STRUCTURAL PHASE TRANSITION OF INDIUM ARSENIDE UNDER INDUCED PRESSURE: A DENSITY FUNCTIONAL THEORY STUDY

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Abstract: We have carried out the first-principles calculations to show phase transition of binary compound semiconductor Indium Arsenide under induced pressure in the light of density functional theory with the generalised gradient approximation of Perdew-Burke-Ernzerhof as exchange correlation potential. The calculated lattice parameters are found to be in good agreement with other theoretical and experimental data. The pressure induced phase transition from zinc-blende to rock salt structure is found to occur at 4.7 GPa pressure with a 17.27% of volume collapse.

Keywords: Density Functional Theory (DFT); energy band diagram; elastic properties; phase transition

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1. Introduction:

The technological importance of group III-V compound semiconductors have increased over the past years due to its electronic and mechanical properties and have received considerable interest from experimentalist and theorists. To understand, the structural phase transition of a material and the influence of band structure parameters on the electronic properties of semi-conductors, the study under induced pressure is found to be an effective tool. Also the study of elastic constants at different pressure plays an important role in mechanical stability, strength, phase transition and a material response to various conditions. One of the interesting phenomena that may occur under applied pressure is a sudden change in the arrangement of the atoms i.e. structural phase transition. Indium Arsenide (InAs) is an important group III-V compound semiconductor having high electron mobility and narrow energy band gap. It is widely used in construction of infrared detectors and diode lasers [1]. It crystallizes in cubic zinc-blende (ZB) structure under ambient conditions. At high pressure it is found to undergo structural phase transition to rock-salt (RS) structure. The pressure-induced phase transition to metallic state was first reported by Minomura and Drickamer at 8.46 GPa pressure from high pressure resistivity measurements [2]. Pitt and Vyas reported the phase transition from the Zinc-blende (ZB) to Rock-salt (RS) through resistivity measurements [3]. Although there have been extensive studies on structural, mechanical and electronic properties of InAs, the experimental and theoretical study of these properties under high pressure is still very scarce. The main aim of this work is to present a detailed study of the structural changes of InAs in ZB to RS phase under induced pressure. The paper is organised as follows. The theoretical and computational method is described in section 2. In section 3, the results and discussion of our study is given and our conclusions are summarized in section 4.

2. Theoretical and Computational Method:

All theoretical calculations of InAs is performed based on the WIEN2K code [4] using the full potential linearized augmented plane wave (FP-LAPW) [5] method with modified Becke-Johnson (mBJ) potential [6] under the framework of Density Functional Theory (DFT) [7,8,9]. The generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof scheme is used for treating the exchange correlation interaction effects [10]. 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. 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. The number of k-points used

for the integration part is 8000 k-points which is reduced to 256 irreducible k-points inside the Brillion zone including five high symmetry points W, L, Γ, X and K. Convergence of the basis set is obtained at $R_{MT}K_{max} = 9.0$ where K_{max} gives us the plane wave cut-off.

3. Results and Discussion:

The energy as a function of the primitive cell volume for ZB and RS phase is shown in figure 1. From the figure, one can clearly see that the InAs-ZB structure is more stable than the RS structure. The equilibrium lattice parameters of the InAs crystal in zinc-blende and rock-salt structure is obtained by fitting the resultant curve to the Birch-Murnaghan equation [11]. The calculated structural parameters are compared with other results [12,13,14,15,16] and are given in table 1. Our results are found to be in good agreement with other results and hence are used for further calculations.
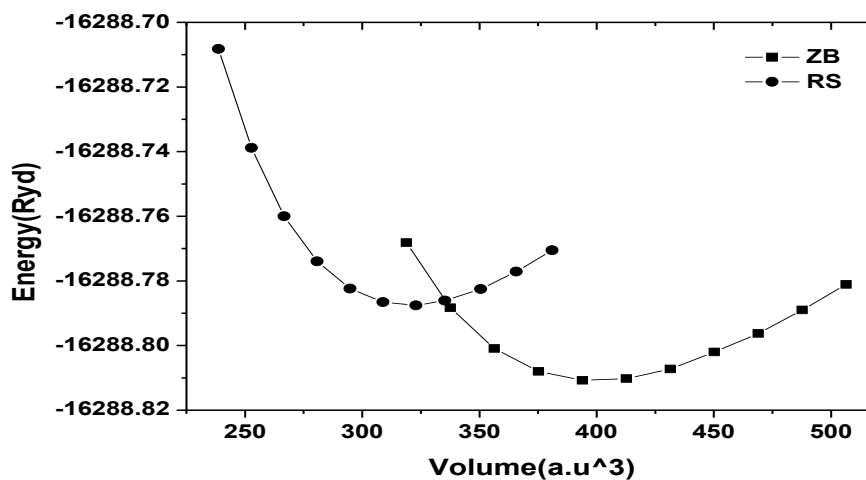

Figure 1. Total energy as a function of primitive cell volume of InAs in ZB and RS phases.

Table 1. Lattice constants, bulk modulus and pressure derivative of bulk modulus of InAs-ZB and InAs-RS at zero pressure.

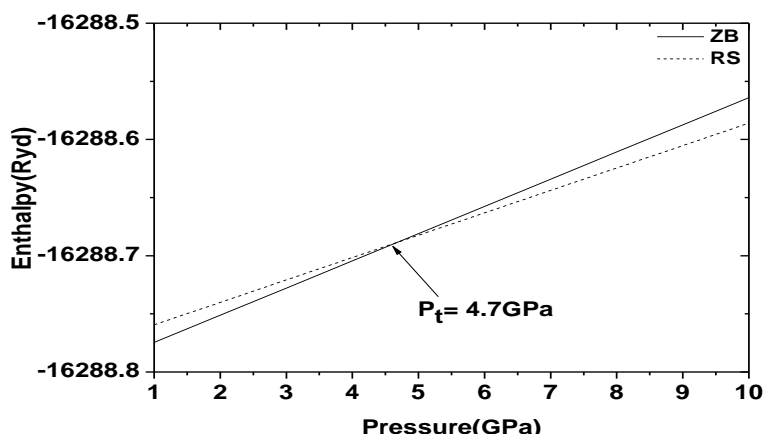| Structure		$a(A^0)$	$B(GPa)$	$B^/$
ZB	Present work	6.188	49.48	4.78
	References	6.058[a], 6.10[b], 6.08[c]	55.51[c], 59.2±5[d]	6.8±2[d]
RS	Present work	5.748	62.98,	4.84
	References	5.65[c], 5.5005[d], 5.514[e]	40.6±14[d]	7.3±1[d]

Ref.12[a], Ref.13[b], Ref.14[c], Ref.15[d], Ref.16[e]

Figure 2. Enthalpy variation of InAs in ZB and RS structures as a function of pressure.

The pressure induced phase transition of InAs-ZB to InAs-RS phase is investigated from a series of ground state optimisation at various pressures. After optimisation, the enthalpy, H = E + PV is used to obtain the pressure induced phase transition. Figure 2 shows the enthalpy as a function of pressure of both the InAs-ZB and InAs-RS structure. It is clearly seen that the phase transition of InAs-ZB structure to InAs-RS structure is found to occur at 4.7 GPa pressure.
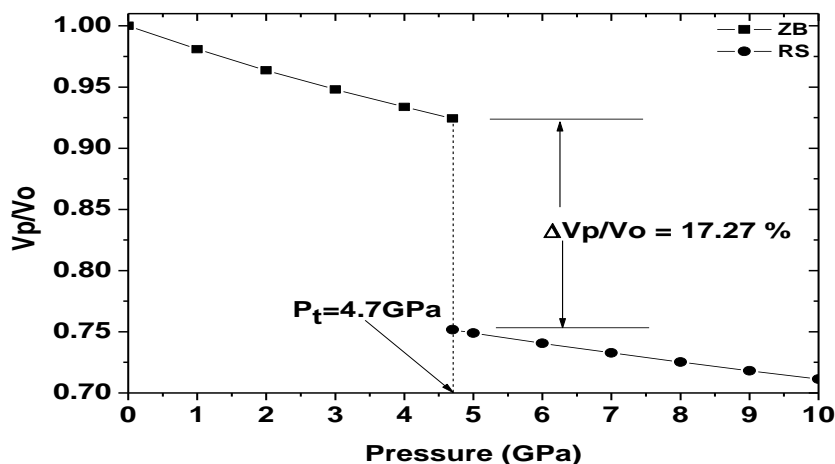

Figure 3. Phase transition between ZB and RS structure of InAs at 4.7 GPa pressure.

Table 2. Phase transition pressure and volume collapse comparisons with other experimental and theoretical data:

	Present calculation	Expt. results	Theoretical results
Transition pressure (P_t) (GPa)	4.7	7[a] , 6.9±0.2[c]	3.9[d], 4.0[e], 6.0[f],
Volume collapse (%)	17.2	17.0±0.2[a], 18.8[b]	17.0[g], 24.0[h]

Ref.15[a], Ref.16[b], Ref.17[c], Ref.18[d], Ref.19[e], Ref.20[g], Ref.21[h]

The normalised volume (V_p/V_o) of the crystal in ZB phase and RS phase is also found to be 0.924 and 0.752 respectively during the phase transition with a volume collapse of 17.2% indicating that ZB phase is more compressible than the RS phase as given in figure 3. Our calculated results of phase transition and volume collapse are compared with other experimental and theoretical results [17,18,19,20,21] and are shown in table 2. We find that our results are closer to the experimental data than other theoretical results.
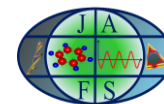
4. Conclusions:

The calculated optimised structural parameter of Indium Arsenide in both zinc-blende and rock salt structure phase are compared with other theoretical end experimental results and are found to be in good agreement. The phase transition of InAs-ZB structure to InAs-RS structure under induced pressure is found to occur at 4.7 GPa pressure. The normalized volume of the crystal in ZB phase and RS phase is also found to be 0.924 and 0.752 respectively during the phase transition with a volume collapse of 17.2% indicating that ZB phase is more compressible than the RS phase.

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