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# Hydrostatic pressure effect on the structural parameters of GaSb semiconducting material: *Ab-initio* calculations

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## Abstract

Ab-initio calculations were performed to investigate the ground state and hydrostatic pressure effect on the structural properties of GaSb semiconducting material. The projected augmented wave pseudopotentials (PAW) approach in the framework of the density functional theory (DFT) as implemented in the Quantum Espresso code was used. The exchange-correlation functional was described with the generalized gradient approximation (GGA). Utilizing the energy - volume (E-V) data, our values of the equilibrium lattice constant, the bulk modulus, and the pressure derivative of the bulk modulus of GaSb semiconductor obtained from the Birch–Murnaghan equation of state were found 6.220 Å, 44.84 GPa and 4.22, respectively. Our obtained data agree well with the available experimental values and other theoretical data of the literature. In addition, the melting point, the lattice thermal expansion coefficient and the microhardness of our material of interest were also calculated and compared with the available experimental data of the literature.

**Keywords:** III-V semiconducting materials, Ab-initio calculations, structural parameters, melting point.

## 1. Introduction

III–V semiconducting materials are made from group III and V elements of the Mendeleev table (the periodic table) [1-4]. III–V compounds are technologically important materials due to their versatile technological usage and flexibility of their physical properties *via* structural engineering, they have been extensively served as substances for electronic and optoelectronic devices [3].

Among III–V semiconducting compounds, the antimonide based compound. At ambient pressure and temperature, III-Sb semiconducting compounds crystallize in the cubic zincblende (ZB) structure. Boron antimonide (BSb) and aluminium antimonide (AlSb) have indirect band gap, while gallium antimonide (GaSb) and indium antimonide (InSb) have direct ones [3].

Recently, GaSb semiconducting compound is considered as promising material for potential applications in field-effect transistors (FET), lasers, multi-junction solar cells (MJSC), infrared detectors (ID), and Shockley diodes [5]. At ambient pressure and temperature, GaSb compound is a

direct semiconductor with a narrow band gap of *Eg* = 0.725 eV [5], a lattice constant is equal to 6.096 Å, a crystal density of 5.615 g/cm$^3$and its melting point of 991 K [6].
Using, full-potential linearized augmented plane wave (FP-LAPW) method, Moussa *et al.* [5] investigated the structural parameters, electronic and optical properties, and elastic constants of cubic $Al_xGa_{1-x}Sb$ ternary alloys. They found that the band gap variations with the composition of the ternary alloys exhibit a small deviation from the Vegard's law, and the obtained results confirm the semiconducting character of the studied materials. Besides, they found that the lattice parameter of the $Al_xGa_{1-x}Sb$ alloys showed a non-linear variation with the Aluminum mole fraction.
In this investigation, we focus on studying the effect of the hydrostatic pressure on the structural properties of GaSb material. Firstly, we explain the method of calculation used in our work; secondly, we present and discuss the results obtained; and finally, we finish with a brief conclusion.

## 2. Method of calculations

In the present work, the Quantum Espresso code with Thermo_PW tool [7-9] were employed to investigate the effect of hydrostatic pressure on the structural properties of GaSb semiconducting material. The Quantum Espresso code is based on the pseudopotential (PP) method and a plane waves basis set. The Ga.pbe-dn-kjpaw_psl.1.0.0.UPF and Sb.pbe-dn-kjpaw_psl.1.0.0.UPF projector augmented wave pseudopotentials (PAW) [10] are used for gallium (Ga) and antimony (Sb) atoms, respectively. As it is well known, the term of exchange and correlation (XC) is not known exactly, therefore, the exchange-correlation potential was calculated using the Perdew-Burke-Ernzerh of generalized gradient approximation (PBE-GGA) [11]. The PBE-GGA functional do not express the XC energy density only as a function of the local density (LD), but it takes into account its gradient.
In the present work, the wave functions were expanded with an energy cut-off of 70 Ry for the plane wave basis set; while the charge density cut-off was taken equal to 700 Ry. The integration over the Brillouin zone was performed using 6x6x6 k-points Monkhorst-Pack mesh [12].With these previous conditions, a convergence with an energy threshold of 1x10$^{-4}$ Ry was achieved.

## 3. Resultsand discussions

### *3.1. Equilibrium structural parameters*

One of the major problems in geophysics science, materials science, and condensed matter physics is the determination of the equation of state and the other thermodynamic properties of materials [13]. As it was mentioned previously, GaSb semiconducting compound crystallizes in the cubic zincblende (B3) structure. The unit cell geometry of B3 phase was assigned as: $a = b = c$ (lattice constants), and $\alpha = \beta = \gamma = 90°$ (lattice angles). In B3 structure, the material is constituted of two different atoms per basis (molecule), with a unit cell of 8 atoms (4 atoms of III element (Ga), and 4 atoms of V element (Sb)) (see Fig. 1) [14], while, the wurtzite (B4) lattice has only four atoms (two molecular units) in the primitive unit cell [6].

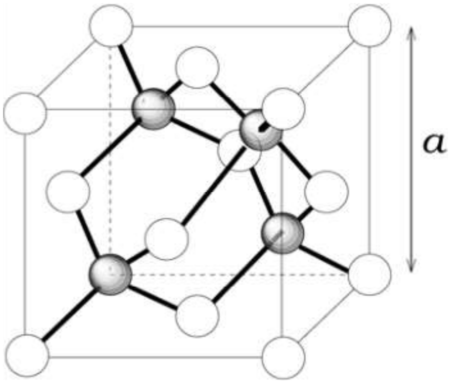

**Figure 1.**Cubic zincblende (B3) crystal structure for III-V semiconducting material [14].

The energies were obtained by hydrostatic compression / dilation of the unit cells. Figure 2 shows the evolution of the total energy as a function of the unit cell volume of cubic zincblende GaSb material.

From the total energy $E_{Tot}$ presented as a function of the cell volume $V$, one can deduce the static structural parameters, such as the equilibrium lattice constant $a_0$ from the volume which gives the minimum energy, the bulk modulus $B_0$ and the derivative of the bulk modulus with respect to pressure $B_0'$ by fitting the total energy with the Birch-Murnaghan's equation of state (BM-EOS), which is expressed as follows [15]:

$$E(V) - E_0 = \frac{9V_0B_0}{16}\left\{B_0'\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^3 + \left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^2\left[6 - 4\left(\frac{V_0}{V}\right)^{2/3}\right]\right\} \tag{1}$$

where, $V_0$ is the equilibrium unit-cell volume, and $E_0$ is the corresponding energy.

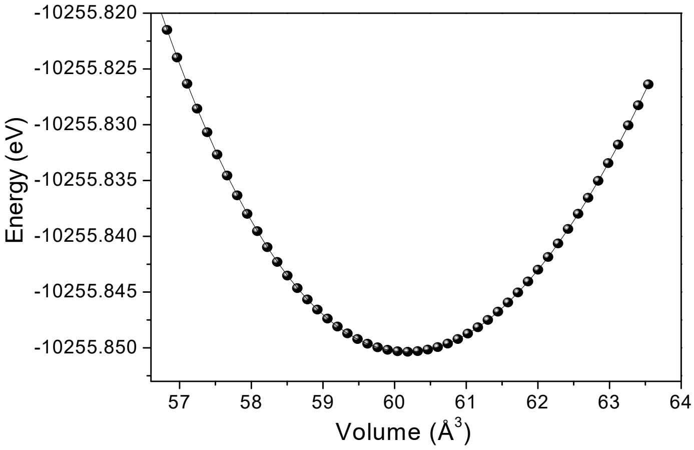

**Figure 2.**Total energy versus the primitive unit cell volume for cubic zincblende (B3) GaSb.

Our calculated values of the equilibrium lattice constant $a_0$, the bulk modulus $B_0$, and its pressure derivative $B_0'$ for GaSb material are summarized in Table. 1, in comparison with the experimental data [6, 16, 17] and other theoretical results [18, 19]. Although our value (44.84 GPa) of $B_0$ is slightly lower than the experimental data one 56.31 GPa reported in Ref. [6], there is a strong evidence that our calculated values of $a_0$, and $B_0'$ coincide well with experimental data [6, 16, 17] and other theoretical results [18, 19]. The deviation between our calculated value (6.220 Å) of the lattice constant $a_0$ and the experimental result (6.130 Å) reported by Böer and Pohl [16] is only around 1.47%.

**Table 1.** Optimized equilibrium structural parameters $a$ (Å), the bulk modulus $B_0$ (GPa), and pressure derivative of bulk modulus $B'_0$ for GaSb semiconducting material.

| Parameter | Our data | Experimental data | Other calculations |
|---|---|---|---|
| $a_0$(Å) | 6.220 | 6.096 [6], 6.130 [16] | 6.005 [18], 5.981 [19] |
| $B_0$ (GPa) | 44.84 | 56.31 [6], 55.4 [17] | 56 [18], 56.7 [19] |
| $B'_0$ | 4.22 | 4.78 [6] | 4.64 [18], 4.662 [19] |

The melting temperature $T_m$ and the Debye temperature $\theta_D$ are two fundamental thermophysical properties of materials [4, 20]. The melting temperature $T_m$ is one of the important information required for the thermal characterization of materials [21]. The melting point $T_m$ of several solids having a cubic structure correlates with the bulk modulus $B$ by this empirical formula [22, 23]: $T_m = 9.3B + 607$, where $T_m$ is expressed in K, and $B$ is expressed in GPa. Although several empirical expressions are not supported by fundamental theory, much important information of semiconducting materials have been obtained on the basis of these equations. Replacing our value (44.84 GPa) of the bulk modulus $B_0$ in the previous equation, the melting point $T_m$ of GaSb material was found equal to 1024 K. This value is slightly higher than the experimental value 991 K reported by Adachi [6]. The deviation between our value (1024 K) of $T_m$ and the result (991 K) [6] is only around 3.33%.

For binary tetrahedral semiconductors, the lattice thermal expansion coefficient α in ($10^{-6}$ $K^{-1}$) is given by this relation [24]: $\alpha = k(T_m \times Z_1Z_2)^{-1/2} - d^{1/2}$, where $T_m$ is the melting temperature in K, $Z_1$ and $Z_2$ are ionic charge of cation and anion, respectively, $d$ ($d = 0.25\sqrt{3}a$) is the nearest-neighbour distance in Å, and $k$ is dimensionless constant. The value of constant $k$ for cubic zincblende type crystal structure is

775 [24]. Replacing our values 1024 K of $T_m$ and 2.69 Å of $d$ in the previous equation, the lattice thermal expansion coefficient α of GaSb material was found equal to $6.43 \text{x} 10^{-6}$ $\text{K}^{-1}$. This value is in excellent agreement with the experimental value ($6.5 \text{x} 10^{-6}$ $\text{K}^{-1}$) reported by Van Uitert [25]. The deviation between our value ($6.43 \text{x} 10^{-6}$ $\text{K}^{-1}$) of α and the experimental one ($6.5 \text{x} 10^{-6}$ $\text{K}^{-1}$) reported by Van Uitert [25] is less than1.1%.

Daoud [4] has shown that for many II–VI and III–V semiconductors having tetrahedral structure, the Debye temperature $\theta_D$ is roughly proportional to the bond-length $d$, they are related by:

$$\theta_D = K_3\,[1/(M^{1/2} d^{5/4})] - K_4 \tag{2}$$

where $d$ is expressed in $10^{-10}$ m, $M$ is the molar mass, and $K_3$ and $K_4$ are two empirical parameters (for group III–V, $K_3 = 112.66$ ($10^{-12}$ $\text{Kg}^{1/2}$ $\text{m}^{5/4}$ K) and $K_4 = 90.74$ K, respectively).

Replacing our value ($2.693 \text{x} 10^{-10}$ m) of $d$ in the previous equation, the Debye temperature $\theta_D$ of GaSb was found equal to 243 K. Although our data of $\theta_D$ is slightly lower than the value 266 K obtained at low-temperature ($T = 0$ K) [6], it is in good agreement with the experimental one 240 K measured at $T = 273$ K [6], and other theoretical ones (233 K, 302 K, and 331 K) reported by Narain [26]. Our value (243 K) of $\theta_D$ deviates from the value (240 K) reported by Adachi [6] by only around 1.25%.

For groups II–VI and III–V, semiconductors having tetrahedral structure, and based on the plasma oscillations theory of solids, Bahadur and Mishra [27] developed an empirical relation for the calculation of the microhardness $H$, which is given as follows: $H = \beta\, r_S^{-5.57}$ [27], where $\beta$ is a constant, (its numerical value is 365.86 for III–V group), and the electron density parameter $r_s$ is expressed as follow: $r_s = 1.388\, a_0 (W/Z'\rho)^{1/2}$ [27], where $a_0$ is the Bohr radius, $W$ is the molecular weight of the compound, $Z'$ is the effective number of electrons taking part in the plasma oscillation, and $\rho$ is the density. The electron density parameter $r_S$ and the bond-length $d$ are also related by: $d = 1.173 r_S$ [27]. Using the previous expressions, the microhardness $H$ of GaSb was found equal to 3.57 GPa, which is slightly lower than the experimental values 4.48–4.68 GPa reported by Adachi [6].

### 3.2. Hydrostatic pressure effect

The study of equation of state means the investigation of pressure, volume and temperature (P–V–T) relation. The study of equation of state (EOS) facilitates to know about the nature of solid state theories [28]. EOS also helps us to determine the values of fundamental thermodynamic parameters of semiconducting compounds and other materials [28]. In order to show how the structural parameter in GaSb compound behaves under external pressure, the volumes of the primitive unit cell were computed at fixed values of applied hydrostatic pressure in the range of 0 to 3.5 GPa. Fig. 3 shows the variation of the primitive unit cell volume $V$ of GaSb as a function of pressure $p$. The fit of our data regarding the volume $V$ as a function of $p$ obeys the following polynomial expression: $V = 60.18 - 1.33p + 0.06p^2$, where $V$ is expressed in $\text{Å}^3$, and $p$ is expressed in GPa.

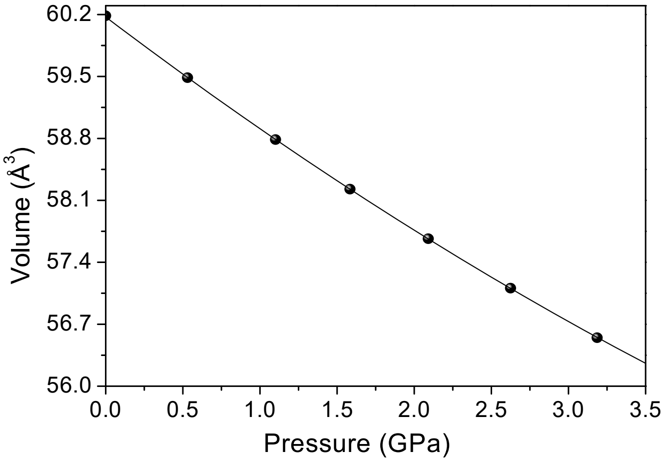

**Figure 3.** Primitive unit cell volume versus pressure for GaSb semiconducting material.

The crystal density ρ of material is related to the atomic arrangement and corresponding electron density map [6]. The crystal density ρ can be calculated as follows [29-31]:

$$\rho = ZM/N_A V \tag{3}$$

where $Z$ is the number of molecules per unit cell, $M$ is the molecular weight, $N_A$ is the Avogadro constant, and $V$ is the volume of unit cell (for binary compounds which crystallizes in the cubic zincblende (B3) structure ($V = a^3$)). The pressure dependence of the crystal density ρ for GaSb material was offered in Fig. 4. From curve of Fig. 4, we observe clearly that the crystal density ρ of GaSb semiconducting material increases with increasing of pressure. Similar qualitative behaviors have been reported for the crystal density ρ versus pressure for cubic zinc-blende AlP semiconducting compound [3], $B_xAl_{1-x}Sb$ ternary alloys [22], (B2-type) Yttrium-Rhodium (YRh) rare earth intermetallic compound [32], cubic zinc-blende thallium phosphide (TlP) compound [33], and cubic zinc-blende boron phosphide (BP) compound [34]. The crystal density ρ of GaSb material started with the value 5.283 g/cm$^3$ at zero-pressure, and it reaches the value of 5.652 g/cm$^3$ at 3.5 GPa. At zero-pressure, our value of ρ is around 5.283 g/cm$^3$, it is slightly lower than the experimental one (5.615 g/cm$^3$) reported by Adachi [6]. The fit of our data regarding the crystal density ρ as a function of pressure $p$ obeys the following expression: $\rho = 5.284+0.118p-3.45\text{x}10^{-3}p^2$, where ρ is expressed in g/cm$^3$, and $p$ is expressed in GPa.

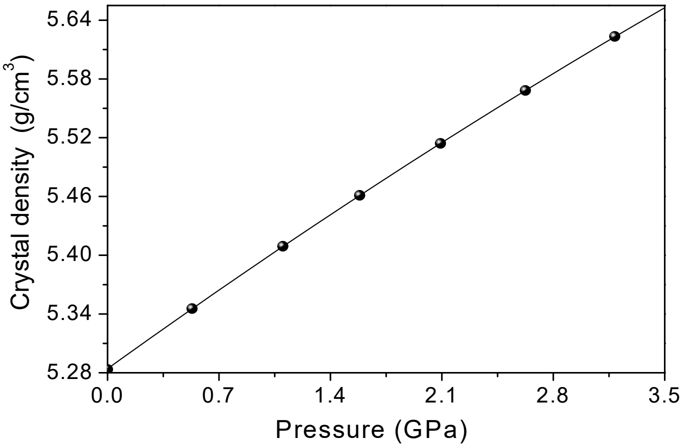

**Figure 4.** Crystal density versus hydrostatic pressure for cubic zincblende (B3) GaSb.

A second way was usually used to present the effect of the compressional behavior on the physical quantities, i.e as a function of the normalized lattice constant ($a/a_0$) [35]. The crystal density ρ of GaSb for different values of ($a/a_0$) is displayed in Fig. 5. The fit of our data regarding the crystal density ρ as a function of $a/a_0$ obeys the following polynomial expression: $\rho = 54.52 - 82.63\ (a/a_0) + 33.40\ (a/a_0)^2$, where $a/a_0$ is dimensionless (without unity), and ρ is expressed in g/cm$^3$.

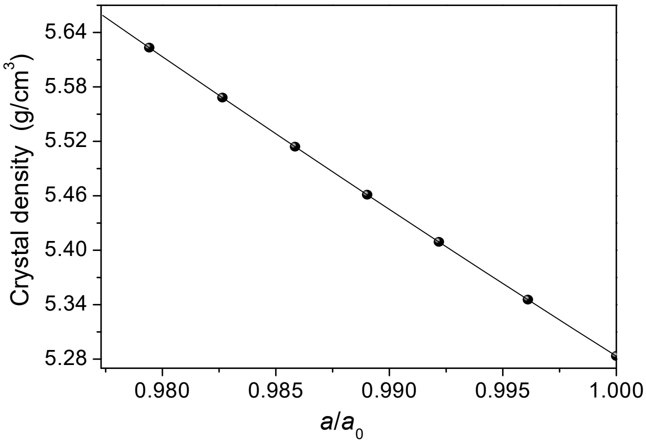

**Figure 5.** Crystal density versus normalized lattice constant $a/a_0$ for GaSb compound.

## 4. Conclusion

In this study, the equilibrium structural parameters as well as the effect hydrostatic pressure on the crystal density of the cubic GaSb semiconducting material were investigated using the projected augmented wave pseudopotentials (PAW) approach in the frame work of the DFT. In general, our calculated structural parameters agree well with other data of the literature. Our calculated value (6.220 Å) of $a_0$ deviates from the experimental one (6.130 Å) by only around 1.47%.

In addition, the melting temperature $T_m$, the Debye temperature, the linear lattice thermal expansion coefficient α, and the microhardness of our material of interest were also calculated. The data obtained in this work are in good agreement with the experimental values of the literature. Our value (1024 K) of $T_m$ deviates from the experimental result (991 K) by about 3.33%, while our predicted data (6.43 x $10^{-6}$ $K^{-1}$) of α deviates from the experimental one (6.5 x $10^{-6}$ $K^{-1}$) by less than 1.1%. These marked results signify the good values obtained for the structural parameters.

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