



An interatomic potential for aluminum arsenide: A molecular dynamics study

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ARTICLE INFO

Article history:

Received 24 March 2010

Accepted 4 May 2010

Keywords:

Semiconductor compound

Aluminum arsenide

Molecular dynamics simulation

Atomistic modeling

Interatomic potential

ABSTRACT

An effective interatomic potential is proposed for AlAs. Molecular dynamics technique was used to simulate the energetics of zinc-blende, wurtzite, rocksalt and NiAs crystal structures of AlAs. The calculated cohesive energy, bulk modulus and C_{11} elastic constant at room temperature and melting temperature agreed very well with experimental values. By constructing a common tangent to the calculated energy versus volume curves for zinc-blende and rocksalt structures of AlAs, the pressure of structural transition between these phases was found to be 10 GPa. Vibrational density of states and specific heat were compared with first-principle calculations, displaying very good agreement. The proposed interatomic potential allows us to predict the temperature dependence of several properties, such as the elastic constants and specific heat.

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1. Introduction

In spite of the well established experimental characterization of $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ heterostructure systems, there is still a lack of experimental data for AlAs III–V semiconductors. The main reason could be the difficulty of growing large good quality samples of this material, due to its hygroscopic property. This is reflected, for instance, in a large range of experimental values for elastic constants, ranging from 119.9 to 151 GPa [1–4]. Most of the properties recorded for pure AlAs, such as Debye temperature and temperature dependence of the specific heat, to cite just two, are obtained by some sort of interpolation based on known values of physical quantities for related compounds [4]. The structural phase transition in AlAs induced by pressure has been studied in a diamond anvil cell by Venkateswaran et al. [5] and by Greene et al. [6]. It was shown that the zinc-blende AlAs phase undergoes a first order transition to the NiAs structure [6], besides the rocksalt form, which is very close in energy [7]. On the other hand, theoretically, most of the studies are based on the *ab initio* pseudo-potential approach, generally carried out to predict the pressure-induced structural phase transition and electronic ground-state properties [7–11]. From the classical point of view, several empirical potentials have been proposed. Kagaya and Soma proposed interatomic force constants and analyzed lattice dynamics, to obtain the phonon dispersion curves for several tetrahedral compounds [12]; Nakamura et al. incorporated Coulomb interaction in the Tersoff conventional potential, in order to study epitaxial growth of III–V semiconductors [13]; Ito and Kangawa proposed an empirical po-

tential to study the wurtzite–zinc-blende structural stability of semiconductors [14,15] and Varshney et al. proposed a more complex effective interatomic potential to describe structural phase transitions and elastic properties induced by pressure [16].

Here we propose an effective interatomic potential which has the same functional form as the interatomic potential used by Ebbsjo et al. to describe topology in amorphous gallium arsenide [17]. This interatomic potential has been used to describe the structural, dynamical, and thermal properties of several materials with very good results [17–28]. In the present paper, the stability of crystal-line structures, their vibrational density of states, specific heat, and elastic moduli are studied as a function of temperature. The aim is to find an interatomic potential able to describe the structural, thermodynamics, dynamical and mechanical behavior of AlAs as well as its structural phase transition under pressure.

2. Interatomic potential

The AlAs interatomic potential introduced here is based on the interatomic potential proposed by Ebbsjo et al. [17], in which two- and three-body interactions were considered. This effective interatomic potential has been used to describe several II–VI and III–V semiconductors, with very good transferability and accuracy.

The total energy of the system is given by:

$$V = \sum_{i<j} \phi_{ij}^{(2)}(r_{ij}) + \sum_{i<j<k} \phi_{jik}^{(3)}(r_{ij}, r_{ik}). \quad (1)$$

The two-body interaction combines steric repulsion, Coulomb, charge-induced dipole and dipole–dipole interactions. It is written as:

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$$\phi_{ij}^{(2)}(r) = \frac{H_{ij}}{r^{\eta_{ij}}} + \frac{Z_i Z_j}{r} e^{-r/\lambda} - \frac{\alpha_i Z_j^2 + \alpha_j Z_i^2}{2r^4} e^{-r/\xi} - \frac{W_{ij}}{r^6}. \quad (2)$$

Here, $r = |\vec{r}_i - \vec{r}_j| \equiv r_{ij}$, Z_i the effective charge in units of electron charge $|e|$, H_{ij} and η_{ij} are respectively the strength and the exponent of the steric repulsion, α_i the electronic polarizability of each element and W_{ij} the strength of the van de Waals attraction. λ and ξ are screening lengths for Coulomb and charge-dipole interactions. The two-body interaction is also truncated at r_{cut} and shifted, for $r \leq r_{cut}$, to make the potential and its first derivative continuous at r_{cut} . The shifted two-body effective interatomic potential is written:

$$\phi_{ij}^{(2)shifted}(r) = \begin{cases} \phi_{ij}^{(2)}(r) - \phi_{ij}^{(2)}(r_{cut}) - (r - r_{cut}) \left[d\phi_{ij}^{(2)}(r)/dr \right]_{r=r_{cut}}, & r \leq r_{cut} \\ 0, & r > r_{cut} \end{cases}. \quad (3)$$

The three-body interatomic potential describes both bond bending and bond stretching effects. It is given by:

$$\phi_{jik}^{(3)}(r_{ij}, r_{ik}) = R^{(3)}(r_{ij}, r_{ik}) P^{(3)}(\theta_{jik}), \quad (4)$$

where

$$R^{(3)}(r_{ij}, r_{ik}) = B_{jik} \exp\left(\frac{1}{r_{ij} - r_0} + \frac{1}{r_{ik} - r_0}\right) \Theta(r_0 - r_{ij}) \Theta(r_0 - r_{ik}) \quad (5)$$

and

$$P^{(3)}(\theta_{jik}) = \frac{(\cos \theta_{jik} - \cos \bar{\theta}_{jik})^2}{1 + C_{jik}(\cos \theta_{jik} - \cos \bar{\theta}_{jik})^2}. \quad (6)$$

$\Theta(r_0 - r_{ij})$ is the step function, B_{jik} the strength of the three-body interaction, θ_{jik} is the angle formed by \vec{r}_{ij} and \vec{r}_{ik} , r_0 the cutoff for these interactions, and $\bar{\theta}_{jik}$ and C_{jik} are constants. Discussion about the three-body term can be found in [24]. As used in previous simulations, the exponent η_{ij} was fixed at 7, 9, and 7, for Al–Al, Al–As, and As–As respectively. The screening lengths were taken as $\lambda = 5.0 \text{ \AA}$ and $\xi = 3.75 \text{ \AA}$ and the cutoff distance for the two-body interaction was fixed at $r_{cut} = 9.3 \text{ \AA}$.

The parameters in the interatomic potential was chosen in order to reproduce the experimental values of the cohesive energy and lattice constant at 0 K, as well as the bulk modulus and C_{11} elastic constant at 300 K. Table 1 summarizes these parameters for the AIs effective interatomic potential. In Table 2 we compare some experimental physical quantities with values derived from the proposed interatomic potential.

Table 1

Parameters for two and three body effective interatomic potential of AIs. These values were used in MD simulations of structural, thermodynamics, dynamical and mechanical proprieties of AIs.

	Z_i (e)	α_i (\AA^3)		
	Al	1.000461	0.0	
	As	-1.000461	2.0	
Two-body	$H_{ij}(\times 10^{-19} \text{ J \AA}^{\eta_{ij}})$	η_{ij}	$W_{ij}(\times 10^{-19} \text{ J \AA}^6)$	
	Al–Al	248.569	7	0
	Al–As	6747.893	9	541.05
	As–As	3898.299	7	0
	$\lambda = 5.0 \text{ \AA}$	$\xi = 3.75 \text{ \AA}$	$r_{cut} = 9.3 \text{ \AA}$	$e = 1.602 \times 10^{-19} \text{ C}$
Three-body	$B_{jik}(\times 10^{-19} \text{ J})$	$\bar{\theta}_{jik}$ ($^\circ$)	C_{jik}	
	Al–As–Al	9.529	109.47	10
	As–Al–As	9.529	109.47	10
	$\gamma = 1.0 \text{ \AA}$	$r_0 = 3.45 \text{ \AA}$		

Table 2

Molecular dynamics results and experimental values for some physical quantities for AIs zinc-blende structure.

	MD	Experiments
Lattice constant (\AA)	5.6524 (at 0 K)	5.6524 (extrapolated to 0 K)
Cohesive energy (eV/N)	-3.850	-3.850
Bulk modulus (GPa)	79.8 (at 0 K)	74 (at 300 K)
	79.4 (at 300 K)	
Elastic constant C_{11} (GPa)	123.3 (at 0 K)	119.9 (at 300 K)
	119.1 (at 300 K)	
Melting temperature (K)	2050 (± 40)	2013

3. Results

In this section, we will first define the lattice energy as a function of volume for several crystalline structures and thence derive an equation of state. This calculation is important to characterize the most stable structure as well as the pressure needed to induce a structural phase transition. For the most stable structure, the zinc-blende AIs structure, several thermodynamics, vibrational and mechanical properties will be discussed. For this analysis, molecular dynamics simulations were performed in the (NPT) ensemble, integrating the equations of motion by the velocity Verlet algorithm, with a time step of 1.5 fs. All results were obtained with a system consisting of 8000 particles (4000 Al + 4000 As). The cubic system has an edge of 56.524 \AA reproducing the extrapolated experimental density at 0 K of 3.748 g/cc .

3.1. Energetics of the structures

The energy per particle was calculated as a function of volume per particle for the zinc-blende, wurtzite, rocksalt and NiAs structures at 0 K. These energies were obtained by compressing/dilating the system hydrostatically. Fig. 1 displays the energies for all four structures. In these figures, the continuous line is a fitting of the Murnaghan equation of states, $E(V) = \frac{BV}{B'(B'-1)} [B'(1 - \frac{V_0}{V}) + (\frac{V_0}{V})^{B'} - 1] + E(V_0)$, to these energies, where B is the bulk modulus, B' its first pressure derivative, and V_0 the equilibrium volume. In this fitting, only the energy data at volumes within $\pm 2 \text{ \AA}^3$ of each minimum was used.

The effective interatomic potential describes the most stable structure, its lattice constant, bulk modulus and its first derivative. From the common tangent to the zinc-blende and rocksalt $E-V$ curves it can be estimated that the transition pressure is around 10 GPa.

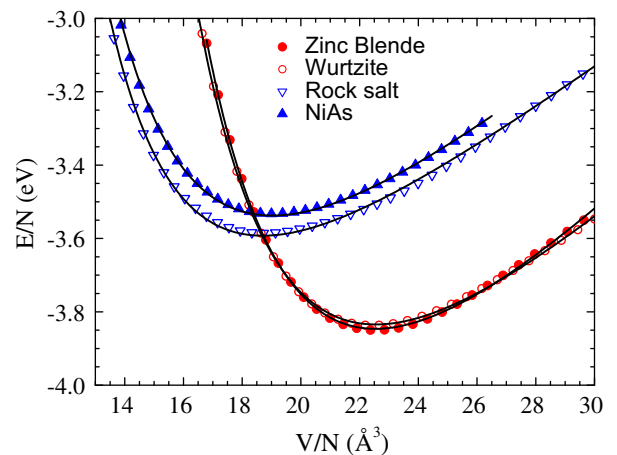


Fig. 1. Energy per particle plotted against volume per particle, for zinc-blende, wurtzite, NiAs and rocksalt structures. The continuous line shows the best-fit Murnaghan equation of states.

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