

Electronic Structures of GaX(X=P, As) under Induced Pressure: A First Principle Study

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Abstract—A first principle study on the electronic structures of GaX (X=P, As) under induced pressure is performed using the modified-becke Johnson potential under the framework of Density Functional Theory. In the present calculation, GaP undergoes a phase transition from B3 to B1 phase at 21.9 GPa pressure with a volume collapse of 14.11% while GaAs undergoes a transition from B3 to B1 phase at 10.7 GPa pressure with a volume collapse of 14.2% indicating that B3 phase of both the compounds is more compressible than the B1 phase. The energy band diagram of GaP-B3 phase and GaAs-B3 phase show an indirect band gap of 2.33eV and a direct band gap of 1.3eV respectively while B1 phase for both the compounds show metallic nature which is in good agreement with other theoretical and experimental studies. Under induced pressure the indirect band gap of GaP-B3 phase and direct band gap of GaAs-B3 phase increases while in the B1 phase, the metallic nature of GaP and GaAs is retained and does not vary with pressure.

1. INTRODUCTION

The development in the field of optoelectronic devices and scientific applications of III-V compound semiconductors has led to its extensive study in recent years [1-3]. GaX (X=P, As) is a III-V compound semiconductor which is being considered of great technological importance due to its potential application in many optoelectronic devices such as light emitting diodes (LED) and laser diodes (LD)[4,5]. The study of the electronic and structural properties helps us in characterizing, understanding and predicting the mechanical properties of a material. Therefore the variation in the energy band gap under induced pressure help us for better understanding of these properties under extreme conditions of pressure.

In literature it has been reported that GaP and GaAs crystallizes in zinc-blende (B3) structure under ambient pressure conditions. In various studies it is reported that when pressure is applied the volume decreases and a structural phase transition to rock salt (B1) structure is found to occur [6-8].

The ab-initio study of the structural and electronic properties of a material has become more systematic and precise with the developments in the computer simulation. It helps us in better understanding and estimation of the properties of a material under induced pressure which are difficult to study

experimentally. Even though there have been many studies on the phase transition and electronic properties of GaP and GaAs, there have been few studies on the effect of pressure on the electronic structure of these compounds. The present paper is mainly focused on the study of the variation in the energy band gap under induced pressure in both B3 and B1 phases using the WIEN2K code based on DFT. The paper has been organized as follows. After this introduction, the methods used in our calculation are described in section 2. In section 3 the results of our study are given and discussed in detailed. The conclusion of our study is given in section 4.

2. COMPUTATIONAL METHODS

The first principle study of GaX(X=P,As) calculation is performed using the first principle full potential linearized augmented plane wave (FP-LAPW) [9] method within the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE-GGA) [10] with modified Becke-Johnson (mBJ) [11] potential under the framework of density functional theory (DFT) [12-14]. This method is used as it is one of the most accurate methods in electronic structure calculation of crystals. In this method, the lattice is divided into non-overlapping atomic spheres surrounding each atomic sites and an interstitial region [15]. 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 part which reduces to 256 irreducible k-points inside the Brillouin zone. 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 position of the first and second atom of the B3 and B1 structures of GaP is taken to be (0,0,0), (0.25,0.25,0.25) and (0,0,0), (0.5,0.5,0.5) respectively. $3d^{10}4s^24p^1$, $3s^23p^3$ and $3d^{10}4s^24p^3$ states are respectively considered as the valence electrons for Ga, P and As respectively. All 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 [16]. The overall calculation is done with WIEN2K [17].

3. RESULTS AND DISCUSSION

The ground state lattice parameter for GaP and GaAs in both B3 and B1 phase are obtained by the structure optimization. A series of different lattice constant are used to calculate the total energy and the corresponding primitive cell volume. The energy versus unit cell volume curves for both GaP and GaAs are shown in Fig. 1(a) and Fig. 1(b). We can clearly see that in both the figures the B3 phase is more stable than the B1 phase which is in good agreement with other theoretical and experimental results.

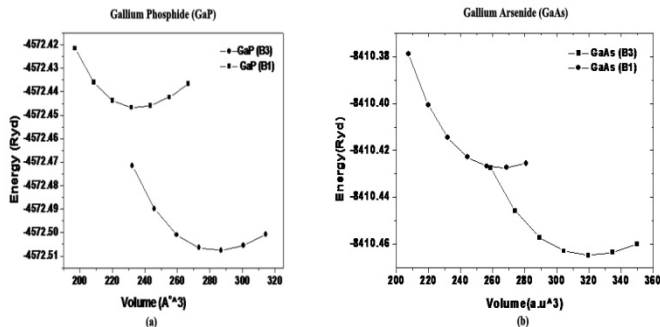


Fig. 1: Total energy versus unit cell volume for B3 and B1 phases of (a) GaP and (b) GaAs.

The phase transition is important for understanding the structural, mechanical and physical properties of a material under pressure. The phase transformation of four-fold coordinated structure (B3) of GaX (X=P, As) to a more denser six fold coordinated structure (B1) under pressure is calculated using the condition of equal enthalpies i.e. the $H=E+PV$. The structural phase transition from B3 to B1 phase for GaP and GaAs are shown in Fig. 2(a) and Fig. 2(b).

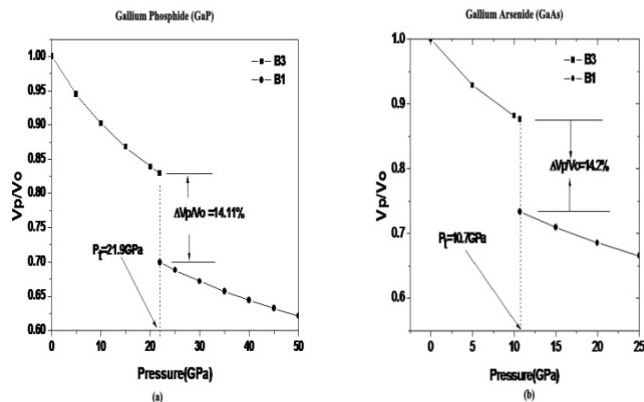


Fig. 2: Phase transition from B3 to B1 phase for (a) GaP and (b) GaAs.

We find that the structural phase transition for GaP-B3 to GaP-B1 occurs at 21.9 GPa pressure with a volume collapse of 14.11% while GaAs undergoes a structural phase transition from B3 to B1 phase at 10.7 GPa pressure with a volume

collapse of 14.2% indicating that in both GaP and GaAs, the B3 phase is more compressible than the B1 phase. The energy band diagram of GaP and GaAs has already been reported in many theoretical and experimental studies [18-20]. In the present study we find that GaP-B3 phase is an indirect band gap semiconductor with a band gap of 2.3eV while GaP-B1 phase is metallic. Also GaAs-B3 phase is a direct band gap semiconductor with a band gap of 1.3eV while GaAs-B1 phase shows metallic nature. Therefore we find that our results for both B1 and B3 phases of GaP and GaAs are in close agreement with previous reported data. We have also calculated the energy band gap of GaX(X=P, As) at different pressures for both B1 phase and B3 phase.

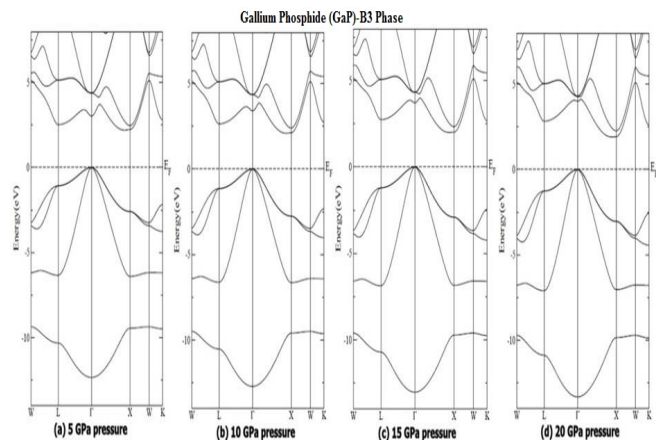


Fig. 3: Energy band diagram of B3-phase of GaAs in (a) 5 GPa pressure (b) 10 GPa pressure (c) 15 GPa pressure and (d) 20 GPa pressure.

Fig. 3(a), 3(b), 3(c) and 3(d) shows the energy band diagram of B3 phase of GaP at different pressures. One interesting thing that we find from the band structure diagrams in Fig. 4 is that as the pressure increases to 5 GPa, 10 GPa 15 GPa and 20 GPa, the gap between the Γ -L increases while the gap between Γ -X decreases towards the fermi level indicating possibilities of crossing over of the conduction band towards the valance band. The variation in the energy band gap with pressure for B3 phase of GaP is also shown in Fig. 6 for clear analysis of the changes between Γ -X and Γ -L with pressure. The energy band diagram of B1 phase of GaP at different pressures after the phase transition is also shown in Fig. 5(a), 5(b), 5(c) and 5(d). From the Fig. we can clearly see crossing over of the conduction band towards the valance band hence confirming the transition from direct band gap nature to metallic at higher pressure.

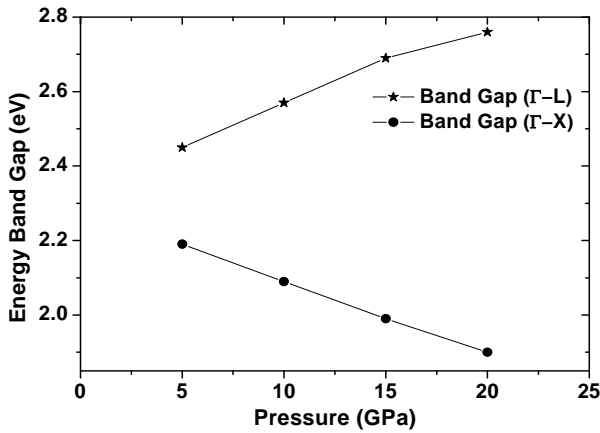


Fig. 4: Variation of Energy band gaps of GaP-B3 phase with pressure.

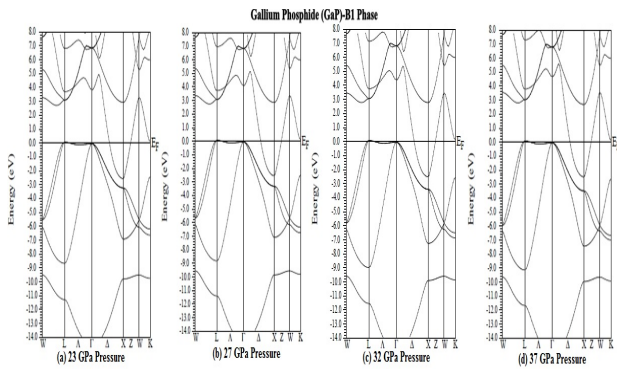


Fig. 5: Energy band diagram of B1-phase of GaP in (a) 23 GPa pressure (b) 27 GPa pressure (c) 32 GPa pressure and (d) 37 GPa pressure.

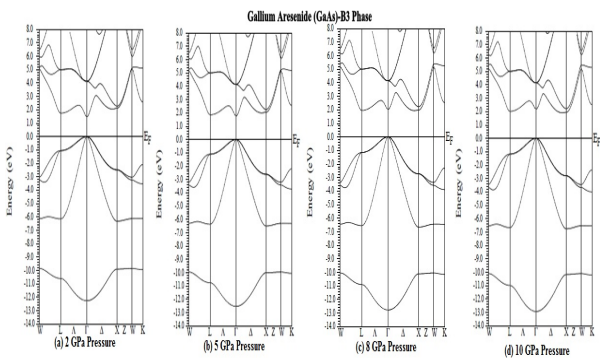


Fig. 6: Energy band diagram of B3-phase of GaAs in (a) 2 GPa pressure (b) 5 GPa pressure (c) 8 GPa pressure and (d) 10 GPa pressure.

In Fig. 6(a), 6(b), 6(c) and 6(d), the energy band diagrams of GaAs-B3 phase at different pressures are given. From the figures we find that the gap between the Γ point increases as

the pressure increases but if we closely study the energy band diagram we find that the gap at the X point decreases which indicates possibility of crossing over at higher pressure as in case of GaP. The variation of gap at the Γ point and X point with increase in pressure is given in Fig. 7.

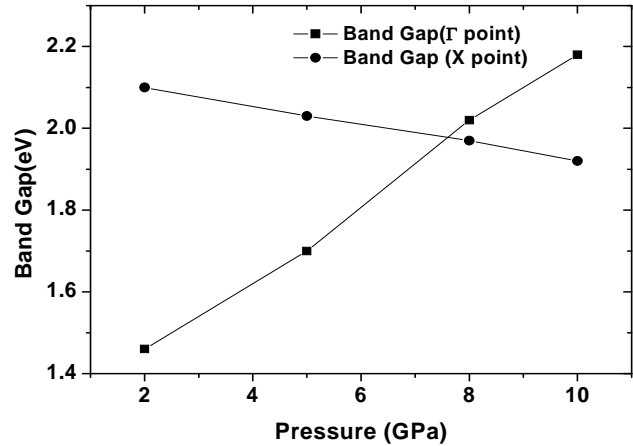


Fig. 7: Variation of Energy band gaps of GaAs-B3 phase with pressure.

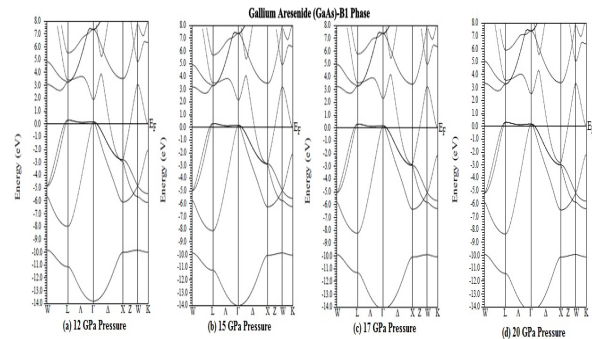


Fig. 8: Energy band diagram of B1-phase of GaAs in (a) 12 GPa pressure (b) 15 GPa pressure (c) 17 GPa pressure and (d) 20 GPa pressure.

Fig. 8(a), 8(b), 8(c) and 8(d) shows the energy band diagram of the B1 phase of GaAs. From the Fig. we find that the metallic nature is retained even at high pressure without much variation. Hence we conclude that the energy band gap of both GaP and GaAs in B3 phase is affected by pressure while the energy band gaps of B1 phase is not much affected by pressure.

4. CONCLUSIONS

The structural properties of GaX (X=P, As) in both B3 and B1 structure are studied and B3 phase is found to be more stable than the B1 phase. A structural phase transition from B3 to B1 is found to occur at 21.9 GPa pressure with a volume collapse

of 14.11% in GaP while GaAs undergoes a structural transition from B3 to B1 phase at 10.7 GPa pressure with a volume collapse of 14.2% indicating that B3 phase of both the compounds is more compressible than the B1 phase. The energy band diagram shows that GaP-B3 is an indirect band gap semiconductor with a band gap of 2.3 eV while GaAs-B3 is a direct band gap semiconductor with a band gap of 1.3 eV. The B1 phase of both the compounds is also found to be metallic which are found to be in good agreement with other experimental and theoretical studies. The energy band gaps for GaP-B3 phase between the Γ -L points, increased while the gap between the Γ -X points decreased under induced pressure. Also GaAs-B3 phase showed an increase in gap at the Γ point and decrease at X point under induced pressure. However the metallic behavior of GaP-B1 and GaAs-B1 phase do not show any change under induced pressure. Thus we conclude that the B3 phase of both GaP and GaAs are affected by pressure while the B1 phase is not affected by pressure.

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