Effect of pressure on some physical properties of gallium based semiconductors

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Abstract. The gallium based semiconductor compounds are very useful materials for optical spectroscopy and optoelectronic applications. we have studied the effect of pressure on various physical properties like total energy, static bulk modulus, energy band gap at the point X on the Jones-zone face, pressure derivative of bulk modulus and equation of state of gallium based binary compounds GaSb, GaAs, GaP and GaN using pseudopotential theory beyond second order with our well established single parametric model potential. We have incorporated Nagy’s static local field correction function to include exchange and correlation effects. The results are compared with those obtained using few other local field correction functions. The present results agree satisfactorily with available experimental and other such theoretical data confirming the application.

1. Introduction

The gallium based semiconductor compounds and their ternary and quaternary alloys are very useful materials for optical spectroscopy and optoelectronic applications. Due to narrow energy gap, group III-V compounds are suitable to fabricate light emitting diodes, infrared detectors and infrared diode lasers, high speed switching devices and communication devices such as emitters, wave guides [1]. The second order perturbation theory based on the pseudopotential formalism, which has been successfully applied to simple metals, their alloys and glasses [2-5] is failed for covalent crystals. When the perturbation treatment is applying to the covalent semiconductors, it is seen that the pseudopotentials are large in these crystal compared with those in simple metals and there is an energy gap on the Jones-zone face corresponding to the Fermi surface. These facts are closely related to the covalent bonding character in covalent crystal, which comes from higher than second order terms and have important role for the stability of lattices of the crystals having zinc-blende structures. While in the second order perturbation theory the crystal are unstable for shear distortion. Therefore higher order terms are considered for covalent crystal to incorporate covalent bonding effect [6-8]. Soma [7, 8] used higher order perturbation theory to calculate total energy and bulk modulus of semiconductor elements and compounds. In the present paper, we have studied effect of pressure on various physical properties like total energy, static bulk modulus, energy band gap at the point X on the Jones-zone face, pressure derivative of bulk modulus and equation of state of gallium based binary compounds
GaSb, GaAs, GaP and GaN using pseudopotential theory beyond second order with our well established single parametric model potential [9, 10]. We have used Nagy’s static local field correction function (N) [11] to include exchange and correlation effects. The results are compared with those obtained using few other local field correction functions due to Hartree (H) [12], Ichimaru et al (I) [13] and Sarkar et al (S) [14].

The paper is organized as follows. In section 1 we give a brief introduction. Section 2 contains a theoretical background for the calculation procedure. Section 3 covers discussion of the results. A summary of our conclusions is narrated in Section 4.

2. Theory
The bare-ion potential used in the present investigations is proposed in r-space [9, 10] is

\[ w^{\text{ion}}(r) = -\frac{Ze^2}{2R_c} \left[ 2 - \left( 2 - \frac{r^2}{R_c} \right) \exp \left( \frac{r}{R_c} \right) \right] \text{ for } r \leq R_c \]

\[ w^{\text{ion}}(r) = -\frac{Ze^2}{r} \text{ for } r \geq R_c \]

(1)

Here \( Z, e \) and \( R_c \) are valency, electronic charge and pseudo core radius respectively and \( R_c \) is estimated through zero pressure condition. It is to be noted that to represent core-core repulsion usually Born-Mayer term is employed. We have also incorporated this feature in our potential through exponential factor. Inside the core, it is represented as the combination of linear and quadratic terms modulated by repulsive exponential factor, which tends to cancel Coulomb potential inside the core. While outside the core, it has the Coulombian tail. The smoothness of the bare-ion potential due to exponential term results in to faster conversions in r-space. It is continuous at the core.

For a covalent metallic crystal with zinc-blende structure, the total energy \( E_T \) per atom using higher order perturbation theory based on pseudopotential method is given as [6, 7]

\[ E_T = E_i + E_0 + E_1 + E_2 + E_{\text{cov}} \]

(2)

Here \( E_i \) is the total Coulomb energy of positively charged pseudo metal ions in a uniformly negatively charged background; \( E_0 \) is the sum of kinetic, exchange and correlation energies of the uniform electron gas; \( E_1 \) and \( E_2 \) represent the first-order and second-order energies of the valence electron due to the pseudopotential, \( E_{\text{cov}} \) is the covalent bond correction to the crystal energy corresponding to the third-order and fourth order terms.

To incorporate the exchange and correlation effects in the dielectric function, Nagy’s static local field correction function [11] is used. It is given by,

\[ f(q) = 1 - g(0,n) + \frac{c_b}{c^2 + q^2} - \frac{g(0,n)}{q} \tan^{-1} \frac{q}{c} \]

(3)

The detailed expressions of form factor, energy terms shown in equation (2) and Nagy’s screening function (N) [11] are given elsewhere [6]. The local field correction functions proposed by H [12], I [13] and S [14] are also employed for comparative study with Nagy’s screening function (N) [11].

The Jones zone of a zinc-blende type crystal is highly symmetrical with twelve \{220\} zone faces and does not deviate too much from a sphere. Heine and Jones [15] have shown that energy band gap at the point X (\( k_x = (110)2\pi/a_0 \)) on the Jones-zone face is given for group III-V can be computed using

\[ E_{gs} = 2 \left[ U_{\alpha}(220) + \frac{a_0^2}{4\pi^2} \left[ U_{\beta}(111)^2 + U_{\delta}(111)^2 \right] \right] \]

(4)

Table 1. Input parameters

| Compound | Structure | Atomic Volume (a.u.)^3 |
|----------|-----------|----------------------|
| GaSb     | Zinc-blende | 193.20               |
| GaAs     | Zinc-blende | 152.50               |
| GaP      | Zinc-blende | 136.70               |
| GaN      | Zinc-blende | 76.90                |
3. Results and Discussion

The input parameters are given in the Table 1. In the present study we have considered only zinc-blende structures of GaSb, GaAs, GaP and GaN. The crystal energy per electron and bulk modulus computed at zero pressure (equilibrium) for the said compounds using N [11], H [12], I [13] and S [14] along with the experimental findings are shown in table 2. It is seen that H [12] produced higher values of energy and bulk modulus while I [13] produced lower values energy and bulk modulus in all screening functions. It suggests that inclusion of exchange and correlation effect is essential for energy calculations. The total energy and bulk modulus computed for all four compounds by N [11] are found in good agreement with the experimental data [8, 16].

Table 2. Total crystal energy and bulk modulus of GaAs, GaSb, GaP and GaN.

| Compound | $-E_T$ (Ryd / electron) | B (GPa) |
|----------|-------------------------|---------|
|          | N [11] | H [12] | I [13] | S [14] | Exp. [8, 16] | N [11] | H [12] | I [13] | S [14] | Exp. [8, 16] |
| GaSb     | 1.984  | 1.776  | 2.057  | 1.936  | 1.965 | 50.26 | 76.05 | 42.61 | 52.44 | 56.3 |
| GaAs     | 2.155  | 1.932  | 2.232  | 2.107  | 2.157 | 2.159 | 72.12 | 100.50 | 63.33 | 73.23 | 75.4, 74.8 |
| GaP      | 2.237  | 2.010  | 2.316  | 2.189  | 2.221 | 2.223 | 85.63 | 114.96 | 76.29 | 86.08 | 88.7 |
| GaN      | 2.700  | 2.471  | 2.778  | 2.656  | 2.634 | 2.635 | 215.48 | 247.4 | 202.32 | 210.19 | 210, 207 |

To study the effect of compression and expansion on the total energy, we have study volume dependency of total energy. The present results of total energy of all four gallium based binary compounds with relative volume using N [11] are shown in figure 1. It is seen that the variations in total energy with volume show same trend for all four compounds. GaN has produced lower value and GaSb has produced higher value of total energy per electron. The energy becomes minimum at equilibrium volumes. The pressure–volume relationship (equation of states) for all four compounds using N [11] is shown in figure 2. In the present study, we have considered compression up to 60%; which is now possible to achieve due to advancement in DAC techniques. It is found that on 60% compression, the pressure become 237 GPa, 316 GPa, 364 GPa and 813 GPa for GaSb, GaAs, GaP and GaN respectively. The pressure of GaN is largely influenced by the volume compression and GaSb showed minimum influence. Our findings of equation of state are compared with those obtained using Murnaghan [17] and Vinet [18] scheme and good agreement is observed.

Figure 1 Total energy as a function of relative volume for GaSb, GaAs, GaP and GaN.

The variations of bulk modulus and energy band gap at point X on the Jones- zone face with pressure (up to 10 GPa) are shown in the figure 3 and 4 respectively. At zero pressure (equilibrium), present results of bulk modulus for all four compounds are agreed with the experimental findings [8]. The computed bulk modulus is increased linearly with the pressure show same trend for all four compounds and increased by 30-35 GPa on pressure changing from 0 to 10 GPa. The values of computed pressure derivatives of bulk modulus at zero pressure are 3.350, 3.193, 3.133 and 2.935 for GaSb, GaAs, GaP and GaN respectively. From figure 4, it is found that the energy band gap at point X on the Jones- zone face is increased by 0.003 to 0.005 eV as pressure is increased up to 10 GPa. Any noticeable change is not observed in $E_{gx}$ with pressure.
4. Conclusions

In the present investigation it is found that total energies computed for all four gallium based binary compounds are matched with the experimental findings. GaN has produced lower value and GaSb has produced higher value of total energy per electron in all four gallium based binary compounds. The present findings of equation of state are found in good agreement with those computed by using Murnaghan [17] and Vinet [18] formalisms. The pressure of GaN is largely influenced by the volume compression in all four compounds. The bulk modulus is linearly increased with the pressure increased up to 10 GPa. But energy band gap at point X on the Jones-zone face is not much influenced by the pressure change up to 10 GPa. The pressure derivatives of bulk modulus are found matching with the experimental results with some deviation. Finally, we conclude that present results using our novel model potential are satisfactory and could be used for further comprehensive study of such system of semiconductor.

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