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Density functional theory study on pressure induced structural transformation, elastic properties and electronic structure of gallium arsenide (GaAs)

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ABSTRACT: The structural phase transformation under induced pressure of the GaAs- zinc blende (ZB) phase to rock salt (RS) phase, elastic properties and electronic structure of the stable (ZB) phase are studied under the framework of the density functional theory (DFT). When pressure is increased up to 10.7 GPa, transition from the GaAs-ZB to GaAs-RS structure occurs and the dependence of volume decrease of ZB to RS structure at the transition pressure is 14.11%. The elastic parameters such as elastic constants C_{11}, C_{12}, C_{33}, Zener anisotropic factor (A), Kleinmann parameter (ζ), Poisson's ratio (υ), Youngs modulus (Y) and energy band gap of GaAs-ZB structure shows a systematic variation with increase in pressure upto transition pressure. The results are found to be in consistent with other experimental and theoretical results.

KEYWORDS: Density Functional Theory (DFT); Energy band structure; Elastic properties; Phase transition.

1 INTRODUCTION

Gallium arsenide (GaAs) is a group III-V binary compound semiconductor utilized in the electronics and telecommunications industries and in the military science [1, 2]. Gallium arsenide chips are found in products such as night vision telescopes, discrete microwave circuitry, and room temperature lasers. It is superior semiconductors to silicon for optoelectronic devices due to its ability to handle signals at higher frequencies, at the same time generate lower noise [3, 4]. It is the most technologically important compound semiconductor material which has been intensively investigated in recent years. The study of electronic and structural properties helps us to understand, characterize and predict the mechanical properties of materials in the surroundings under extreme conditions. This study plays an important role in physical condensed matter [5]. With technological development, study of structural properties, phase diagram and high pressure phases of GaAs has aroused considerable scientific interest in the past decades. Froyen and Cohen [6] first reported the structural phase of GaAs in 1983. The structural transformation in GaAs was also investigated by Besson *et al* [7] and Weir *et al* [8] using the single-crystal x-ray absorption spectroscopy and elastic neutron scattering. Studies on electronic structures, high-pressure properties have been reported by various groups [9-12]. In literature, works on the phase transformation, band structure, density of states (DOS) and elastic properties with variation of pressure is still rare. To the best of our knowledge none of the papers in open literature has considered the variation of energy band gap and elastic properties from the induced pressure perspective and investigated the behavior of the same with the available experimental data. The present paper is mainly focused on study of the phase transition from the zinc-blende to rocksalt structure, band structure and elastic properties of GaAs with increasing pressure using WEIN2K code based on DFT. This paper is organised as follows: Section 2 describes the theoretical and computational method used in this study. The results are discussed in section 3 and conclusions are given in section 4.

2 THEORETICAL AND COMPUTATIONAL METHOD

The calculation of GaAs has been performed with modified Becke-Johnson (mBJ) [13] exchange potential using full-potential linearised augmented plane wave (FP-LAPW) method [14] within the framework of density functional theory (DFT) [15, 16, 17] with Perdew-Bruke-Ernzerhof-Generalized Gradient Approximation (PBE-GGA) for the exchange correlation potential [18] as implemented in the WIEN2K code [19]. Within DFT formalism, the total energy can be expressed as a functional of density of electron system, ρ and can be written by the following functional,

$$E[\rho] = T_o[\rho] + V_H[\rho] + V_{xc}[\rho] + V_{ext}[\rho] \qquad (1)$$

where, $T_o[\rho]$ is the kinetic energy of a non-interacting electron system, $V_H[\rho]$ and $V_{XC}[\rho]$ are the Hartree and exchange-correlation contributions to the energy and $V_{ext}[\rho]$ is the energy due to the external potential of the system. Thus the corresponding Hamiltonian called the Kohn-Sham Hamiltonian is

$$\begin{aligned}\widehat{H}_{KS} &= \widehat{T}_o + \widehat{V}_H + \widehat{V}_{XC} + \widehat{V}_{ext} \\ &= -\frac{\hbar^2}{2m_e}\vec{\nabla}^2{}_i + \frac{e^2}{4\pi\varepsilon_o}\int\frac{\rho(\vec{r}^{\,/})}{|\vec{r}-\vec{r}^{\,/}|}d\vec{r}^{\,/} + V_{XC} + V_{ext}\end{aligned} \qquad (2)$$

The exact density of N electron system can be expressed in ground state by:

$$\rho(\vec{r}) = \sum_{i=1}^{N} \phi_i(\vec{r}) * \phi_i(\vec{r})$$

where the single particle wave functions ⍰*ᵢ*(r*)* are the N lowest energy solutions of the Kohn Sham equation: $\hat{H}_{ks}$⍰ᵢ = ⍰ᵢ⍰ᵢ of the N electron system.

These equations can be solved self consistently in an iterative process. In this method, the lattice is divided into non-overlapping spheres (called atomic or muffin tin sphere) surrounding each atomic sites and an interstitial region [20]. Inside the muffin tin (MT) region, the potential is a product of radial function and spherical harmonics and expanded up to order l = 10. For the interstitial regions that are outside the muffin tin spheres, the potentials are expanded in plane waves. 8000 k-points are used for the integration procedure as we find that above 8000 k-points the energy remains same and this 8000 k-points reduces to 256 irreducible k-points inside the Brillion zone including five high symmetry points W, L, Γ, X and K. Convergence is obtained at $R_{MT}K_{max}$ = 9.0 where R_{MT} is the atomic sphere radii and K_{max} gives the plane wave cut-off. The calculations are performed with the equilibrium lattice constants which are determined from the plot of the total energy against the unit cell volume by fitting to the Birch-Murnaghan equation of states [21].

3 RESULTS AND DISCUSSION

3.1 STRUCTURAL PROPERTIES

The total energy curve as a function of unit cell volume for GaAs in zinc-blende and rocksalt structure is shown in figure 1. It is clearly seen that ZB structure of GaAs is more stable than the RS structure which is in good agreement with previous results [22, 23, 24]. The obtained zero pressure equilibrium lattice constant (a_0) for GaAs-ZB structure is found as 5.74 A^o. This lattice constant corresponding to the optimized structure is slightly larger than experimental values as given in table 1. It has an error of about 1.8% which is quite acceptable under the 2% error and is used for further calculation. Thus the agreement between our result and other available theoretical and experimental data [25, 26, 27, 28, 29, 30] is well good indicating that our calculation can proceed for further study.

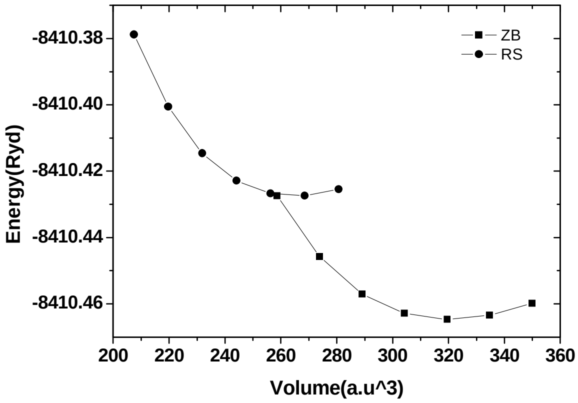

Fig.1. Energy versus volume for ZB and RS structure of GaAs.

Table 1. Lattice Constants, Bulk Modulus And Pressure Derivative Of Bulk Modulus Of ZB And RS Structure Of Gaas At Zero Pressure.

Structure		A_0 [A^0]	B_0 [Gpa]	$B_0^{/}$
ZB	Present Work	5.74	61.08	4.86
	References	5.65[a], 5.64[b],5.59[c]	60.4[d],74.7[a]	4.8[e],4.71[c],4.56[f]
RS	Present Work	5.39	71.10	4.90
	References	5.32[g],5.31[h],5.28[i]	73.54[c],69.95[i]	4.05[c],4.77[g],4.87[i]

Ref[a][22], Ref[25][B], Ref[26][C], Ref[27][D], Ref[28][E], Ref[29][F], Ref[23][G], Ref[24][H], Ref[30][I],

3.2 PHASE TRANSITION AND ELASTIC PROPERTIES

The zero temperature pressure induced phase transition between the GaAs-ZB structure and GaAs-RS structure has been determined using the usual condition of equal enthalpies i.e. H = E + PV. The enthalpy as a function of energy is shown in figure 2. The phase transition from ZB to RS structure is found to occur at a pressure of 10.7 GPa which is close to the experimental values [31, 32] and other theoretical results as shown in table 2.

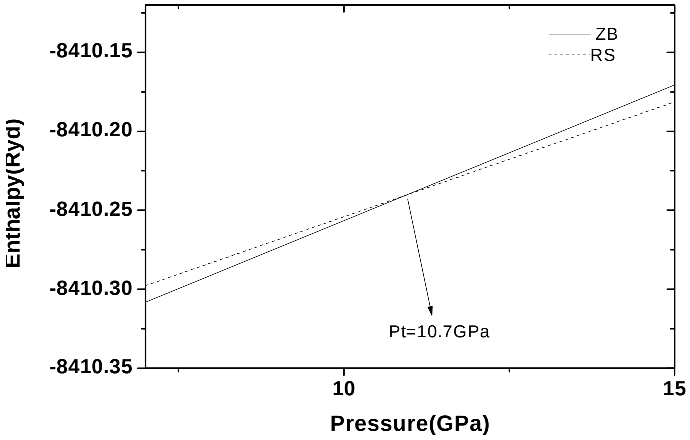

Fig.2. Enthalpy as a function of pressure.

Table 2. Transition pressure from ZB to RS in GaAs.

ZB-RS	Pressure [GPa]
Present work	10.7
Ref [7]	12±1.5
Ref [30]	10.5
Ref [31]	11.8
Ref [32]	12.3

To understand the volume collapse at the transition, the unit cell volume at different pressures (V_P) are normalised by dividing with volume at zero pressure (V_O). The normalised volume (Vp/Vo) of ZB and RS structure of GaAs at different pressure is shown in figure 3. With increase in pressure the relative volume is found to decrease for the two structures. During phase transition, the normalised volume of ZB phase is found to be occurring at 0.876 and for RS phase at 0.734. It is clearly seen that volume collapse occurs at 14.2% indicating that the ZB phase is more compressible than the RS phase.

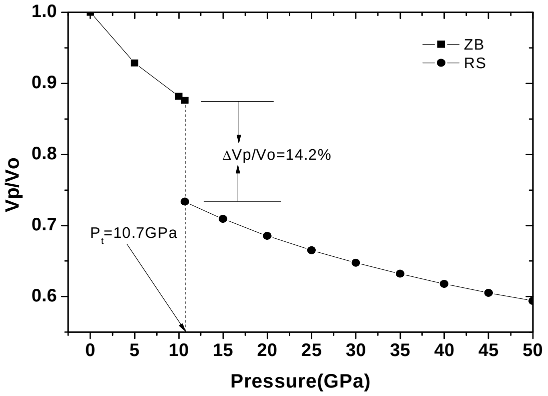

Fig. 3. Phase transition between ZB and RS structure of GaAs at 10.7 GPa pressure.

Since the transition pressure occurs at 10.7 GPa, the three independent observable elastic constants are obtained from 0 to 10 GPa pressure for ZB phase and 12 GPa to 25 GPa pressure for RS phase and is shown in figure 4. Figure 4 shows the linear increase in C_{11}, C_{12}, C_{44} value with increase in pressure for ZB phase. Also these values satisfy the mechanical stability conditions: $(C_{11}+2C_{12}) > 0$; $C_{11}C_{12} > 0$; $C_{44} > 0$; $C_{11} > 0$. In case of RS phase after transition pressure, even though there is a little variation in C_{44} value with linear increase in C_{11}, C_{12} values, and the stability conditions are found to be satisfied.

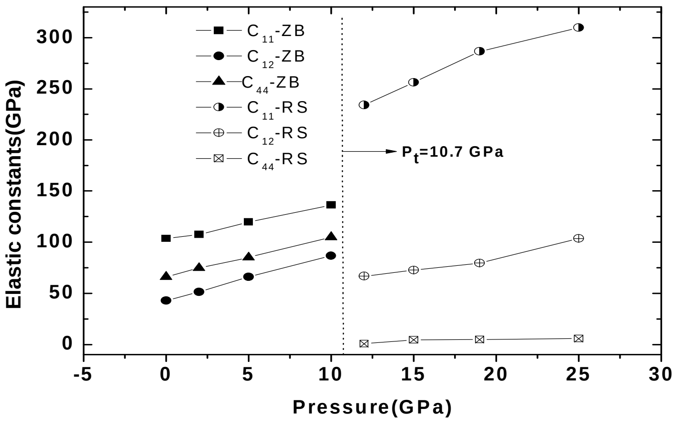

Fig. 4. Elastic constants (C_{11}, C_{12}, C_{44}) as a function of pressure for GaAs-ZB and GaAs-RS structure.

In this light of observations, we are confined our calculation for the elastic parameters on ZB structure up to a higher pressure of 10 GPa. The Zener anisotropic factor (A), Poisson's ratio (υ), Kleinmann parameter (ζ), Youngs modulus (Y), and Debye's temperature (θ_D) are important elastic parameters which determine the mechanical and thermal behaviour of a material.

The Zener anisotropic factor (A), Poisson's ratio (υ), Kleinmann parameter (ζ), Youngs modulus (Y) are calculated using the relation given by Mayer *et. al* [33]. The Zener anisotropy factor gives us an insight on the elastic isotropy of the material. For an elastically isotropic material, A = 1. If A > 1, it is stiffest along <111> plane body diagonals and when A < 1, it is stiffest along <100> cube axes. It is expressed as:

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \tag{3}$$

Kleinmann parameter describes the relative position of the cation and anion sub-lattices and is given by the relation:

$$\zeta = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}} \tag{4}$$

The Poisson's ratio gives us the stability of crystal against shear and provides a sharp criterion for differentiating the brittleness and ductility in solids and it is calculated using the relation,

$$\upsilon = \frac{1}{2}\left(\frac{B - (2/3)G}{B + (1/3)G}\right) \tag{5}$$

The Young's modulus is determined to measure the stiffness of the solid and is given by:

$$Y = \frac{9GB}{G + 3B} \tag{6}$$

where, $G = \frac{G_V + G_R}{2}$ is the isotropic shear modulus , G_v is the Voigt's shear modulus corresponding to the upper bound of G values, and G_R is the Reuss's shear modulus corresponding to the lower bound of G values. G_v and G_R can be expressed as

$$G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5} \tag{7}$$

$$G_R = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})} \tag{8}$$

Debye's temperature is an important parameter which determines the thermal characteristics of a material. Debye's temperature also gives us explicit information about lattice vibrations. It is calculated using the average sound velocity (υ_m) given by the common relation [34]

$$\theta_D = \frac{h}{k}\left[\frac{3n}{4\pi}\left(\frac{N_A \rho}{M}\right)\right]^{1/3} \upsilon_m \tag{9}$$

Where *h* is the Plank's constant, *k* is the Boltzmann constant, N_A is the Avogadro's number, *n* is the number of atoms per formula unit, *M* is the molecular mass per formula unit, *ρ* is the density and υ_m is given by [35]

$$\upsilon_m = \left[\frac{1}{3}\left(\frac{2}{\upsilon_t^3} + \frac{1}{\upsilon_l^3}\right)\right]^{-(1/3)} \tag{10}$$

where υ_t and υ_l are the transverse and longitudinal velocities respectively, which are obtained from Navier's equation [36] as

$$\upsilon_t = \sqrt{\frac{3B + 4G}{3\rho}} \tag{11}$$

$$\upsilon_l = \sqrt{\frac{G}{\rho}} \tag{12}$$

The calculated elastic parameters for ZB phase with variation of pressure up to 10 GPa are shown in figure 5(a) and figure 5(b). A consistent pattern of linear increase in elastic parameters with increase in pressure can be observed from these figures.

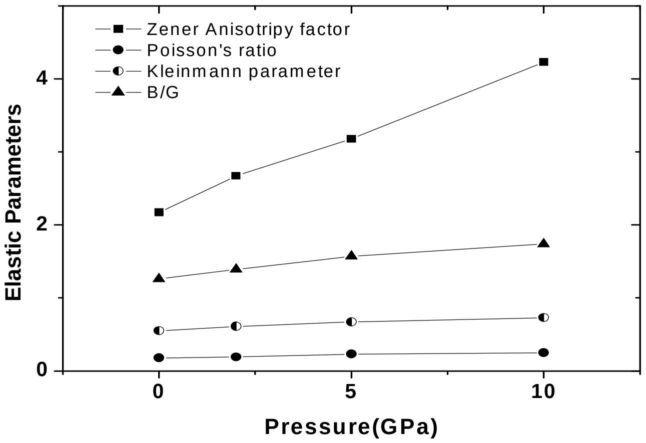

Fig. 5a. Elastic parameters (Zener anisotropic factor, Poisson's ratio, Kleinmann parameter and B/G ratio) as a function of pressure.

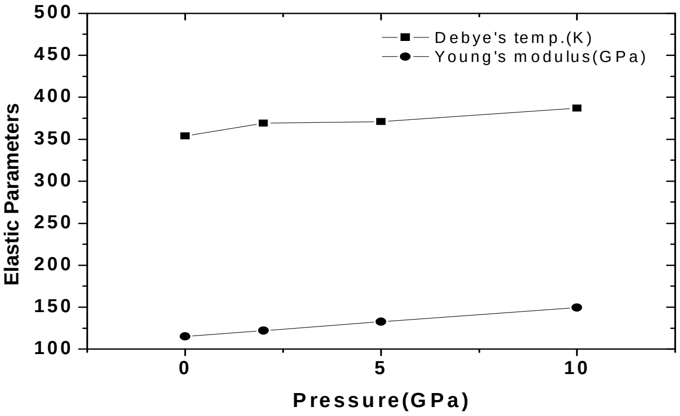

Fig. 5b. Debye's temperature and Young's modulus as a function of pressure.

The Kleimann parameter quantifies internal strain and thus indicates the relative ease of bond bending against the bond stretching. It also implies resistance against bond bending or bond angle distortion. In a system, minimizing bond bending leads to Kleinmann parameter, ζ = 0 and minimizing bond stretching leads to ζ =1. In the present study, the parameter ζ is found to be 0.55 to 0.73 with the variation of pressure, indicating the shrinkage in bond-stretching. Also the value of the Zener anisotropic factor varies from 2.17 to 4.23 with increase in pressure showing the degree of elastic anisotropy. The empirical malleability measure of a material is determined by the value of B/G [37]. A material is found to be brittle if B/G < 1.75 and ductile if B/G > 1.75. B/G value of the present studies varies from 1.26 to 1.74 with increase in pressure and hence it is found that GaAs-ZB structure is brittle and with increase in pressure it tends to become ductile. The larger the value of Young's modulus, the stiffer is the material and since the value of Y varies from 114.96 GPa to 149.456 GPa as pressure increases, we find that GaAs-ZB pahse becomes more rigid. Poisson's ratio gives us the degree of directionality of the covalent bonds. For covalent materials, $\upsilon = 0.1$, whereas for ionic materials, $\upsilon = 0.25$ [38]. Our calculations show that with increase in pressure the value of υ varies from 0.18 to 0.25 showing that with increase in pressure the ionic contribution to inter atomic bonding becomes dominant. Fu *et al* [39] reported that for central force solids the lower and upper limits for υ are 0.25 and 0.5 respectively. Our values also indicates that as pressure increases, inter atomic forces tends to be more central. The value of Debye's temperature is also found to vary from 354K to 387K suggesting that with increasing pressure the Debye's temperature also increases indicating stiffer lattice and better thermal conductivity.

3.3 BAND STRUCTURE AND DENSITY OF STATES

The energy band diagram of GaAs-ZB structure and GaAs-RS structure at zero pressure and zero temperature is calculated using mBJ as it gives us more accurate results closer to the experimental values and the results are given in figure 6(a) and figure 6(b) respectively. From figure 6(a) we observed that the conduction band minimum as well as the valance band maximum is located at the middle of the Brillioun zone, Γ point. From these observations we can conclude that the band gap of GaAs-ZB structure is direct band gap with an energy band gap of 1.3eV while the experimental value is 1.4 eV. Again from figure 6(b) we find that the conduction band crosses the Fermi level and lies within the valance band making the GaAs-RS structure metallic in nature. The reason for the metallic nature in the RS structure is due to broadening of the band with increase in pressure and overlapping of the filled valance band and conduction band.

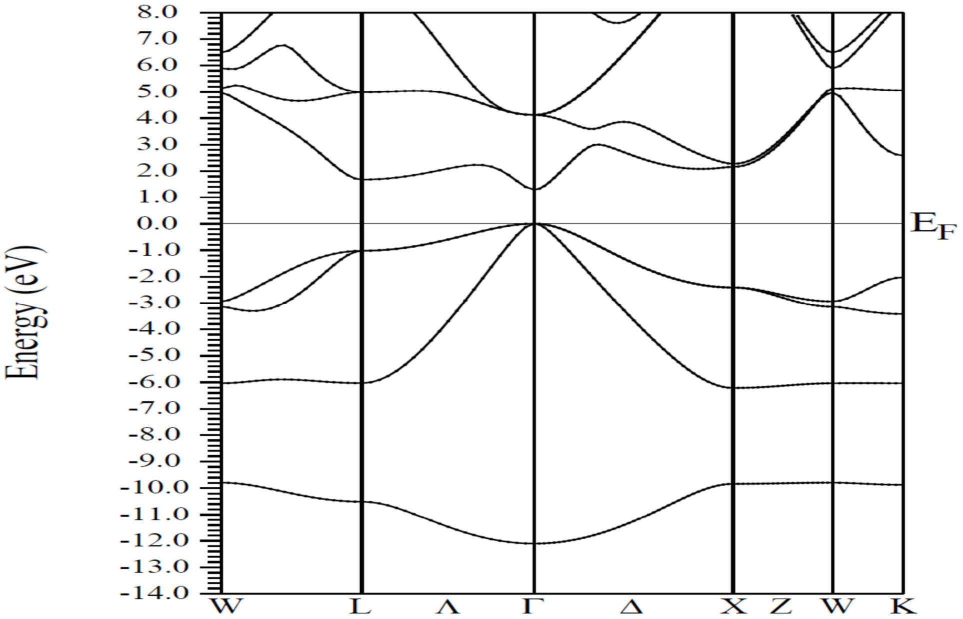

Fig. 6a. Band structure of GaAS-ZB structure.

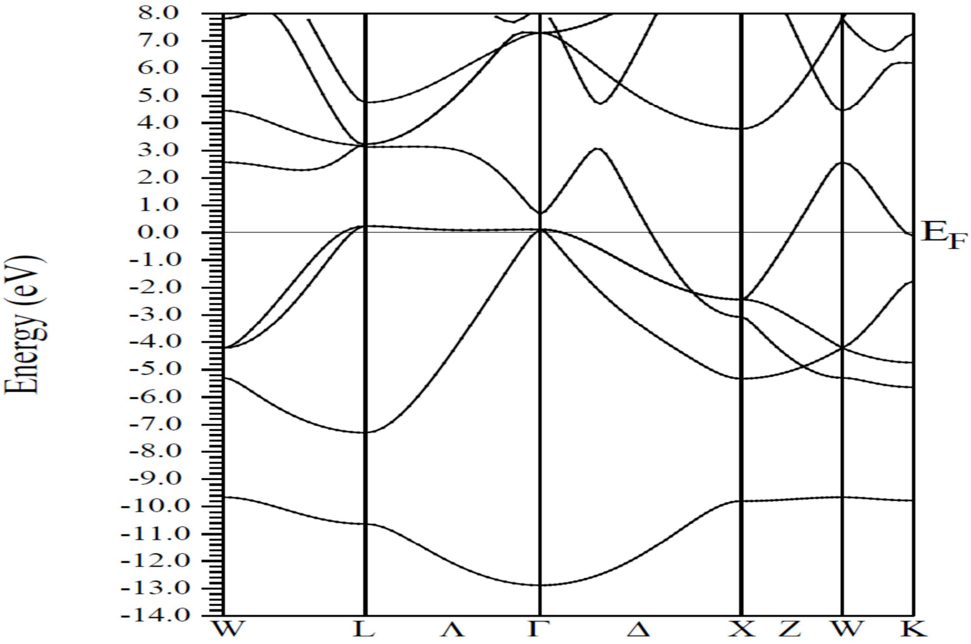

Fig. 6b. Band structure of GaAs-RS structure.

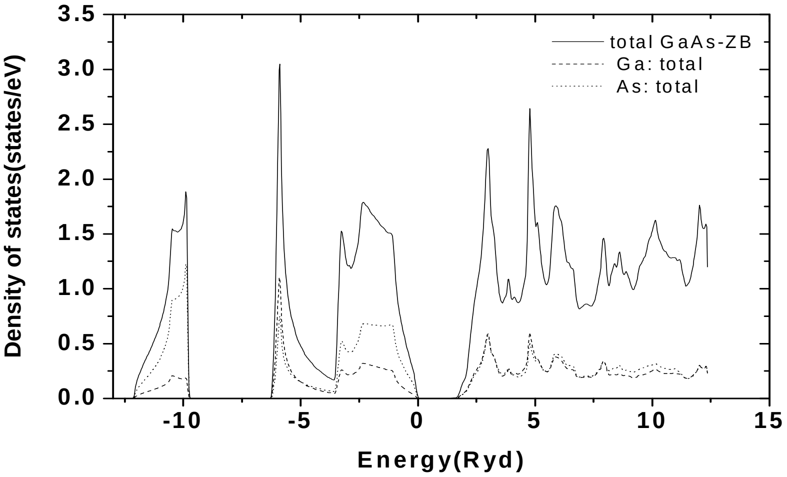

Fig. 7a. Total DOS of GaAs -ZB structure.

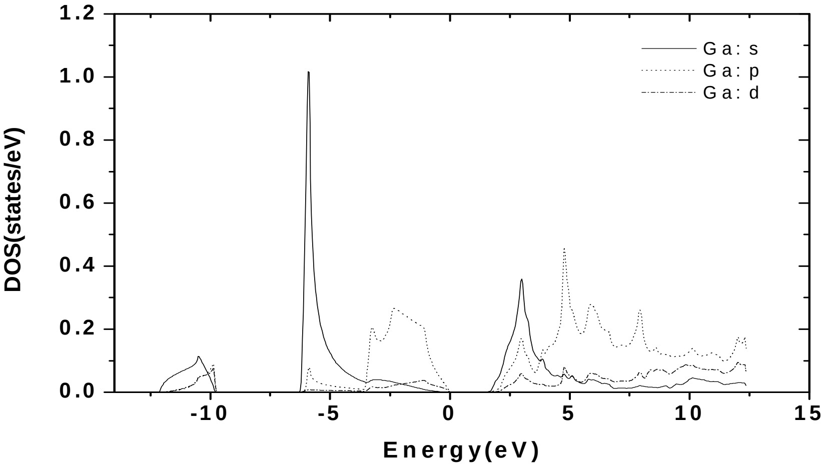

Fig. 7b. Partial DOS of Ga atom in GaAs-ZB structure.

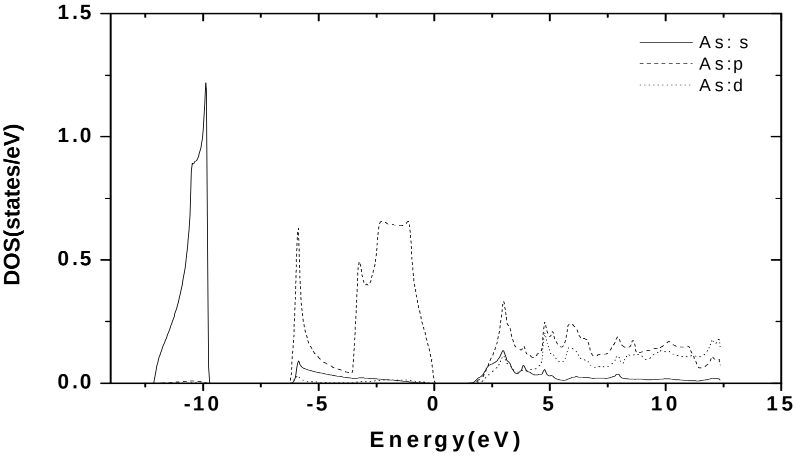

Fig. 7c . Partial density of As atom in GaAs-ZB structure.

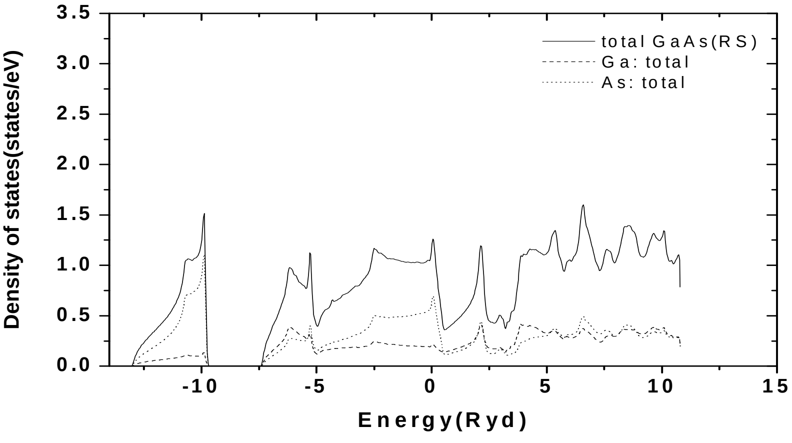

Fig. 8a. Total DOS of GaAs-RS structure.

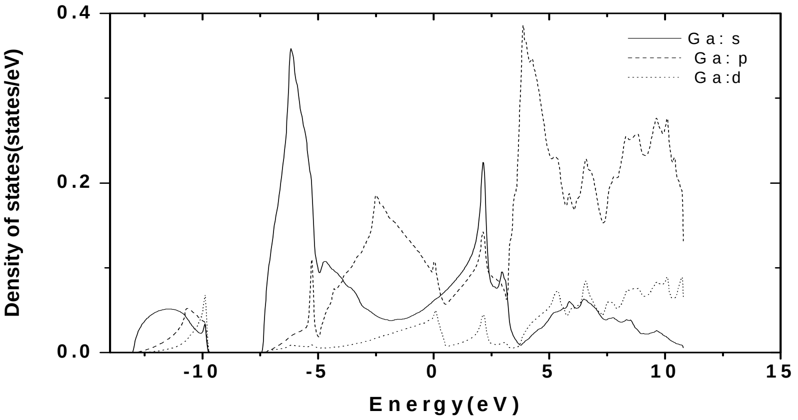

Fig. 8b. Partial DOS of Ga atom in GaAs-RS structure.

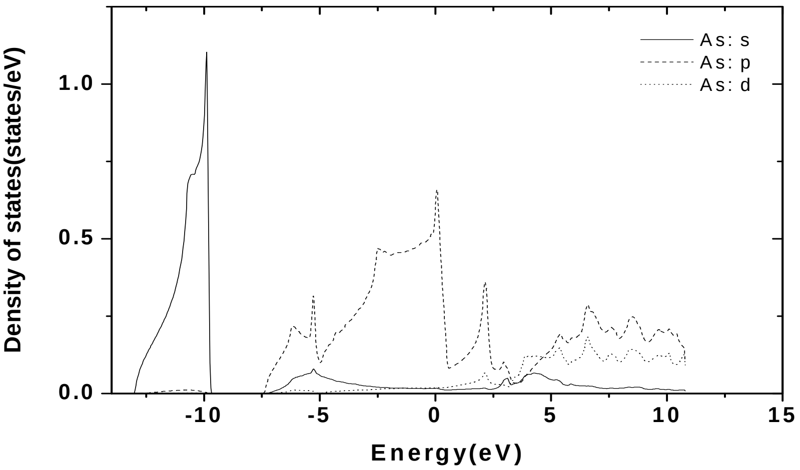

Fig. 8c. Partial DOS of As atom in GaAs-RS structure.

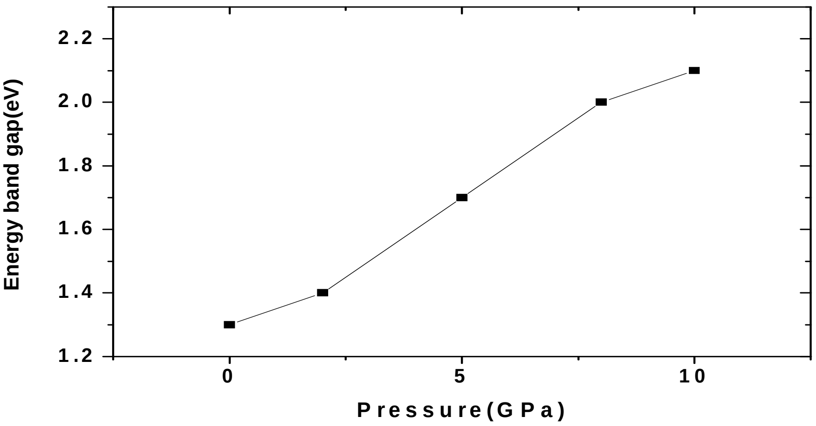

Fig. 9. Variation of energy band gap with pressure in GaAs ZB structure.

Figure 7(a,b,c) shows the total and partial DOS of GaAs in ZB phase and figure 8(a,b,c) shows the same in RS phase. From the partial DOS as shown in figure 7(b) and figure 7(c), one can observe that the lowest band appears in energy band diagram of ZB phase is mainly contributed from s-non metal (As atom) orbital and the valance band is mainly contributed by the s-metal (Ga atom) orbital and p-non metal (As atom) orbital with little contribution from the p-metal (Ga atom) orbital. The contribution of the s, p orbital of metal and non-metal in DOS in the lowest and valence band is found to decrease with increase in pressure. Similar behaviour is observed in partial DOS of GaAs-RS structure in figure 8(b) and figure 8(c) as the lowest band is mainly contributed by the s-non metal orbital while the valence band is mainly contributed by the p-non metal orbital and s- metal orbital with little contribution from the p-metal and d-metal orbital. An important observation in the energy band diagram of GaAs-RS structure is the crossing of the conduction band towards valence band and hence results in metalic nature. It is interesting to see the variation of band gap with pressure for the direct band gap in GaAs-ZB phase. These variations of the energy band gap with increase in pressure is shown in figure 9 and observe that with increase in pressure the band gap also increases. The resaon is that the energy eigenvalues corresponding to s, p, and d orbital's lies in the higher region with increasing pressure.

4 CONCLUSION

In this paper we present a detailed study of pressure induced structural transformation, elastic properties and electronic structure of GaAs. The phase transition from ZB to RS structure is obtained at 10.7 GPa and ZB structure is found to be more stable. During the phase transition, the relative volume of ZB structure occurs at 0.876 and the RS structure at 0.734 and volume collapses at 14.2% indicating that ZB structure of GaAs is more compressible as compared to RS structure. The calculated equilibrium lattice parameter, bulk modulus, pressure derivative of the bulk modulus and elastic constants are found to be in good agreement with the other experimental and theoretical studies. The elastic constants satisfy the mechanical stability condition from 0 to 10 GPa pressure for ZB structure and 12 GPa to 25 Gpa pressure for RS structure. The elastic parameters for the stable GaAs-ZB phase such as Zener anisotropic factor, Kleinmann parameter, Poisson's ratio and Youngs modulus show a systematic variation with increase in pressure up to 10 GPa pressure before transition. The GaAs-ZB structure is found to be direct band gap semiconductor of 1.3 eV and the band gap increases with increase in pressure.

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