

Pressure Effects on The Elastic and Lattice Dynamics Properties of AIP from First-Principles Calculations

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Abstract. We have performed first-principles calculations to investigate the behavior under hydrostatic pressure of the structural, elastic and lattice dynamics properties of aluminum phosphide crystal (AIP), in both zinc-blende (B3) and nickel arsenide (B8) phases. Our calculated structural and electronic properties are in good agreement with previous theoretical and experimental results. The elastic constants, bulk modulus (B), shear modulus (G), and Young's modulus (E), Born effective charge and static dielectric constant ϵ_0 , were calculated with the generalized gradient approximations and the density functional perturbation theory (DFPT). Our results in the pressure behavior of the elastic and dielectric properties of both phases are compared and contrasted with the common III–V materials. The Born effective charge Z_B decreases linearly with pressure increasing, while the static dielectric constant decreases quadratically with the increase of pressure.

Keywords: DFT, DFTP, elastic properties, dielectric properties.

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INTRODUCTION

Aluminum phosphide (AIP) is a wide-indirect band gap semiconductor. At normal conditions, AIP crystallizes in the zinc-blende (ZB) structure [1]. High-pressure experiments on this compound are difficult because of sample handling problems; AIP is unstable in air [2]. The zb form has been reported theoretically to be metastable. The zinc-blende phase is known to transform to the nickel arsenic (NiAs) phase at about (9.5 – 17) GPa [3]. Although other studies have placed this transformation at a somewhat smaller pressure (7- 9.3) GPa [4]. At a pressure of about 36 GPa the NiAs phase has been reported to undergo a Cmc₂m-like distortion with no significant change in volume. The CsCl phase is a possible candidate for AIP at very high pressures [2]. AIP is a subject of extensive theoretical studies ranging from the semiempirical to the first principles methods [5] within the density functional theory (DFT) framework using both pseudopotential [2], and all-electron approaches. For the bulk phase of AIP,

theoretical calculations based on the Hartree-Fock [6], and potential model [7] have obtained a very good description of its structural and electronic properties.

Over the last few years, the study of materials under high pressure has become an extremely important subject. This is primarily due to both theoretical and experimental developments, which have facilitated such work [8].

The pressure is a continuously varying parameter that can be used in systematic studies of the properties of solids as a function of inter-atomic 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 of atomic arrangement. The ultimate pressures in the experiment can lead to a reduction in the volume by a factor of two causing enormous changes in the inter-atomic bonding [9].

The aim of this work is to investigate the above properties by employing the pseudo potential method, the density functional theory and the density functional perturbation theory to study the linear response of this compound under pressure. The calculated structural parameters and electronic properties are compared with previous experimental and theoretical studies. The evolution under pressure of the elastic constants, the Born effective charges, the dielectric tensor $\epsilon(0)$ are compared with the available experimental data. To our knowledge many of the present results have been not previously reported and we hope that this work will stimulate new experimental studies in the future.

COMPUTATIONAL METHOD

The calculations were performed using the plane wave pseudo potential approach within the framework of the density functional theory (DFT) with CASTEP [10]. The exchange–correlation energy of the electrons was described in the generalized gradient approximations (GGA) given by Perdew Burke Eenzershof (PBE) [11]. The valence electron ion interaction was treated by ab initio norm-conserving pseudo potentials [12]. The aluminum $3s^23p^1$ electrons and phosphore $3s^23p^3$ electrons were treated as valence electrons. Well converged results were obtained using a kinetic energy cutoff of 850 eV and with a Monkhorst–Pack k-points $10 \times 10 \times 10$. The total energy converged to better than 1 meV/atom. The static dielectric tensor $\epsilon(0)$ and the Born effective tensor charges Z_B were calculated using the self-consistent density functional perturbation theory (DFPT [13-16] which avoids the use of a supercell and allows calculation of the dynamical matrix at an arbitrary q vector. The elastic stiffness coefficient was determined using a finite strain technique [17] from a linear fitting of the computed stress based on adding small strains, where six strains amplitude up to a maximum of 0.3% were used.

RESULTS and DISCUSSION

Structural Properties and Phase Transformation

The equilibrium lattice constants are calculated by minimizing the total crystal energy obtained from different volumes and fitted to the Murnaghan's equation of state [18].

The calculated values of equilibrium lattice constants (a,c), bulk modulus (B_0), and first pressure derivative of bulk modulus (B_0') for AIP with the B_3 and B_8 structures are all listed in Table 1 with available theoretical calculations and available experimental data results [19-23]. The variations of enthalpy with pressure of B_3 structure (solid line) and B_8 structure (dashed line) are shown in Fig. 1. It is clear that the pressure induced phase transition from the B_3 structure to the B_8 structure occurs at a transition pressure of 14.51 GPa, which is larger than other theoretical studies [4-22-24] as shown in Table 2. However, the present predicted transition pressure is in good agreement with the available experimental data with (9.5 – 18) [3].

Table 1. Calculated values of equilibrium lattice constants (a,c), bulk modulus (B_0), and first derivative of bulk modulus with pressure (B_0') for AIP in B_3 and B_8 structures.

Phase	a(A)	c(A)	B_0 (GPa)	B_0' (GPa)
B3	5.52		86.5	3.82
	5.46 [21]		90.46[22]	3.72[22]
	5.48 [20]			
	5.40 [19]			
	5.43 [22]			
B8	3.53	5.74		
	3.55 [22]	5.71 [22]		
	3.46 [23]	5.57 [23]		

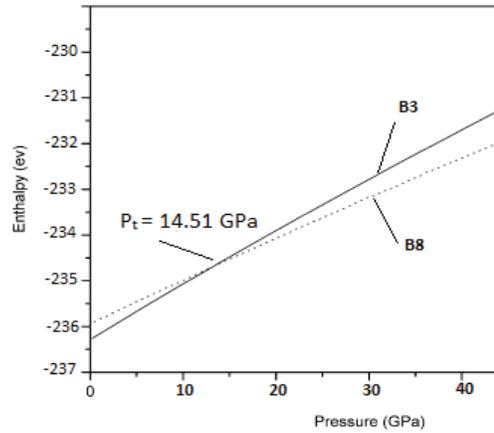


Figure 1. Calculated enthalpy versus pressure of AIP.

Table 2. Calculated values of the phase transition pressure.

Phases	P_T / GPa		
	This work	Cal.	Exp.
B3→B8	14.51	6.78 [22] 7.7 [24]	(7- 9.3) GPa [4] (9.5 – 17) [3]

Elastic Properties

The elastic constants for AIP with zinc Blend (B3) and NiAs (B8) structures are listed in the following Table 3. From Table 3, the elastic constants of B3 structure are all in good agreement with the theoretical data [20-25]. To the best of our knowledge, no results on elastic constants with pressure for the NiAs structure have been reported, that is, the present calculated elastic constants with pressure can be considered as predictions. The pressure dependences of the elastic constants of AIP for both of the phases are shown in Fig. 2. It is clear that the value of C_{ij} increases linearly with pressure increasing. From the calculated results of single crystal elastic constants bulk modulus (B), shear modulus (G), and Young's modulus (E) are determined using the Voigt–Reuss–Hill averaging scheme [26–27]. The pressure dependences of the Young's modulus (E), bulk modulus (B) and shear modulus (G) are shown in Table 4.

Table 3. Elastic constants of AIP in the B3 structure at zero pressure and in B8 structure at $P = 16.0$ GPa.

		C_{11} (GPa)	C_{12} (GPa)	C_{13} (GPa)	C_{33} (GPa)	C_{44} (GPa)	C_{66} (GPa)
	This work	134.10	62.00			64.38	
B3	Ref.[20]	132	63			61.5	
	Ref.[25]	132.25	67.5			76.55	
	Ref.[22]	132.28	68.46			62.15	
B8	This work	231.5	110.2	76.25	281	72.45	62.3
	Ref.[22]	229.95	106.38	78.53	274.84	71.71	61.78

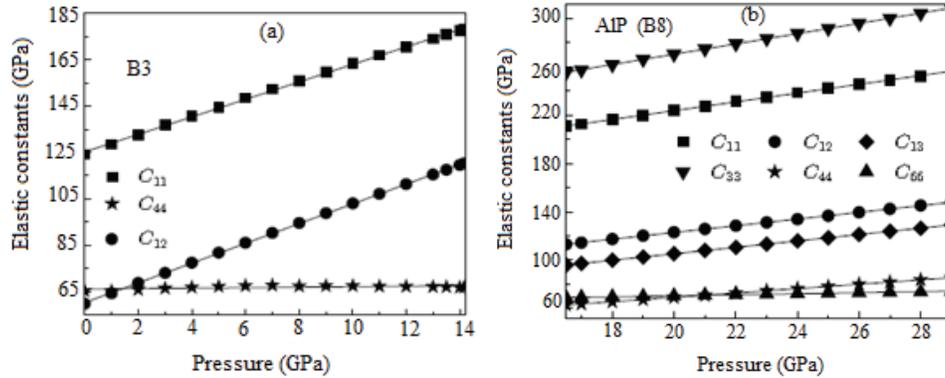


Figure 2. Elastic constants (C_{ij}) of AIP versus pressure in the B3 (a) and B8 (b) phases.

Table 4. The pressure dependences of the Young's modulus E ,bulk modulus B and shear modulus G and poisson's ratio ν .

P(GPa)	E(GPa)	B(GPa)	G(GPa)	ν
0	94.90	86.037	51.02	0.316
2	94.81	91.25	50.98	0.326
4	94.75	99.59	50.83	0.341
6	94.41	107.74	50.72	0.354
8	94.99	116.46	50.83	0.364
10	92.45	124.00	48.82	0.376
12	91.20	131.70	48.11	0.382

Dielectric Properties

Since the B₃-AIP has cubic symmetry, only one dielectric tensor component can completely characterize the linear optical properties. This component is $\epsilon_2(\omega)$, the imaginary part of the frequency-dependent dielectric function is expressed as [28] :

$$\epsilon_2(\omega) = \frac{1}{\pi} \left(\frac{e}{m\omega} \right)^2 \sum_{ij} \int_{BZ} f_{ij} P_{ji} P_{ij} \delta(E_{ji} - \hbar\omega) dk$$

where m is the mass, ω is the frequency, k is the wave vector, $E = \hbar\omega$, $E_{ji} = E_j - E_i$, and $f_{ij} = f_i - f_j$, with f_i being the Fermi occupation factor of the single-particle state i , P_{ij} is the momentum matrix element. The subscripts i and j indicate the conduction and valence band, respectively. It should be noted that the BZ stands for Brillouin zone.

The imaginary parts of the dielectric function of B₃-AIP at $P = 0.0$ GPa and $P = 10$ GPa are shown in Fig. 4. The pressure makes both the shape and the position of the main peaks of the $\epsilon_2(\omega)$ vary successively, which accords well with the previous first-principles studies [29]. The curve of calculated energy of the main peak of $\epsilon_2(\omega)$ versus pressure is shown in Fig. 5. The calculated energy of the main peak varies almost linearly as pressure increases.

To deal with the macroscopic electric field associated with the longitudinal optical mode and the relevant non analytic behavior of the dynamical matrix at G point, we calculate static dielectric constant ϵ_0 and Born effective charge Z_B tensors for AIP in the B₃ structure, which are isotropic scalars in cubic symmetry. The Born effective charge is a fundamental quantity that specifies the leading coupling between lattice displacement and electrostatic field in insulator. The pressure dependence of Born effective charge Z_B and static dielectric constant ϵ_0 for the B₃ phase are shown in Fig. 6. The Born effective charge Z_B decreases linearly with pressure increasing, while the static dielectric constant decreases quadratically with the increase of pressure.

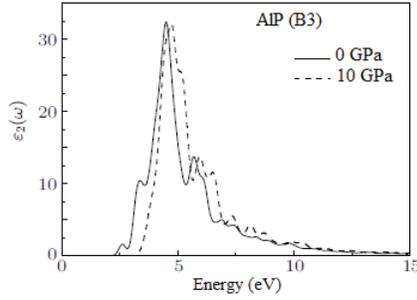


Figure 4. Imaginary parts of the dielectric function of AIP in the B3 phase at $P = 0$ GPa and $P = 10$ GPa.

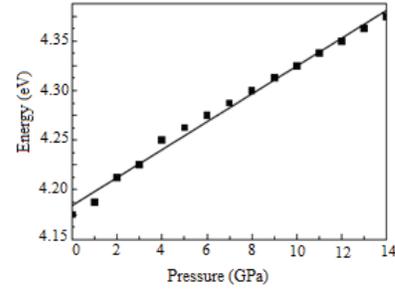


Figure 5. Calculated energy of the main peak of $\epsilon_2(\omega)$.

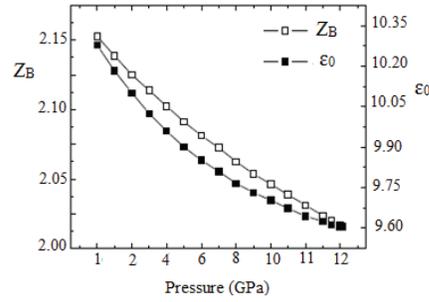


Figure 6. Born effective charge and static dielectric constant of AIP versus pressure in the B3 phase.

CONCLUSION

In summary, ab initio calculations are adopted to investigate the structural, elastic and dielectric properties of AIP with zinc-blende (B3) and nickel arsenide (B8) phases under hydrostatic pressure. The calculated values of lattice, bulk modulus, and elastic constants are all in good agreement with experimental data and other first principles calculations. We find that elastic constants, Bulk modulus and static dielectric constants vary almost linearly hydrostatic pressure. However, Born effective charge Z_B decreases linearly with pressure increasing, while the static dielectric constant decreases quadratically with the increase of pressure. We hope that our work will stimulate future high-pressure Raman and X-ray experiments in AIP.

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