**Metastable phases, phase transformation and properties of AlAs based on
first-principle study**

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ABSTRACT

By utilizing an evolutionary methodology on crystal structure search, we propose three new metastable phases for aluminum arsenide (AlAs) as follows: (1) a $P6_422$ symmetric structure ($hP6$ -AlAs), (2) a $C222$ symmetric structure ($oC12$ -AlAs), and (3) a $I3d$ symmetric structure ($cI24$ -AlAs). By controlling the unloading pressure rate, $oC12$ -, $hP6$ -, and $cI24$ -AlAs may be acquired through quenching NiAs-AlAs. The elastic constants and phonon dispersion spectra are calculated to certify the mechanical and dynamic stabilities of three newly discovered phases. On the basis of first-principle study, we explore phase transformations under pressure for several AlAs polymorphs. The calculation of mechanical properties illustrates that $oC12$ -, and $hP6$ -AlAs possess similar hardness levels, which are higher than that of $cI24$ -AlAs. Meanwhile, $oC12$ -, and $hP6$ -AlAs hold similar shear anisotropic factors, which are smaller than that of $cI24$ -AlAs. Electronic band structure calculation reveals that at **zero** pressure, $oC12$ -, and $hP6$ -AlAs possess indirect band gaps of 0.468 eV and 1.356 eV, respectively. $cI24$ -AlAs is a direct semiconductor with a gap value 1.761 eV.

Keywords: aluminum arsenide; phase transformation; mechanical property; electronic property; first-principle.

1. Introduction

At ambient conditions, aluminum arsenide (AlAs) exists stably with zinc blende structure (zb-AlAs), which is a common crystal form of III-V compounds. **AlAs has excellent physical performances[1], including a high thermal expansion coefficient $5.20 \times 10^{-6} \cdot K^{-1}$, thermal conductivity 0.9 W/cm·K, and, high melting points 2013 K and, and is an advantageous material for the manufacture of optoelectronic devices, such as light emitting diodes [2].** Given the almost identical lattice constants, AlAs and gallium arsenide (GaAs) can form a superlattice $Al_xGa_{1-x}As$ with small induced strain. With unique electrical and optical characteristics, $Al_xGa_{1-x}As$ holds important applications in optoelectronic devices, such as Bragg reflector superlattices, heterojunction bipolar transistors, solid-state lasers, high electron mobility transistors, and light emitting diodes [2, 3].

In 1983, Froyen and Cohen studied the structural properties of AlAs under pressure, and

suggested that the high pressure structure transformed from zb-AlAs could be either rocksalt or NiAs (NiAs-AlAs) [4]. Several years later, Weinstein et al. observed a phase transformation within a high pressure experiment via diamond-anvil cell [5], and afterward, in a Raman study [6] at ~ 12.4 GPa on unloading, however the structure was unknown. In the following years, experimental studies that explored the phase transition of AlAs have attracted increasing research attention. In 1994, Greene et al. first observed a first order phase transition from zb-AlAs to NiAs-AlAs at the equilibrium transformation pressure 7 ± 5 GPa through an energy-dispersive X-ray diffraction study on AlAs [7]. Subsequently, by X-ray diffraction and electrical resistivity measurements, zb-AlAs $\rightarrow$ NiAs-AlAs transformation was detected at 14.2 GPa on loading [8].

Theoretical research also achieved great progress in phases and phase transformation of AlAs under high pressure. The calculated pressure of zb-AlAs $\rightarrow$ NiAs-AlAs phase transition ranges from 6.1 GPa to 9.15 GPa [9-11]. Mujica et al. predicted that NiAs-AlAs becomes unstable and forms CsCl-AlAs at 77.9 GPa [11]. Other structures such as cmcm, cinnabar, and sc16 of AlAs have been considered [11, 12]. Research indicated cmcm structure AlAs (cmcm-AlAs) can stably exist within a certain pressure range, whereas the cinnabar and sc16 structures are not thermodynamically stable at any pressure and could occur only as metastable phases [11, 12]. In 1992, wurtzite structure of AlAs has been proposed theoretically [6], and extensively investigated [13, 14].

In the present work, we proposed three new AlAs metastable phases. By analyzing elastic constants and phonon spectra, these AlAs polymorphs are found to be mechanically and dynamically stable, respectively. Then, we studied the phase transition behaviors under pressure, as well as the mechanical and electronic properties of these AlAs polymorphs.

2. Computational methods

The potential AlAs polymorphs' structures were explored by using the CALYPSO code without any experimental information [15-17], which has been widely used and has achieved substantial advances in structural prediction [18-22]. Once the structures were generated from the CALYPSO, geometric optimization, elastic constants and phonon frequency calculation, and physical property research were implemented in CASTEP code [23]. The exchange correlation potential generalized

gradient approximation (GGA) of Perdew–Burke–Ernzerhof (PBE) was adopted [24, 25], and atomic electronic configuration was described with the ultrasoft pseudopotential [26]. To ensure calculation precision at 1 meV, the plane-wave pseudopotential method was employed under an energy cutoff of 550 eV and the k-points for Monkhorst–Pack grid was generated by a k-point separation ($2\pi \times 0.04 \text{ \AA}^{-1}$) [27].

GGA-PBE generally underestimates the energy gap by 30% ~ 40% relative to the experimental value when calculating for **band gap** [28]. Hence, we adopted the Heyd–Scuseria–Ernzerhof hybrid functional (HSE06) [29] on the primitive cells; such method can obtain an accurate prediction of band gaps. Geometric optimization was carried out using the BFGS minimization algorithm [26], during which iterations were continued until the following criteria were satisfied: (1) the force on atom is less than 0.01 eV/Å; (2) the atoms' displacement is below $5 \times 10^{-4} \text{ \AA}$; (3) the energy change does not go beyond $5 \times 10^{-6} \text{ eV/atom}$; (4) the stress component does not exceed 0.02 GPa. The efficient stress–strain method with the maximum strain amplitude 0.003 and 9 steps for each strain is employed to calculate the elastic constants. To inspect dynamically stability of the obtained structures, the phonon frequencies are calculated via the linear response method [30] as implemented in CASTEP code [23].

3. Results and discussion

3.1. Optimisation of crystal structures

Fig. 1. Structure graphs for *o*C12-AlAs (a), *h*P6-AlAs (b), and *c*I24-AlAs (c). The balls in dark green

1 and indigo represent the Al and As atoms, respectively. The Al-As bonds are represented by gold
2 sticks.

3
4 A wide selection of candidate structures of AlAs was calculated. In addition to zb-AlAs,
5 NiAs-AlAs, cmcm-AlAs and the structures predecessors studied, three new structures attracted our
6 attention. The first new structure we proposed is a C-centered ($1/2, 1/2, 0$) orthorhombic crystal
7 system (space group $C222$) with 12 atoms per unit cell, denoted as *oC12*-AlAs. The second one is a
8 primitive centered hexagonal ($P6_422$) structure with 6 atoms/unit cell, denoted as *hP6*-AlAs. The last
9 one is a body centered cubic structure ($I3d$) with 24 atoms per unit cell, denoted as *cI24*-AlAs. All
10 atoms in *oC12*-, *hP6*-, and *cI24*-AlAs contain four coordination atoms, which combine to form Al-As
11 bonds, indicating that no Al-Al (As-As) bonds were present in the three newly discovered structures.
12 Information about *oC12*-, *hP6*-, and *cI24*-AlAs, such as space group number, crystal system, lattice
13 parameter, density, and atomic Wyckoff positions, are listed in Table 1.

14 For *oC12*-AlAs (Fig. 1a), the atoms Al2, As1, Al1 and As2 are distributed in the plane marked
15 by P0, P1, P2 and P3, respectively. In *oC12*-AlAs, three kinds of bonds with similar bond lengths are
16 displayed as follows: the first one between P0 and P1 with length 2.512 Å; the second one between
17 P1 and P2 with length 2.502 Å; and the last one with length 2.517 Å are in P2 and P3. For *hP6*-AlAs
18 (Fig. 1b), there is only one kind of Al-As bond with length 2.508 Å. It is a halved unit cell about the
19 plane $c = 0.5$, represented by a red line. Similar to *hP6*-AlAs, only one kinds of bonds is shown
20 present in *cI24*-AlAs with bond length of 2.500 Å. The central atom Al/As forms a tetrahedron
21 $[AlAs_4]/[AsAl_4]$ with its 4 coordination As/Al atoms, presented by a polyhedron in lavender/aqua,
22 respectively. The tetrahedron $[AlAs_4]$ is similar to $[AsAl_4]$. The six edges that form the tetrahedron
23 comprise one L1 (black), one L2 (wine) and four L3 (pink), marked by a polyhedron in aqua. L1 and
24 L2 hold the same length of 4.562 Å; whereas the four L3 possess a uniform length of 3.817 Å. L1 is
25 perpendicular to L2, however the two do not intersect as L1 and L2 are not in the same plane. One
26 central atom connects with two coordination atoms and forms three atoms chain, the angle values of
27 atoms chain are 99.594° and 131.810° .

28 Referring to the optimized structures at **zero** pressure, *cI24*-AlAs exhibits a slightly higher

density than that of zb-AlAs (3.604 g/cm³) by about 3.7%. Meanwhile, both the *o*C12- and *h*P6-AlAs possess higher densities than that of zb-AlAs by about 11.7% and 11.8%, respectively.

Table 1

Space group (S.G.), crystal system (C.S.), lattice parameter (L.P.) (Å), density ρ (g/cm³), and atomic Wyckoff positions (A.W.P) for three new AlAs polymorphs.

Structure	S.G.	C.S.	L.P.	ρ	A.W.P.
<i>o</i> C12-AlAs	<i>C</i> 222 (21)	orth	$a=6.975; b=3.977$ $c=9.094$	4.025	Al1: $4k$ (0.25, 0.25, 0.167); Al2: $2d$ (0, 0, 0.5) As1: $4k$ (0.25, 0.25, 0.666); As2: $2b$ (0.5, 0, 0)
<i>h</i> P6-AlAs	<i>P</i> 6 ₄ 22 (181)	hex	$a=4.0260; c=8.973$	4.031	Al: $3c$ (0.5, 0, 1); As: $3d$ (0.5, 0, 0.5)
<i>c</i> I24-AlAs	<i>I</i> 3 $\bar{d}$ (217)	cub	$a=8.161$	3.736	Al: $12a$ (0.375, 0, 0.25); As: $12b$ (0.25, 0.125, 0.5)

orth: orthorhombic; hex: hexagonal; cub: cubic

3.2. Stability analysis

To verify the mechanical stability of *o*C12-, *h*P6-, and *c*I24-AlAs, the elastic constants were calculated and listed in Table 2.

For an orthorhombic crystal system, the mechanical stability under zero pressure can be evaluated by [31]

;;

;;

(1)

For cubic crystal system [31]:

;;;

(2)

For hexagonal crystal system [31]:

;;;

(3)

The calculated elastic constants at zero pressure satisfy the mechanical stability criteria, suggesting that *o*C12-, *h*P6-, and *c*I24-AlAs all possess mechanical stability.

Table 2

Independent elastic constants C_{ij} for three newly discovered AlAs polymorphs.

Structure	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}
<i>o</i> C12-AlAs	126.9	121.2	152.8	46.6	38.2	42.8	38.8	45.0	51.6
<i>h</i> P6-AlAs	125.7	—	146.8	44.3	—	—	38.1	50.8	—
<i>c</i> I24-AlAs	104.0	—	—	41.9	—	—	49.1	—	—

The appearance of soft phonon modes denotes the dynamical instability and will lead to distortion of crystal. Phonon dispersions of *o*C12-, *h*P6-, and *c*I24-AlAs at **zero** pressure are calculated and plotted in Fig. 2. There is no imaginary frequency in the entire Brillouin zone, suggesting these new phases are all dynamically stable.

Fig. 2. Phonon dispersion spectra for *o*C12-AlAs (a), *h*P6-AlAs (b), and *c*I24-AlAs (c).

3.3. Phase transformation under pressure

Pressure, as a fundamental physical variable, notably affects the chemical and physical properties of material. High-pressure technology is an interesting domain for material research. The

enthalpy (per formula unit, f.u.) curves relative to zb-AlAs as a function of hydrostatic pressure up to 60 GPa for the AlAs polymorphs are presented in Fig. 3. It is clearly seen that zb-AlAs transforms to NiAs-AlAs under the pressure 9.2 GPa, which not only agrees with experimental values (7 ± 5 GPa [7] and 14.2 GPa [8]) but also matches the theoretical values (5.34 [32], 6.1 [9], 6.99 [33], 7 [11], 9.15 [10] and 6.68 [34]). The calculated transformation pressure for NiAs-AlAs to cmcm-AlAs is 34.4 GPa, which was consistent with the reported value 36 GPa [12]. *o*C12-, *h*P6-, and *c*I24-AlAs are all pressure driven structures and hold lower energies than those of NiAs- and cmcm-AlAs at ambient pressure. The decompression rate plays an important role during the metastable phase formation, for example, the Si-XII, Si-III and Ge-III phases can be acquired by slowly releasing pressure from Si-II and Ge-II, respectively [35, 36]. However, rapid depressurization causes the formation of Ge-IV phase and Si-VIII/IX phases [37, 38]. *h*P6-AlAs will obtain its energy advantage over that of zb-AlAs at 5.7 GPa during decompression. Meanwhile, *o*C12-AlAs and *c*I24-AlAs attain its energy favorable than that of zb-AlAs at 2.3 GPa and 2.5 GPa, respectively. Therefore, *o*C12-, *h*P6-, and *c*I24-AlAs may be obtained by following steps: a) zb-AlAs loading pressure, b) forming NiAs-AlAs, c) quenching NiAs-AlAs with controlled unloading rate.

Fig. 3. Enthalpy curves (relative to zb-AlAs) as functions of pressure for various AlAs polymorphs. b is the zoomed in views of the selected region on the left panel.

3.4. Mechanical properties

The pressure versus volume curves of *o*C12-, *h*P6-, and *c*I24-AlAs are fitted to Birch-Murnaghan equation of state (BM-EOS) [39].

$$; \quad (4)$$

Herein, V_0 and V represent the volume per formula unit at zero pressure and given pressure, respectively; B_0 and B_0' represent the isothermal bulk modulus and its first pressure derivative, respectively. The fitting results and a series value of pressure versus volume are presented in Fig. 4. The obtained values of V_0 , B_0 and B_0' are listed in Table 3. Among the three new AlAs structures, *c*I24-AlAs has the largest volume ($45.30 \text{ \AA}^3$) per formula unit at zero pressure and the largest volume compressibility (32.70%); *o*C12-AlAs and *h*P6-AlAs have the similar ($42.06 \text{ \AA}^3$ and $41.97 \text{ \AA}^3$, respectively) and volume compressibility (31.82 % and 31.65 %, respectively).

Fig. 4. Volumes of *o*C12-, *h*P6-, and *c*I24-AlAs as functions of pressure. The scatter symbol and solid lines represent the calculated data and fitting results, respectively.

Elasticity anisotropy is important for understanding the micro-cracks produced in ceramic materials and significantly influences materials' engineering application [40]. As a widely used criterion, the degree of anisotropy in the bonding between atoms in different planes can be measured by the shear anisotropy. The shear anisotropic factors A_1 , A_2 and A_3 are described for shear planes (1 0 0) between $\langle 0\ 1\ 1 \rangle$ and $\langle 0\ 1\ 0 \rangle$ directions, (0 1 0) between $\langle 1\ 0\ 1 \rangle$ and $\langle 0\ 0\ 1 \rangle$, (0 0 1) between $\langle 1\ 1\ 0 \rangle$ and $\langle 0\ 1\ 0 \rangle$, respectively [41].

;;

(5)

For a cubic structure

(6)

For a hexagonal structure,

;

(7)

For isotropic crystals, A_1 , A_2 and A_3 are all equal to 1. Any value deviation from 1 indicates the degree of shear anisotropy. Our calculated shear anisotropic factors are given in Table 3. Among three new AlAs polymorphs, *cI24*-AlAs has the highest shear anisotropic factor, *hP6*-AlAs has the isotropy for (0 0 1) shear plane, and slight anisotropy for (1 0 0) and (0 1 0) shear planes. For *oC12*-AlP, all the shear planes (1 0 0), (0 1 0) and (0 0 1) exhibit anisotropy.

The bulk modulus (B) and shear modulus (G) are calculated based on the elastic constants [42-44], then Young's modulus (E) and Poisson's ratio (μ) are obtained via Eq. (8). As one basic physical property of solid material, hardness of three new AlAs polymorphs are calculated based on Chen's empirical scheme in accordance with Eq. (9) [45].

;

(8)

;

(9)

The calculated B , G , E , σ , ν , and κ are all presented in Table 3. The value of B agrees well with the fitted value of B derived from the BM-EOS, suggesting the calculation is correct. B and G represents the capacity to resist volume change under load and reversible deformations upon shear stress [46]. Among three newly discovered AlAs polymorphs, *oC12*-AlAs exhibits the similar B , G and E with *hP6*-AlAs, whereas *cI24*-AlAs has the smallest B , G and E . Generally speaking, a higher

E denotes a stiffer material, which indicating that $hP6$ -AlAs and $oC12$ -AlAs are both stiffer than $cI24$ -AlAs. A similar conclusion is achieved in . Generally speaking, for solid material, larger volume means smaller density and larger volume compressibility, imply smaller mechanical modulus, and lower hardness, the relationship has also confirmed by $oC12$ -, $hP6$ -, and $cI24$ -AlAs. The calculated B , G , E and signify that $oC12$ -, $hP6$ -, and $cI24$ -AlAs possess appropriate mechanical properties and these AlAs compound polymorphs extend the industrial applications of aluminum compounds.

Table 3

BM-EOS fitting results (, , and), shear anisotropic factors (, , and), and mechanical parameters (B , G , κ , E , μ , and) for three new AlAs polymorphs. , B , G , E , and are expressed in GPa; whereas is expressed in $\text{\AA}^3$, and the others hold dimensionless units.

structure							B	G	κ	E	μ		
$oC12$ -AlAs	74.2	3.90	42.06	0.983	0.895	1.004	74.0	43.0	0.581	108.1	0.257	6.57	
$hP6$ -AlAs	75.6	3.89	41.97	1.037	—	1.000	74.8	43.6	0.583	109.5	0.256	6.68	
$cI24$ -AlAs	69.1	3.95	45.30	1.526	—	—	67.4	35.4	0.525	90.4	0.277	4.59	

3.5. Electronic properties

Based on the hybrid functional HSE06, the band structures of zb -, $oC12$ -, $hP6$ -, and $cI24$ -AlAs at zero pressure are calculated and presented in Fig. 5. For zb -AlAs (Fig. 5a), the valence band maximum (VBM) and conduction band minimum (CBM) are located at G point and X points, respectively. The VBM and CBM are separated by a forbidden band of 2.081 eV, in agreement with the earlier theoretical value (2.1 eV [47], 2.24 eV [48]) and experimental value (2.16 eV [49], 2.2 eV [50] and 2.23 eV [51]). At zero pressure, $oC12$ -AlAs (Fig. 5b) and $hP6$ -AlAs (Fig. 5c) are both semiconductors with indirect band gaps of 0.468 eV and 1.356 eV, respectively. For $oC12$ -AlAs, VBM and CBM are located at Z point and Y points, respectively. For $hP6$ -AlAs, VBM is located at G point and CBM at M point, respectively. $cI24$ -AlAs (Fig. 5d) is also a semiconductor with a direct band gap (1.761 eV) at G point.

Fig. 5. Calculated band structures for zb-AlAs (a), oC12-AlAs (b), hP6-AlAs (c), and cI24-AlAs (d) at ambient pressure. The Fermi level is represented by a horizontal red line.

4. Conclusion

In summary, oC12-, hP6-, and cI24-AlAs are proposed by employing CALYPSO. The elastic constants and phonon dispersion spectra are calculated to certify the mechanical and dynamic stabilities of the three newly discovered phases. Based on calculated enthalpy curves relative to zb-AlAs as functions of pressure for various AlAs polymorphs, oC12-, hP6-, and cI24-AlAs all hold energy advantages over those of cmcm-, and NiAs-AlAs at ambient pressure. The new AlAs polymorphs are all pressure driven phases. zb-AlAs first transforms into NiAs-AlAs at 9.2 GPa and then to cmcm-AlAs at 34.4 GPa. oC12-, hP6-, and cI24-AlAs may be obtained by quenching NiAs-AlAs with controlled unloading rate. Calculation for mechanical properties reveals that the hardness of oC12-, and hP6-AlAs are similar, (6.57 GPa and 6.68 GPa, respectively), both higher than that of cI24-AlAs (4.59 GPa). The shear anisotropic factors of oC12-, and hP6-AlAs are similar,

and both smaller than that of *c*I24-AlAs. The electronic band structures calculation illustrate that all the three newly discovered AlAs polymorphs are semiconductors with gaps smaller than that of *zb*-AlAs. *o*C12-AlAs and *h*P6-AlAs are both indirect semiconductors with band gaps 0.468 eV and 1.356 eV, respectively. *c*I24-AlAs is a direct semiconductor with a gap value of 1.761 eV.

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