Using first principles FPLAPW methods, Ferhat et al. [1] have found that the zinc-blende structure is the most stable for AlBi and GaBi while InBi prefers the tetragonal PbO structure. In the zinc blende (B3) phase, first principle calculations show that GaBi and InBi are conductors, while AlBi is found to be a semiconductor with a small and direct band gap of 0.042 eV at Γ with a linear relation between the bulk modulus and the cell volume for the zinc blende phase [2].

The purpose of this work is to provide some additional information to the existing data on the physical properties of AlBi with state-of-the-art first-principles calculations. Additionally to the structural and electronic properties, the thermodynamic properties have also been investigated. The latter are the basis of solid-state science and industrial applications and their study is of importance to extend our knowledge on their specific behaviour when undergoing severe constraints of high-

pressure and high temperature environments. This is particularly true since the coming of modern technologies (geophysics, astrophysics, particle accelerators, fission and fusion reactors, etc.) from which we always expect new advances and innovations in materials science to reach higher performances.

THEORETICAL FRAMEWORK :

We have employed the first principles full potential linear augmented plane wave (FP-LAPW) method [3] as implemented in the WIEN2k code [4]. The exchange and correlation effects are described in the framework of the density functional theory [5, 6] with the parameterization of Perdew et al. [7]. The unit cell is divided into non overlapping muffin-tin spheres of radius R_{MT} and an interstitial region, the Kohn-Sham wave functions being expressed in spherical harmonics within spheres and in plane waves in the interstitial regions. To ensure the correctness of our calculations, we have taken $l_{max} = 10$, $R_{MT} K_{MAX} = 8$, $R_{MTS} = 2.3$ a.u for Al and 2.7 a.u for Bi. The number of the irreducible Brillouin zone special K-points and the total number of plane waves involved in the calculations were 47 and 1088 respectively.

To investigate the thermodynamic properties, we used the quasi harmonic Debye model [8] in which the non-equilibrium Gibbs function $G^*(V; P, T)$ is written in the following form :

$$G^*(V; P, T) = E(V) + PV + A_{vib}[\theta(V); T] \quad \dots(1)$$

where $E(V)$ is the total energy per unit cell, PV corresponds to the constant hydrostatic pressure condition, $\theta(V)$ is the Debye temperature and A_{vib} is the vibrational term which can be written using the Debye model of the phonon density of states as [9, 10]:

$$A_{vib}(\theta; T) = nkT \left[\frac{9\theta}{8T} + 3 \ln(1 - e^{-\theta/T}) - D\left(\frac{\theta}{T}\right) \right] \quad \dots(2)$$

where n is the number of atoms per formula unit, $D(\theta/T)$ represents the Debye integral and for an isotropic solid, θ is expressed as [9]:

$$\theta_D = \frac{h}{k} [6\pi^2 V^{1/2} n]^{1/3} f(\sigma) \sqrt{\frac{B_s}{M}} \quad \dots(3)$$

M being the molecular mass per unit cell, B_s is the adiabatic bulk modulus, which is approximated given by the static compressibility [8]

$$B_s \cong B(V) = V \frac{d^2 E(V)}{dV^2} \quad \dots(4)$$

Details on $f(\sigma)$ can be found elsewhere [11, 12]. Therefore, the non-equilibrium Gibbs function $G^*(V; P, T)$ as a function of V , P and T can be minimized with respect to volume V :

$$\left[\frac{\partial G^*(V; P, T)}{\partial V} \right]_{P, T} = 0 \quad \dots(5)$$

By solving Eq. (5), one can obtain the thermal equation-of-state (EOS) $V(P, T)$. The heat capacity C_V and the thermal expansion coefficient α are given by [13].

$$C_V = 3nk \left[4D \left(\frac{\theta}{T} \right) - \frac{3\theta/T}{e^{\theta/T} - 1} \right] \quad \dots(6)$$

$$\alpha = \frac{\gamma C_V}{B_T V} \quad \dots(7)$$

where γ is the Gruneisen parameter which is defined as

$$\gamma = - \frac{d \ln \theta(V)}{d \ln V} \quad \dots(8)$$

Through the quasi-harmonic Debye model, one could calculate the thermodynamic quantities of any temperatures and pressures of AlBi from the calculated E–V data at $T = 0$ and $P = 0$.

RESULTS AND DISCUSSION :

First, we have calculated the total energy of zinc blende AlBi as a function of the volume, then the equilibrium volume, the equilibrium lattice constant, the bulk modulus B and its derivative were obtained by fitting to the Murnaghan equation of state [14]. The results are presented in Table – 1. The calculated lattice parameters and bulk modulus are in general in good agreement with literature. The cohesive energy is calculated using the following formula : $E_{coh}^{AlBi} = E^{Al} + E^{Bi} - E_{tot}^{AlBi}$. E_{Al} , E_{Bi} being the atomic energies for Al and Bi respectively and E_{total}^{AlBi} is the total energy of AlBi. The elastic constants are also listed and enable us to infer the Young modulus $Y = 33.53$ GPa, the Poisson ratio $\sigma = 0.3556$ and the shear modulus $C = 12.124$. It is clear that AlBi is elastically stable in the zinc blende (B3) phase since $C_{12} < B < C_{11}$ and all the following quantities are positive : $C_{11} - C_{12}$, $C_{11} + 2C_{12}$, C_{11} and C_{44} . Unfortunately, there are no experimental data to check our results.

TABLE - 1

Lattice constant a , bulk modulus B , pressure derivative of bulk modulus B' and elastic constants parameters of AlBi at zero pressure and zero temperature, compared with the experimental data and other theoretical works.

| | Present work | Other theoretical works |
|-----------------------------|--------------|--|
| $E_{\text{coh}}(\text{eV})$ | 4.004 | |
| a (Å) | 6.448 | 6.31 ^{a)} 6.266 ^{b)} |
| B (GPa) | 38.750 | 45.58 ^{a)} 48.2 ^{b)} |
| B' | 4.576 | 4.23 ^{a)} 5.237 ^{b)} |
| C_{11} (GPa) | 48.498 | |
| C_{12} (GPa) | 29.001 | |
| C_{44} (GPa) | 14.5 | |

[a] – Ref. [1] [b]- Ref. [2]

Fig.-1 shows the band structure of AlBi for the equilibrium volume. We remark an almost zero Γ - Γ direct fundamental gap. Its magnitude is found to be about ~ 0.02 eV which is underestimated by LDA so that AlBi is probably a semiconductor.

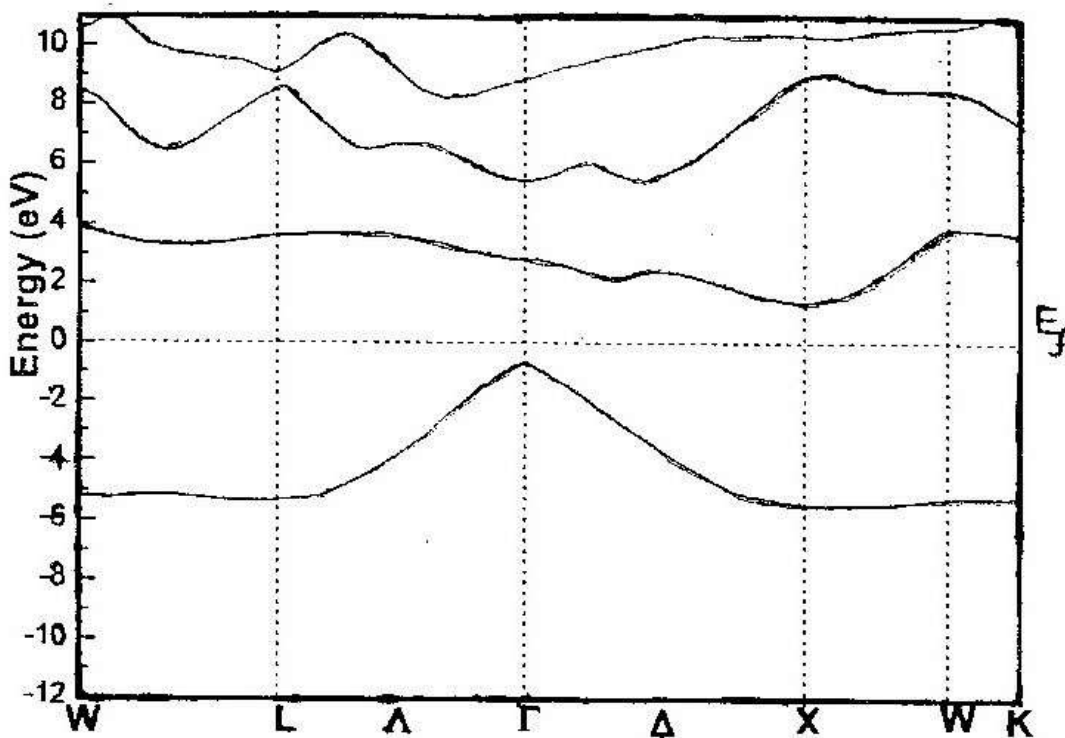


Fig.-1 : Band structure calculated along high-symmetry directions of AlBi. The energy zero is taken at E_f .

CONCLUSION :

In summary, we have applied the FPLAPW method and the quasi-harmonic Debye model to investigate the structural, elastic, electronic and thermal properties of AlBi. In particular, we confirm the semiconducting nature of AlBi with a small and direct bandgap which makes it a good candidate for opto electronic applications. Various useful data have been calculated and may be checked in further works.

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