Structural and electronic properties of gallium arsenide crystal using INDO method

Khalid H. B. AL-Ammar **Fuaad Sh. Hashim** **Hamad R. Jappor**

Babylon University, College of Education, Department of Physics

Abstract

We present the structural and electronic properties of GaAs under the effect of pressure using large unit cell method within the framework of intermediate neglect of differential overlap (LUC-INDO) calculations. It is found that the results are consistent with the available experimental data and other theoretical results. Energy gap, valence bandwidth, bulk modulus and cohesive energy increase with increasing pressure, while the conduction bandwidth decreases. All the aforementioned properties are obtained by selecting empirical parameter sets for LUC-INDO calculation.

الخلاصة

تم عرض الخواص التركيبية والالكترونية لارسنيد الكاليوم تحت تأثير الضغط باستعمال طريقة خلية الوحدة الكبيرة ضمن اطار حسابات الاهمال المتوسط للتداخل التفاضلي (LUC-INDO). وقد وجد ان النتائج متوافقة مع النتائج العملية المتوفرة والنتائج النظرية الاخرى. ان فجوة الطاقة وعرض حزمة التكافؤ ومعامل المرونة الحجمي وطاقة الترابط تزداد مع زيادة الضغط، بينما يقل عرض حزمة التوصيل مع زيادة الضغط. جميع الخواص تم الحصول عليها باختيار عوامل تجريبية لحسابات الاهمال المتوسط للتداخل التفاضلي.

1. Introduction

Theoretical studies of properties continue to be of great importance. Among these are the complete (CNDO) and intermediate (INDO) neglect of differential overlap. The extension of the semiempirical calculations to solids had begun in approximately one decade after its application to molecules [Evarestov and Lovchikov, 1977]. The extension made use of the large unit cell (LUC) method to implement periodic boundary of solid. LUC-INDO calculations have the ability to include large number of atoms including surfaces, interstitials, or vacancies. Previous LUC-INDO calculations for semiconductors had focused on diamond and silicon [Harker and Larkins, 1979; Craig and Smith, 1987]. Other calculations applied the method to F centers [Eglitis *et al.*, 1997] titanium oxides [Evarestov *et al.*, 1997], etc.

The calculation of energy levels of electrons in solids, that is, the determination of energy bands, in central theoretical problem of solid state physics. Knowledge of these energies and electron wave functions is required, in principle, for any calculation of more directly observable properties including mechanical properties, vibrational spectra, magnetic order, electrical and thermal conductivities, optical dielectric function, and so on. On the other hand, calculation of the bulk ground state properties, such as lattice constants, bulk modulus, cohesive energy, and atomic positions, play an important role in the physics of condensed matter [Wachowicz and Kiejna, 2001], bulk calculations help us to understand, characterize, and predict mechanical properties of materials in surroundings, under extreme conditions.

Gallium arsenide (GaAs) is the most technologically important and the most studied compound semiconductor material. Many band structure parameters for GaAs are known with a greater precision than for any other compound semiconductor. This is especially true of the fundamental energy gap with a value of 1.519 eV [Sze and Ng, 2007].

Gallium arsenide has been intensively investigated in recent years. Particular properties studied are its direct band gap for photonic applications [Jovanovič1 *et al*., 2008], Nanotubes [Ghosh *et al*., 2007] and its internally-carrier transport and higher mobility for generating microwaves [Ng, 2002].

Pressure has been proved to be a valuable tool for studying the influence of the band-structure parameters on the electronic properties of semicond- uctors, bulk crystals, or two dimensional systems, thus, we have studied the effect of pressure on the some properties of GaAs using the self-consistent large unit cell within intermediate neglect of differential overlap (LUC-INDO) method in the linear combination of atomic orbitals approximation [Abdulsattar and Al-Bayati, 2007; Radi *et al*., 2007]. This method, gives surprisingly accurate results considering the computing time and effort involved, and can be applied successfully to account for the band structure and physical properties of semiconductors using appropriate parameters [Abdulsattar and Al-Bayati, 2007].

2. Structural Properties and Phase Transition of GaAs

GaAs crystallizes in the zinc-blende structure. Under ambient conditions and up to 13GPa adopts the zinc-blende structure. At high pressures [Kelsey *et al.,* 1998] it adopts a site-ordered (orthorhombic) Cmcm structure [Nelmes and McMahon, 1998]. Yu *et al.*[Yu *et al.*,1978] reported it to be orthorhombic, with an onset at about 17 GPa, and although it could not be conclusively solved at the time using EDX methods, all later experimental studies agreed on its orthorhombic symmetry (Baublitz and Ruoff, 1982). A second transition was reported by Weir *et al.* [Weir *et al.,* 1989] at about 24 GPa to another orthorhombic structure, Imm2, which then gradually approaches a "sh-type" structure. First-principles calculations by Mujica and Needs (Mujica and Needs, 1996) show that the Cmcm and Imm2 phases are close in enthalpy at high pressures and are clearly favored over other structures. First-principles studies had predicted the existence of a field of stability for a sc16 phase, which was, however, close to the numerical precision of the calculations (Mujica *et al.*, 1995). Under compression, sc16 transforms into the Cmcm phase at 22 GPa, which remain stable up to at least 108 GPA (Weir *et al.,* 1989). However, it is believed that only in the range 13–14.5 GPa (where the temperature induced Cmcm→sc16 transition is observed) is the sc16 phase stable [Mujica *et al*., 2003]

3. Method of Calculation

We use large unit cell in the intermediate neglect of differential overlap (LUC-INDO) to obtain a self-consistent solution for the valence electrons in bulk phases of GaAs, at various lattice constants. In a first step, we calculate the lattice constant.

We choose the large unit cell of eight atoms with zinc-blende structure. The calculations are carried by forming a cube of a side 3a where a is the lattice constant of the Bravais lattice. The number of Bravais lattices in this cube is 27 lattices. The interaction of the atoms in the central Bravais with the surrounding atoms up to the fourth neighbors is included.

These calculations require the determination of wave functions and positions of 864 electrons and 216 nuclei. We choose ZB phase since it has fewer atoms per unit cell, and is therefore computationally easier to treat.

In the band structure calculations, the valence electronic configurations assumed for the atoms of GaAs are: Ga $4s^2 4p^1$ and As $4s^2 4p^3$. The semicore 3d electrons of Ga were found to have as valence electrons and essential to describe accurately structural properties. Spin-orbit splitting will be used to obtain the original nonsplit levels, Experimental spin-orbit splitting Δ_{so} is given the value 0.341 eV for diamond [Aspnes and Studna, 1971].

The Fock matrix elements (F_{pp}) in their final forms in the LUC-INDO formalism are used in this work [Radi *et al.,* 2007]:

$$F_{pp(0)} = U_{op,op} - \sum_{A \neq B} \sum_{v} Z_B \gamma_{AB}^{ov} + \sum_{v} \beta_A^0 (S_{op,vp} - \delta_{ov}) + \sum_{r} \sum_{v} P_{rr}(0) \gamma_{AB}^{ov} - \frac{1}{2} \sum_{v \neq 0} P_{pp}(0) f(x) \gamma_{AA}^{ov} - \frac{1}{2} \sum_{r} P_{rr}(0) (\phi_p^r \phi_r^o | \phi_p^o \phi_r^o) \tag{1}$$

$$F_{pq(0)} = \sum_{v} \beta_{AB}^0 S_{op,vp} - \frac{1}{2} \sum_{v} P_{pq}(0) f(x) \gamma_{AB}^{ov} \tag{2}$$

For p and q on different atomic centers, and

$$F_{pq(0)} = \sum_{v} \beta_{A}^{0} S_{op,vp} - \frac{1}{2} \sum_{v \neq 0} P_{pq}(0) f(x) \gamma_{AA}^{ov} + \frac{1}{2} P_{pq}(0)[(\phi_{p}^{o}\phi_{q}^{o} | \phi_{r}^{o}\phi_{s}^{o}) - (\phi_{p}^{o}\phi_{r}^{o} | \phi_{s}^{o}\phi_{q}^{o})] \tag{3}$$

for p and q on the same atomic center.

where β_{AB} is the bonding parameter, P is the density matrix, Z is the nuclear charge, S_{pq} is the overlap integral for atomic function ϕ_q and ϕ_p, γ_{AB}^{ov} is the average electrostatic repulsion between any electron on atom A and any electron on atom B, δ_{ov} is the Kronecker delta and U_{pp} is the local core matrix element and can be written as [Pople and Beveridge, 1970]:

$$U_{pp} = -\frac{1}{2}(I_p + A_p) + (Z_A - \frac{1}{2})\gamma_{AA} \tag{4}$$

where I_p and A_P are the ionization potential and electron affinity, respectively, *f(x) is* the modulating function and is given by [Szymanski, 1984]

$$f(x) = \left(\frac{\sin x}{x} \right)^2 \tag{5}$$

for the 8 atom LUC x is given by

$$\mathrm{x} = \frac{\pi \, \mathrm{R}_{\mathrm{AB}}}{\mathrm{a}} \tag{6}$$

R_{AB} is the distance between the atom A at the central lattice o and the atom B at the v lattice.

Computer programs are prepared to perform computations using FORTRAN as a programming language. Many subroutines are written to simulate the crystalline solids. Position and properties of atoms, which compose these crystals, are entered as input data. The final modified LUC-INDO k=0 equations are embodied in these computer routines and solved by iterative methods.

4. The Results and Discussion

4.1 Choice of Parameters

Empirical parameters in INDO method include the orbital exponent ζ the Slater-type orbital, the bonding parameter β, the electronegativity of s-orbital E_s, and the electronegativity of p-orbital E_p. The main assumptions of these methods can be summarized by considering only valence electrons, replacing the overlap matrix by unit matrix, neglecting differential overlap in two-electron repulsion integrals, reducing the remaining set of two-electron integrals to one value per atom pair, neglecting monatomic differential overlap in the interaction integrals involving the cores of other atoms, and finally taking diatomic off-diagonal core matrix elements to be proportional to the corresponding overlap integrals [Abdulsattar and Al-Bayati, 2007].

These parameters are varied firstly to give nearly the exact value of the equilibrium lattice constant, cohesive energy, energy gap and valence bandwidths. The optimum values of these parameters used for GaAs in the present work are listed in Table 1.

Table 1. Present parameter sets of GaAs for LUC-INDO.

Parameter	Ga	As
$\zeta_{4s,4p}(\mathrm{a.u})^{-1}$	١.7038	2.3240
β (eV)	-5.7127	-4.0113
E_{4s} (eV)	14.9800	19.4300
E_{4p} (eV)	11.9000	16.000

4.2 The electronic and structural properties

Based on the total energy results, we obtained the cohesive energy (E_{coh}) as follows:

$$-E_{coh}=E_{tot}/8-E_{free}-E_0 \tag{7}$$

where E_{tot} is the total energy, E_{free} is the free atom sp shell energy, and E_0 is the zero – point vibration energy. In this work E_{free} =113.394 eV, and this value is taken from ionization potential of GaAs, so E_0= 0.067 eV, is calculated by the formula $E_0= (9/8)\ k_B\Theta_D$ (per atom) [Born and Huang, 1954], where k_B is Boltzmann constant, with Θ_D being the Debye temperature which is equal to 360 K [Pässler, 1999].

The results of cohesive energies as a function of lattice constant are obtained by the above method at 0 k and zero pressure. Figure 1 displays the cohesive energy versus lattice constant of GaAs, obtained using the same set of parameters. The curve is fitted to the Murnaghan's equation of state [Ziambaras and Schröder, 2003], from which we obtain the equilibrium lattice constant a_0, the bulk modulus B, and its derivative B'_0.

The results of structural and electronic properties of GaAs are given in Table 2, along with the experimental measurements and other results. We notice that the lattice constant and the cohesive energy for GaAs are in a good agreement with experimental results. For example, the calculated lattice constant and the cohesive energy are 5.6542Å and -

6.50 eV/atom, respectively, in good agreement with the corresponding experimental values of 5.65 Å and -6.52 eV/atom, respectively (see Table 2), The lattice constant for GaAs presented here is slightly larger than experimental calculations, the difference between the experimental data and our results are very small, i.e., only 0.0042 Å. The results of B and B'_0 are essentially identical to those obtained by using other method. Figure 2 shows the band structure in the vicinity of the energy gap of GaAs throughout the first Brillouin zone [Vurgaftman *et al.*, 2001].

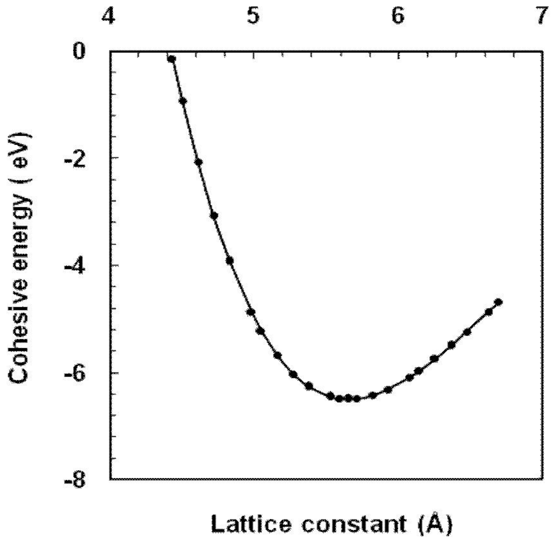

Figure 1. Cohesive energy as a function of lattice constant for GaAs.

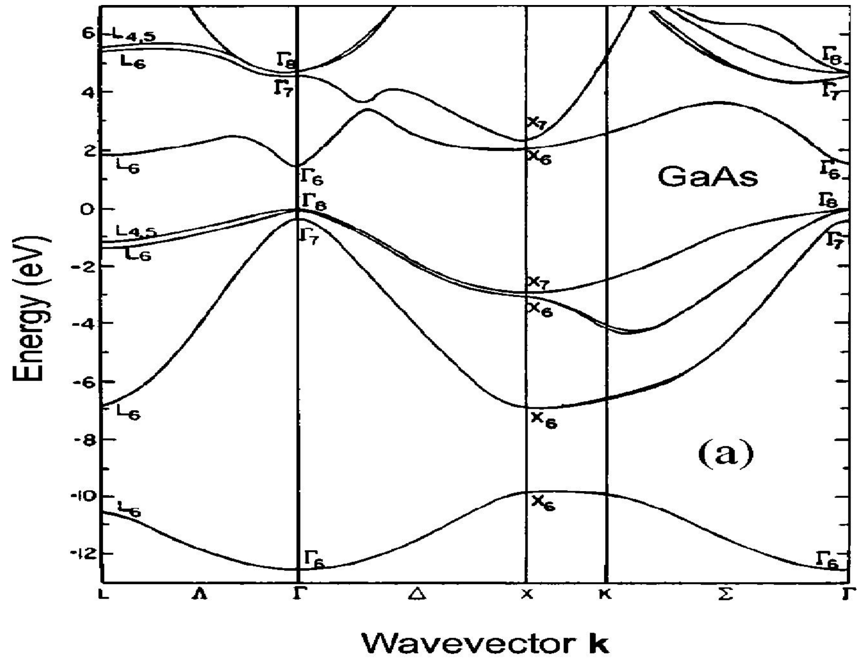

Figure 2. Diagram of the band structure in the vicinity of the energy gap of GaAs throughout the first Brillouin zone [Vurgaftman *et al.*, 2001].

The valence band in the zinc-blende structure, such as that for GaAs consists of four subbands when spin is neglected in the Schrodinger equation, and each band is doubled when spin is taken into account. Three of the four bands are degenerate at k = 0 (r point) and form the upper edge of the band, and the fourth band forms the bottom. Furthermore, the spin-orbit interaction causes a splitting of the band at k = 0.

The conduction band consists of a number of subbands. The bottom of the conduction band can appear at the center k = 0, or off center along different k axes. Symmetry considerations alone do not determine the location of the bottom of the conduction band. The conduction-band minimum can be aligned or misaligned in k-space in determining the band gap.

We obtain an energy gap (E_g) of 1.91eV which is larger than the other results [Ye, 2008; Madelung, 1982] (see Table 2 for comparison); this is, mainly, a consequence of two approximations made in this calculation. First, the core structure was ignored, through some compensation results from using semiempirical parameters. Second, using minimal basis set atomic orbitals (without considering any excited levels). However, the INDO method predicts a one - electron eigenvalues band gap that is too large and conduction bands that is much narrower than the band model values. This result in energy gap for GaAs bears significant consequences when carriers transfer between this minimum gap in that momentum is conserved for energy gap

The valence-band maximum (E_v) occurs at Γ, The total valence bandwidth or the difference between the top of the valence bands (Γ_{15v}) and the lowest energy of valence band (Γ_{1v}) is 13.22 eV for GaAs. The obtained total valence bandwidth is in agreement with previous results. Our work gives a value of the conduction bandwidth to be 6.709eV, but no experimental results are found to the conduction bandwidth of the zb of GaAs.

Hybridization state show an increasing s-state occupation and p-state occupation with the increasing atomic number of the compound where the occupation of s and p orbital of arsenide is larger than of that for gallium. This reflects the weaking of the directional character of these bonds represented by the sp^3 hybridized orbitals with increasing the atomic number.

Table 2. Electronic and structural properties calculated within LUC-INDO method at ground state (zero pressure and 0 temperature) compared to experiment and other references.

Property	**Present**	**Experimental**	**Others**
Lattice constant (Å)	5.6542	5.65 [Madelung, 1982]	5.56 [Lee *et al.*, 1997] 5.51 [Remediakis and Kaxiras, 1999]
Cohesive energy (eV/atom)	- 6.50	- 6.52 [Juan and Kaxiras, 1993]	- 6.21, - 6.51 [Lee *et al.*, 1997]
Conduction bandwidth (eV)	6.709	.....	.....
Valence bandwidth (eV)	13.22	13.21 [Froyen and Cohen, 1983]	12.69 [Froyen and Cohen, 1983]
Energy gap (eV)	1.91	1.42 [Ye, 2008] 1.52 [Madelung, 1982]	1.062 , 1.717 [Remediakis and Kaxiras, 1999]
Hybridization state of Ga	$s^{0.7435}p^{2.0706}$	s^2p^1	.....
Hybridization state of As	$s^{0.9667}p^{4.2966}$	s^2p^3	.....
Bulk modulus (GPa) B	٧٩.٨	74.7 [Madelung, 1982]	75.4, 60.4 [Lee *et al.*, 1997]
B'_0	٣.٦٨٦	3.36 [Zhang, and Cohen, 1987]	.....

The energy eigenvalues for GaAs crystal are calculated at various high symmetry points of the Brillouin zone and the results are listed in Table 3, along with the results of the GW method [Rohlfing *et al.*, 1993]. We also include experimental data in Table 3, for comparison to theoretical results. For folding reasons, the electronic structure is only studied at Γ and X points of the fcc Brillouin zone. The most important band states are considered. They are the valence bands Γ_{1v}, Γ_{15v}, X_{1v}, and X_{5v}. In the case of the conduction bands we consider the states X_{1c}, X_{5c}, Γ_{15c}, and Γ_{1c}. The agreement between the present calculations, LUC-INDO results, and the experimental data is in a good agreement.

Table 3. Eigenvalues (in electron volts) at Γ and X high-symmetry points from the present (LUC-INDO) method, compared with other results.

Symmetry point	**LUC–INDO**	**Experimental [Rohlfing *et al.*, 1993]**	**Theoretical [Rohlfing *et al.*, 1993]**
Γ_{1v}	-13.22	-13.21	-12.69
Γ_{15v}	0.0	0.0	0.0
Γ_{1c}	2.251	1.52	٠.٥٧
Γ_{15c}	6. 41	4.61	3.57
X_{1v}	-9.521	-10.68	-10.37
X_{5v}	-6.88	-6.81	-6.79
X_{1c}	3.90	1.90	1.8
X_{5c}	8.96	----	10.33

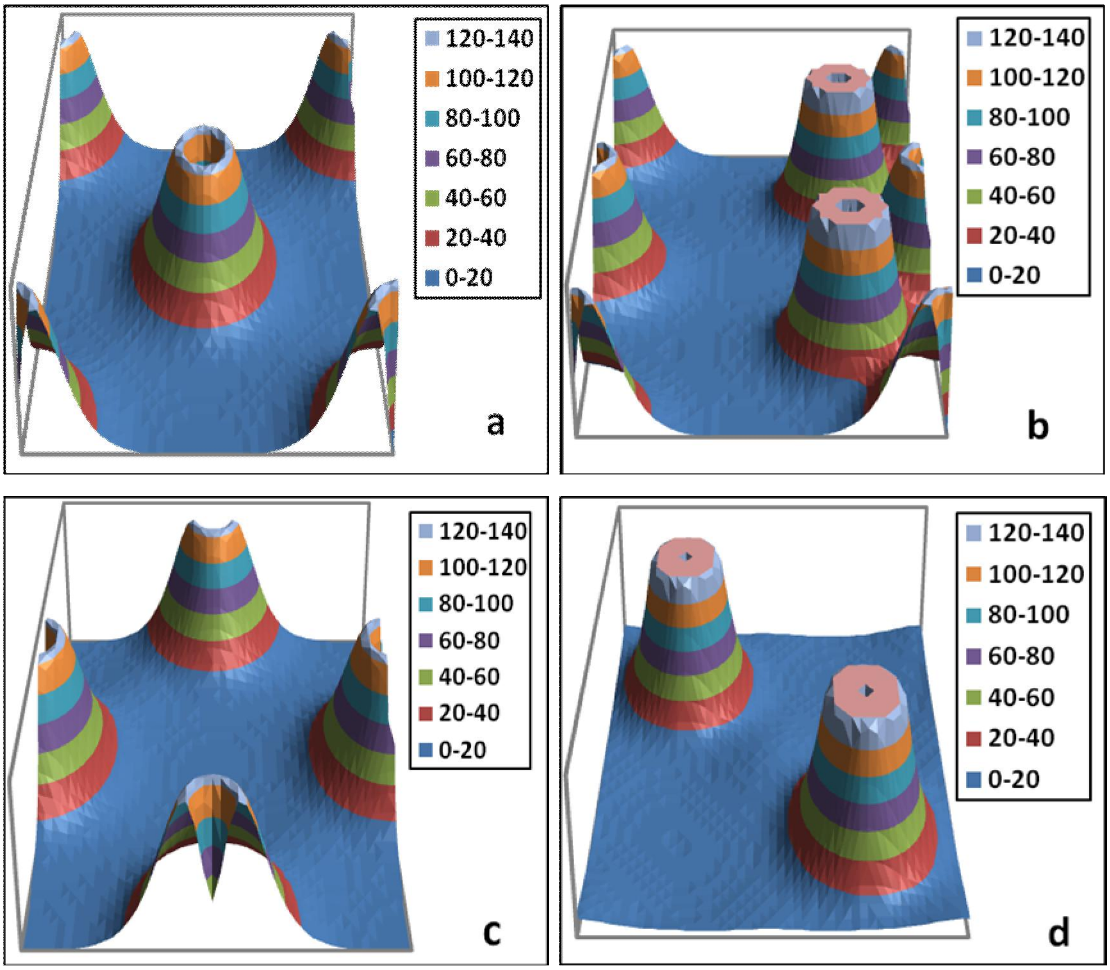

Figure 3. The valence charge density for GaAs at zero pressure in the planes (a) (100), (b) (110), (c) (200), and (d) (400).

The total valence charge densities for GaAs are displayed along the Ga-As bonds in the (100), (110), (200), and (400) planes in Figure 3. This figure also shows the charge density associated with the dangling bond lab at the As site. Figure 3a shows the charge density for the (100) surface, where a buildup of charge density along the GaAs bond length on the surface is clearly visible. LUC- INDO studies have revealed that this method give a reasonable description of the exchange-correlation potential in regions close to a molecule.

. 4.3 Effect of pressure on the properties

The pressure is a continuously varying parameter which can be used in systematic studies of the properties of solids as a function of interatomic distances. An interesting phenomenon that may occur at the applied pressure is a sudden change in the arrangement of the atoms, i.e., a structural phase transition**.** The effect of pressure on the electronic structure and other properties can be calculated from the present theory and computational procedure. The conversion from pressure dependence to the relative lattice change is performed using the following equation [Wang *et al.*, 2006]:

$$\mathrm{P} = \frac{\mathrm{B}_0}{\mathrm{B}_0'}\left[\left(\frac{V_0}{V}\right)^{\mathrm{B}_0'} - 1\right] \tag{8}$$

where V is the lattice volume at pressure P, V_0 is the equilibrium volume at zero pressure, B_0 the bulk modulus equal to 79.8 GPa, and its pressure derivative, equal to 3.686. We use a pressure up to 14 GPa, because this structure transforms to another phase, Cmcm structure, when pressure exceeds nearly 14 GPa [Nelmes and McMahon, 1998]. The calculated lattice constant as a function of pressure is shown in Figure 4. The relative pressure changes of the unit cell constant were found to be linear.

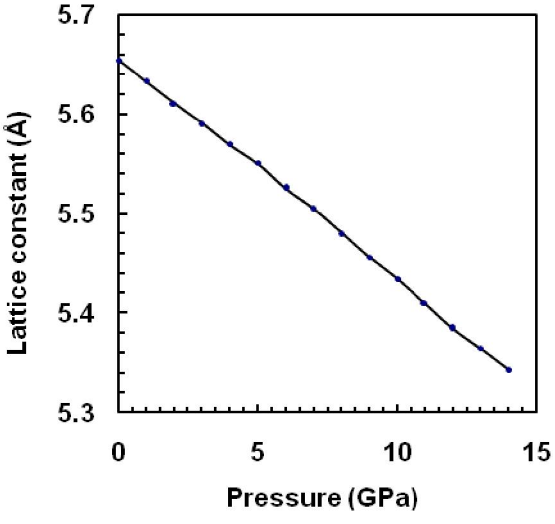

Figure 4. Lattice constant as a function of pressure for GaAs.

The pressure dependence of the cohesive energy and the bulk modulus are illustrated in Figure 5. It is shown that the absolute value of the cohesive energy decreases as the pressure increases. On the other hand, the bulk modulus increases linearly with pressure.

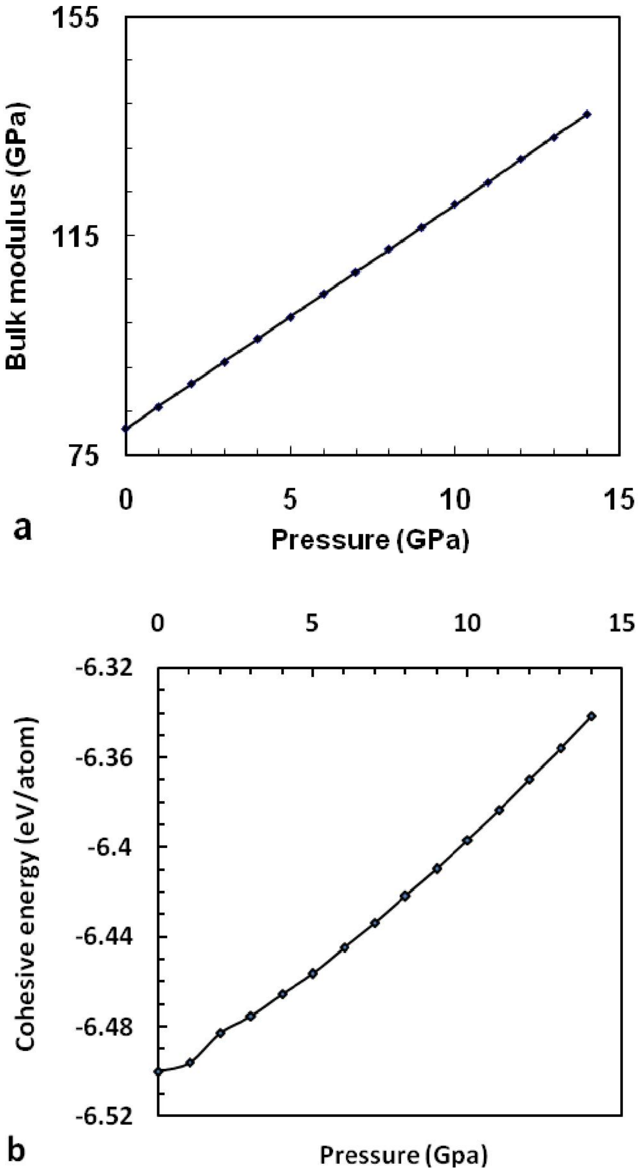

Figure 5. Effect of pressure on (a) the bulk modulus, and (b) Cohesive energy of for GaAs.

The pressure derivative of the high symmetry points (Γ_{1v}, Γ_{15v}, X_{1v}, $X_{5v,}$ X_{1c}, X_{5c}, Γ_{15c}, and Γ_{1c}) is shown in Figure 6, from this figure one can see that the eigenvalues at conduction band (X_{5c}, Γ_{15c}, Γ_{1c}, X_{1c}) are increase with pressure, whereas eigenvalues at valence band (X_{5v}, X_{1v}, Γ_{1v}) decrease with pressure. However, the decrease of X_{5v}, $X_{1v,}$ and Γ_{1v} with pressure is very small.

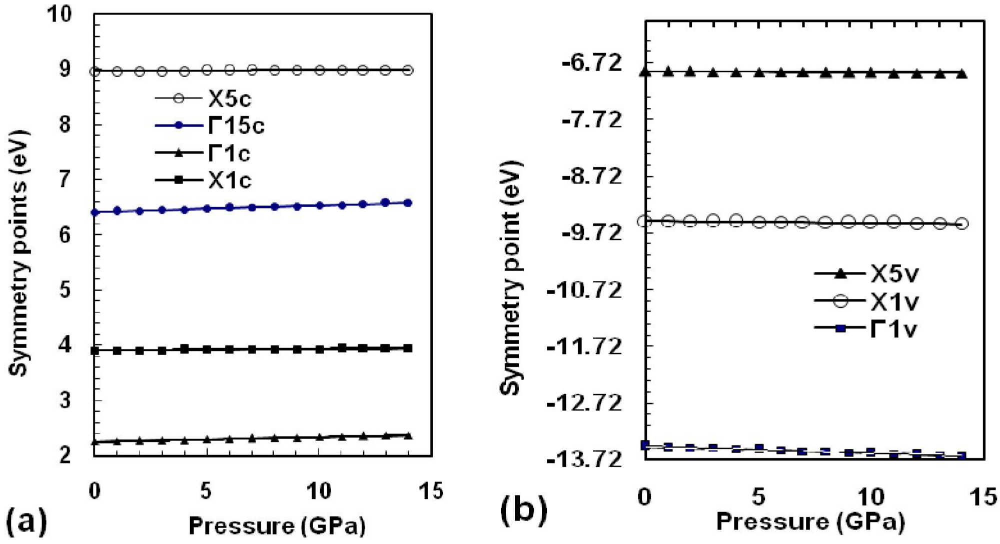

Figure 6. Effect of pressure on the high symmetry points in (a) conduction band (X_{5c}, Γ_{15c}, Γ_{1c}, X_{1c}), and (b) valence band (X_{5v}, X_{1v}, Γ_{1v}).

The pressure derivative of the direct band gap is shown in Figure 7, from this figure we can see that the direct band increase with the increase of pressure. The predicted effect of pressure on the valence bandwidth and conduction bandwidth is illustrated in Figure 8. The valence bandwidth increases with the increase of pressure, while the conduction bandwidth decreases with the increase of pressure. Our calculations give pressure derivative of ~ 0.136 eV/GPa for the valence bandwidth, and ~ -0.63 eV/GPa for the conduction bandwidth.

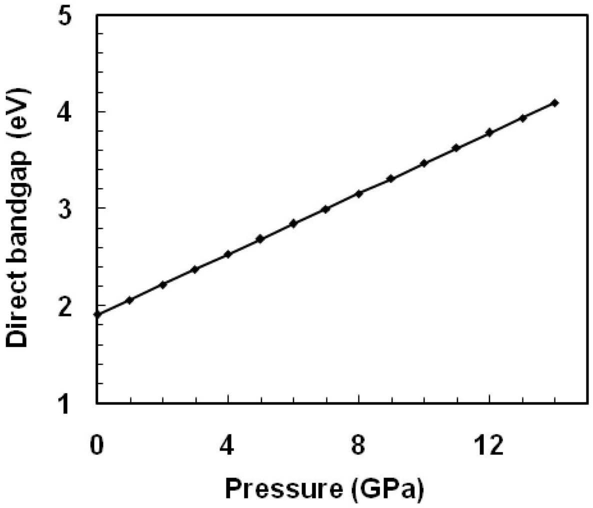

Figure7. Effect of temperature on direct gaps for GaAs, calculated within the LUC-INDO method

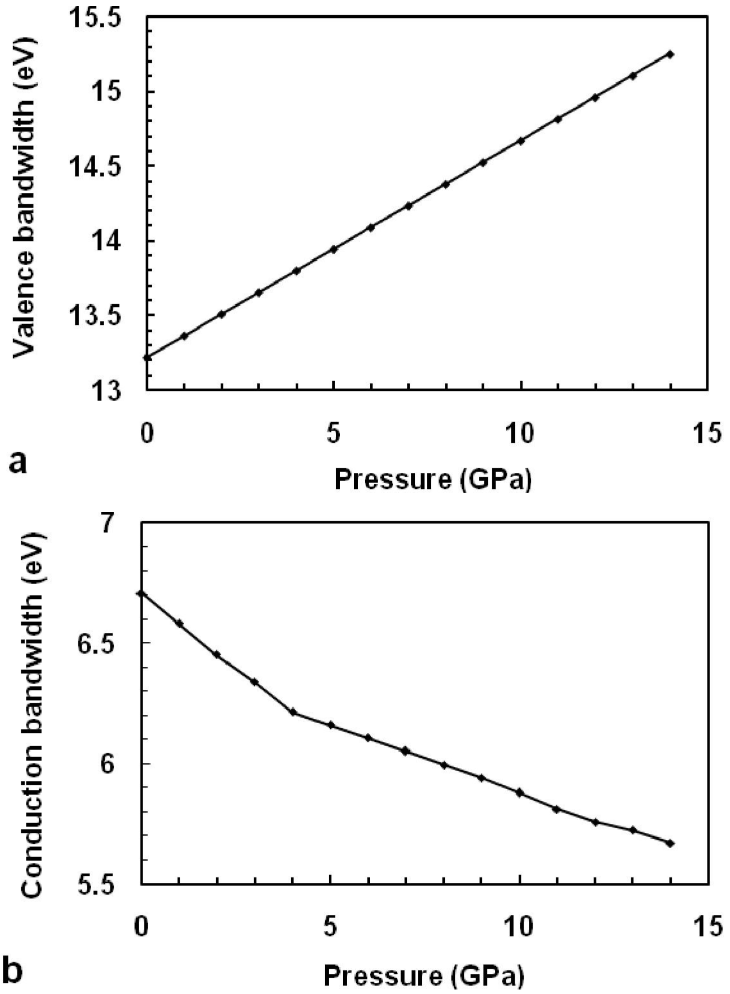

Figure 8. Effect of pressure on (a) the valence bandwidth, and (b) conduction bandwidth.

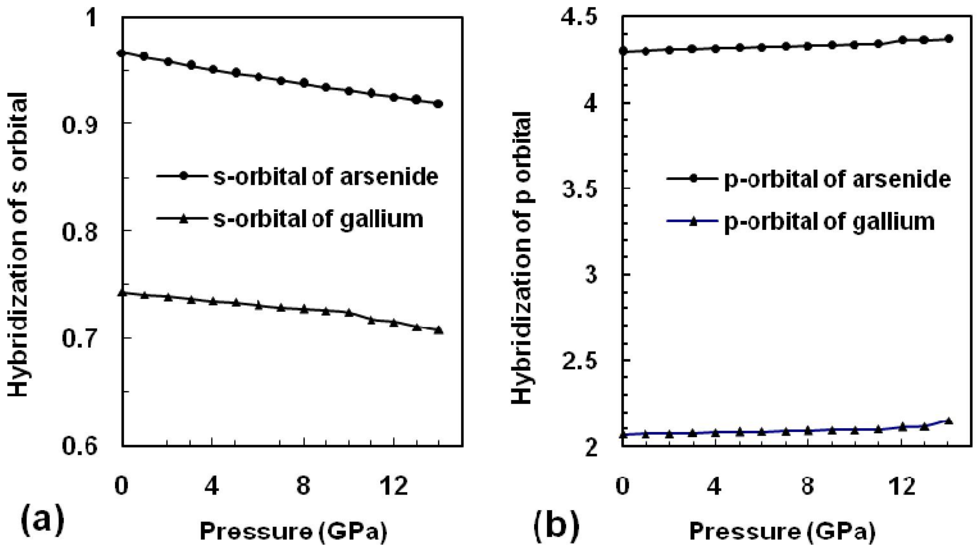

Figure 9. Effect of pressure on the hybridization of (a) s- state and (b) p-state.

We found that the s- state occupation for Ga and As decreases with the increase of pressure, whereas the p states occupation for Ga and As increases in this case. The occupation of s and p states for Ga and As with pressure is shown in figure 9. The increase of pressure causes an increase of the probability of electron transition from s-orbital to p-orbital. This phenomenon is known and leads to a phase transition due to the change of electronic distribution such as the s-d transition in alkali metals [Takemura and Syassen, 1983].

Conclusions

We applied large unit cell within the intermediate neglect of differential overlap method to studies the structural and electronic properties of GaAs semiconductor under effect of pressure. The properties obtained are in very good agreement with the existing experimental data and with others results except the energy gap which is greater than the experimental data, this difference is due to the neglect to the core states and to the approximations incorporated with the computational formalism and INDO methods neglect a large number of two electron integrals. The increasing of pressure on GaAs is predicted to cause the following effects; an increase of the valence bandwidth and energy gap, a decrease of the conduction bandwidth. In addition to this we have found that the parameter values resulting from the fittings by this method are as a rule physically reasonable and the present self-consistent semiempirical theory can be applied successfully to account for the band structure and physical properties of semiconductors using appropriate parameters. Transforming the calculations to larger unit cells gives generally acceptable results. Relativistic effect is added to the calculation of the energy gap, also zero point energy is added to the calculation of the cohesive energy. Finally, this method is shown to give a good description to the charge density of GaAs and it is expected that this method could give reliable description for other materials that have zinc-blende and cubic structures.

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