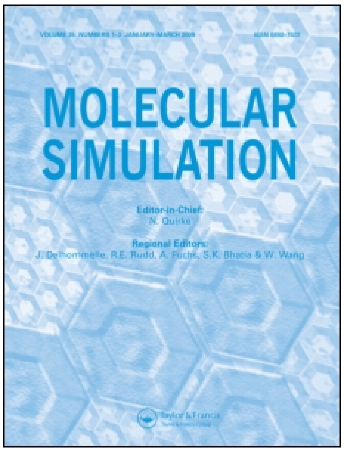

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MOLECULAR DYNAMICS STUDY OF ZINC-BLENDE GaN, AlN AND InN

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We present a result of the molecular dynamics calculations with used a three-body empirical Tersoff potential. The parameters of the Tersoff potential are determined for nitride compound semiconductors such as GaN, AlN and InN. The structural and thermodynamic properties of GaN, AlN and InN in zinc-blende structure are presented. We report the equilibrium lattice constants, the bulk moduli, the cubic elastic constants, thermal expansion coefficient and specific heat. Good agreement is obtained with recent experimental and theoretical results for all constants.

Keywords: Semiconductors; Tersoff potential; lattice constants; cubic elastic constants

1. INTRODUCTION

The group III nitrides are currently being actively investigated in view of their potential (GaN, AlN and InN) for short-wavelength electroluminescent devices and the extreme hardness and high thermal conductivity. All these materials also have potential for high-temperature, high-power and high-frequency electronics. These properties are closely related to their wide band gaps and strong (mixed ionic and covalent) bonding. An overview of the recent interest in wide -band-gap semiconductors and the particular

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role of the group III nitrides can be found in several recent conference proceeding [1–4] while general information on the properties of group III nitrides is available in a recent compilation [5].

At ambient conditions, the materials were known to crystallize only in the structure Wurtzite (space group C_{6v}^4) form, which differs from the zinc-blende structure (group space T_d^2) mainly at the relative positions of the third neighbors and beyond. Zinc-blende GaN, which is thermodynamically metastable phase of GaN, has been epitaxially stabilized on β – SiC and MgO(100) substrates [6,7] which are closely lattice matched to β – GaN, and GaAs [8,9] and Si substrates [10]. The more ionic compound AlN, which is generally reported to be non polymorphous, crystallizes at ambient condition in the wurtzite structure [11]. However; several works report the occurrence of a metastable zinc-blende polytype of AlN [12]. Because of the reactivity of AlN, high-purity source material and an oxygen-free environment are required to grow AlN crystals of good quality. Therefore, AlN is not a particular easy material to study experimentally and most researchers in the field have concentrated on GaN. The position of the aluminum and the nitrogen atom in the periodic table indicates that the physical properties of AlN should be similar to those of SiC.

Nitride compound semiconductors such as GaN and InN have recently attracted much attention as promising materials for optical devices such as displays and for high-density optical data storage. Despite the importance of the nitride compound semiconductors, very little attempt has been made to obtain the empirical interatomic potentials for them. This is because of the lack of reference data on structural and thermodynamic properties for nitride compound semiconductors needed to determine a large number of empirical potential parameters in cubic phase. Experimentally very little is known about the electronic, optical and mechanical properties of the cubic group III-V nitrides. In recent study, Rubio *et al.* [13] performed a theoretical calculation for cubic GaN and AlN.

In this work, we have used a model potential developed by Tersoff [14] coupled with molecular dynamics (MD) method [15]. We adjust the parameters for the potential using data from *ab-initio* calculations and experimental results to reproduce the relative stability between zinc blende and rocksalt structures. Theses potentials are tested by calculating the elastic constants for nitride-compounds semiconductors, equilibrium lattice parameters, bulk modulus, pressure derivatives and cohesive energies in the cubic structure. We tested with this parameters the transferability of the potential by calculating the thermal expansion coefficient and the specific heat. We briefly describe this model potential and calculation method in Section 2. Then, the results of our calculation are presented and discussed in Section 3.

2. SIMULATION DETAILS

The Tersoff potential is based on the bond-order concept [14]. The interatomic potential energy between two neighboring atom i and j is written as

$$V_{ij} = f_c(r_{ij})[A\exp(-\lambda_1 r_{ij}) - \chi B b_{ij}\exp(-\lambda_2 r_{ij})] \tag{1}$$

$$f_c(r_{ij}) = \left\{ \begin{array}{c} 1, r \prec R - D \\ \frac{1}{2} - \frac{1}{2}\sin[\frac{\pi}{2}(r - R)/D],\ R - D \prec r \prec R + D \\ 0,\ r \succ R + D \end{array} \right\} \tag{2}$$

Where b_{ij} is the many-body bond-order parameter describing how the bond-formation energy (the attractive part of V_{ij}) is affected by local atomic arrangement due to the presence of other neighboring atoms-the k atoms. It is a many-body function of the positions of atoms i, j and k. It has the form [14].

$$b_{ij} = (1 + \xi_{ij}^{n_i})^{-1/(2n)}. \tag{3}$$

with

$$\xi_{ij} = \sum_{k \neq i,j} f_c(r_{ij})\beta_i g(\theta_{ijk})\exp[\lambda_3^3(r_{ij} - r_{ik})^3] \tag{4}$$

$$g(\theta) = 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h - \cos\theta)^2} \tag{5}$$

$$a_{ij} = (1 + \alpha^n \eta_{ij}^n)^{-1/(2n)} \tag{6}$$

$$\eta_{ij} = \sum_{k \neq i,j} f_c(r_{ik})\exp[\lambda_3^3(r_{ij} - r_{ik})^3] \tag{7}$$

Where ξ is called the effective coordination number and $g(\theta)$ is a function of the angle between r_{ij} and r_{ik} that has been fitted to stabilize the tetrahedral structure.

The nitrides form a specific subgroup of the III-V compounds characterized by high ionicity, very short bond lengths, as a results of the short

TABLE I The adjusted Tersoff parameters for GaN, AlN and InN

	GaN	*AlN*	*InN*
A(eV)	2975.4	1730.00	3297.0
B(eV)	540.310	246.1	3297.0
λ_1(Å^{-1})	3.3718	3.20	3.3
λ_2(Å^{-1})	2.220	1.853	1.853
β	1.572410^{-6}	1.110^{-6}	1.110^{-6}
n	0.72751	0.72	0.72
c	38049	10039	10039
d	4.384	16.217	16.217
h	−0.57058	−0.598	−0.598
r_{cut}(Å)	2.40	2.34	2.6405
d_{cut}(Å)	0.20	0.15	0.15

bonds of the nitrides, these materials show many the properties with diamond, notably exceptional hardness, high lattice thermal conductivity and a wide band gap [17]. No parameters in the literature have been found for the Tersoff potential which fits crystalline GaN, AlN and InN. So, we start our fitting with the Tersoff parameters of carbon [18] as input parameter for our simulation. The parameters are fitted to polytype energies [16, 19–22]. Table I gives the adjusted parameters of group III-Nitrides.

2.1. Computer Simulations

Molecular Dynamics (MD) is a direct simulation technique at the atomic level. Almost all the physical properties of a material may be determined using molecular dynamics. It requires generally an inter-particle potential. Thus molecular-dynamic computer simulations have been performed to determine the prediction of Tersoff potential for solid structure under temperature and pressure effect. The MD cell is formed of a cube of side L with $3 \times 3 \times 3$ diamond units cells, where 216 particles are included. The periodic boundary conditions are applied. The atomic structure of solid has been calculated by using a NVT Molecular Dynamics simulation. The MD routine is based on a fifth-order Gear-Predictor-Corrector algorithm of the Newtonian equations of motion using a neighbor list technique with a time step $\Delta t = 1.86\,\mathrm{fs}$ and an efficient network cube algorithm for nearest-neighbor book keeping, details are given elsewhere [23].

After an equilibration period, a histogram of atomic separations is produced in order to compute the pair correlation function [24] $g(r)$ and other various properties which are computed along the trajectory of the system in phase space.

2.2. Calculation of the Elastic Moduli

The elastic moduli of a cubic crystal may be divided into two classes, the bulk modulus $B=(C_{11}+2C_{12})/3$ and the two shear moduli $(C_{11}-C_{12})$ and C_{44}. The bulk modulus is related to the curvature of $E(V)$

$$B(V) = -VP'(V) = VE''(V) \tag{8}$$

where V is the volume of the unit cell, $E(V)$ is the energy/unit cell at volume V and $P(V)=-E'(V)$ is the pressure required to keep the cell at volume V. Here begin by making a least squares fit of the computed energies to the form proposed by Birch [25]

$$\begin{aligned} E(V) = E_0 + \frac{9}{8}B_0V_0[(V_0/V)^{2/3}-1]^2 + \frac{9}{16}B_0(B_0'-4)V_0[(V_0/V)^{2/3}-1]^3 \\ + \sum_{n=4}^{N}\gamma_n[(V_0/V)^{2/3}-1]^n \end{aligned} \tag{9}$$

where E_0, B_0 and B_0' are, respectively, the equilibrium energy, volume, bulk modulus and pressure derivative of the bulk modulus, while N is the order of the fit.

The shear moduli require knowledge of the derivative of the energy as a function of a lattice strain [26]. In the case of a cubic lattice, it is possible to choose this strain so that the volume of the unit cell is preserved. The strain can be chosen so that the energy is an even function of the strain, whence an expansion of the energy in powers of the strain contains no odd powers. Thus for the calculation of the modulus $C_{11}-C_{12}$. We have used the volume-conserving orthorhombic strain tensor,

$$\vec{\varepsilon} = \begin{pmatrix} \delta & 0 & 0 \\ 0 & -\delta & 0 \\ 0 & 0 & \delta^2/(1-\delta^2) \end{pmatrix} \tag{10}$$

Application of this strain changes the total energy from its unstrained value to

$$E(\delta) = E(-\delta) = E(0) + (C_{11}-C_{12})V\delta^2 + O[\delta^4] \tag{11}$$

Where V is the volume of the unit cell and $E(0)$ is the energy of the unstrained lattice at volume V. For the elastic modulus C_{44}, we have used the volume-conserving monoclinic strain tensor

$$\vec{\varepsilon} = \begin{pmatrix} 0 & \frac{1}{2}\delta & 0 \\ \frac{1}{2}\delta & 0 & 0 \\ 0 & 0 & \delta^2/(4-\delta^2) \end{pmatrix} \tag{12}$$

which changes the total energy to

$$E(\delta) = E(-\delta) = E(0) + \frac{1}{2}C_{44}V\delta^2 + O[\delta^4] \tag{13}$$

Note that there is no pressure or stress term [27] in either (11) and (13) since the strains (10) and (12) are constructed so that $\Delta V = 0$.

The strain (10) and (12) can be used for any cubic lattice. In the general case, the internal parameters of the lattice must be chosen to minimize the total energy of the strained structure. Fortunately, the lattices discussed here fall into a restricted subset of the cubic lattices, where all of the atoms sit at inversion sites, even under the reduced symmetry caused by the strains (11) and (13). For isotropic cubic crystal, the bulk modulus is given exactly by

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{14}$$

just as for a cubic crystal [28].

3. NUMERICAL RESULTS

3.1. Partial Pair Distribution Function

In order to test the stability of our zinc-blende structure of GaN, AlN and InN at finite temperature within the Tersoff potential model, we have calculated the pair distribution functions, at 300 K. Figure 1 shows the pair distribution function of GaN, AlN and InN. In Table II the amplitude and peaks positions are given.

The first peak position is 1.93 Å, 1.87 Å and 2.13 Å for GaN, AlN and InN, respectively, they represent the distance between a zinc-blende lattice point and its first neighboring tetrahedral site. The coordination numbers are evaluated by the equation

$$\eta = 4\pi\rho_0 \int_0^R r^2 \rho(r) dr \tag{15}$$

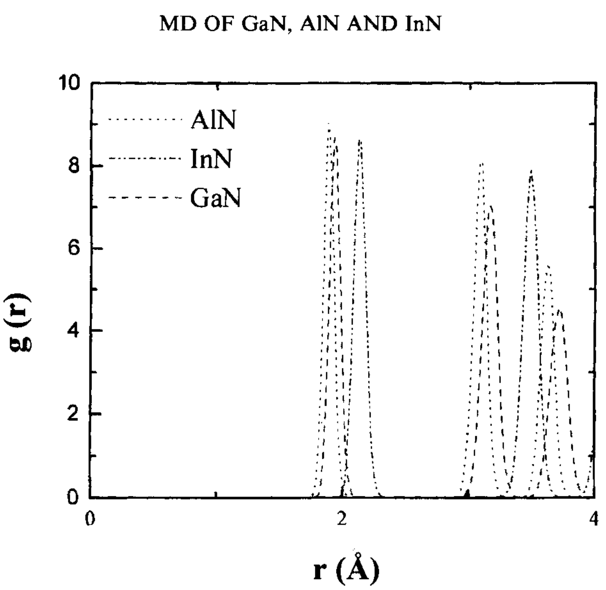

FIGURE 1 Partial pair distribution functions for GaN(a), AlN(b) and InN(c).

TABLE II Values of peak distances and coordinate numbers of pairs for (GaN, AlN, InN) in the zinc-blende structure at 300 K. Experimental values in parenthese (from Ref. [26])

		GaN	*AlN*	*InN*
1st pick	distance (Å)	1.939(1.944)	1.879(1.896)	2.138(2.142)
	number of pair	3.97(4)	3.97(4)	3.971(4)
2nd pick	distance (Å)	3.717(3.174)	3.101(3.096)	3.489(3.498)
	number of pair	11.941(12)	11.942(12)	11.945(12)
3rd pick	distance (Å)	3.717(3.722)	3.626(3.631)	4.098(4.103)
	number of pair	11.951(12)	11.950(12)	11.955(12)
4th pick	distance (Å)	4.485(4.490)	4.375(4.380)	4.944(4.949)
	number of pair	5.971(6)	5.978(6)	6.01(6)

where ρ_0 is the number density of atoms, it is in good agreement with experimental values [26]. This confirm the accuracy of our fitting for group III-Nitrides.

3.2. Ground-state Properties

The calculated ground-state energies plotted as functions of the volume for group III-Nitrides are shown in Figure 2 for the zinc-blende phase. The equilibrium parameters from the Birch equations [25] fit (E_0, V_0, B_0 and B'_0) are listed in Table III. Our calculated equilibrium lattice constants for GaN and AlN is in agreement with the experimental result [16, 19, 20].

Our values of bulk modulus are also in agreement with theoretical studies of Christensen *et al.* [29] which used the LMTO method [30] in its

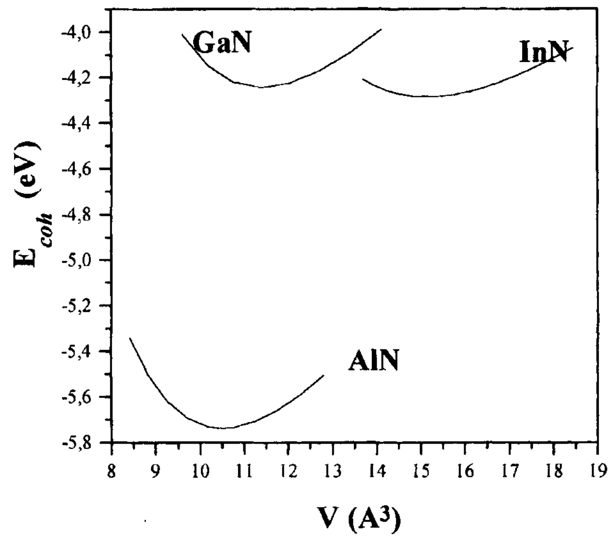

FIGURE 2 Calculated total energies of GaN(a), AlN(b) and InN(c) in the zinc-blende structure as a function of volume *V*.

TABLE III The Calculated equilibrium lattice constant a, bulk moduli B, the pressure derivatives and the cohesive energies for (GaN, AlN, InN) in the zinc-blende structure

	GaN	*AlN*	*InN*
Present	4.501	4.379	4.949
a(Å) Calc.	4.46^{a}, 4.46^{b}	4.37^{a}, 4.32^{b}	4.95^{a}, 4.92^{b}
Exp.	4.5^{c}	4.37^{d}	4.98^{e}
Present.	1.897	2.083	1.429
B(Mbar) Calc.	2.01^{b}, 1.84^{a}	2.03^{b}, 2.15^{a}	1.39^{b}, 1.37^{a}
Exp.	1.90^{f}	2.02^{f}	–
Present.	4.607	4.139	4.672
B′(Mbar) Calc.	3.9^{b}, 4.6^{a}	3.2^{b}, 4.0^{a}	4.4^{b}, 4.3^{a}
Exp.	–	–	–
Present.	4.320	5.815	4.363
E_{coh}(eV) Calc.	–	–	–
Exp.	4.45^{g}	5.75^{g}	–

[a]Ref. [39]; [b]Ref. [34]; [c]Ref. [19]; [d]Ref. [20]; [e]Ref. [16]; [f]Ref. [21]; [g]Ref. [22].

scalar-relativistic form in conjunction with the local density approximation (LDA) for zinc-blende type semiconductors. The differences between calculated Nitrides modulus and calculated values of N. E. Christensen [29] are within 3.1 – 4.3% for all the elastic constants. The deviation from the experimental values [21] is smallest 0.1% and 2.9% for GaN and AlN. However, no experimental data is available for the bulk modulus of InN.

It is interesting to compare our results for B_0 with the values obtained using the empirical relation [31] $B_0 = 1761d^{-3.5}$, where d is the nearest-neighbor distance in Angstroms. This relation gives $B_0 = 1.70$, 1.889 and 1.222 Mbar for GaN, AlN and InN, respectively, in excellent agreement with our results. This suggests that the Tersoff potential describes well the homogeneous response of group III-Nitrides to hydrostatic compression.

3.3. Elastic Properties

We have determined the elastic constants at 300 K: C_{11} and C_{12} from Eq. (11) combined with Eq. (14) and C_{44} from Eq. (13). Figure 3 plots the energy of GaN, AlN and InN as a function of orthorhombic strain (10) for the fixed volume associated with the cubic lattice constant ($a_{\mathrm{GaN}} =$ 4.501, $a_{\mathrm{AlN}} = 4.379$, $a_{\mathrm{InN}} = 4.949$) Å. Figure 4, display the energy of the monoclinic strain (12). The slop of these curves yield $C_{11} - C_{12}$ and C_{44}.

Table IV shows our zinc-blende elastic constants C_{11}, C_{12} and C_{44} together with results from two earlier theoretical studies; Wright *et al.* [32] for GaN, AlN and InN using a method based with DFT *ab-initio* pseudopotential and plane wave expansions. We have also compared our results with the theoretical studies of Kim *et al.*, using DFT [33] implemented *via* the full potential linear muffin-tin orbitals (FP-LMTOs) method. The agreement with experimental is good.

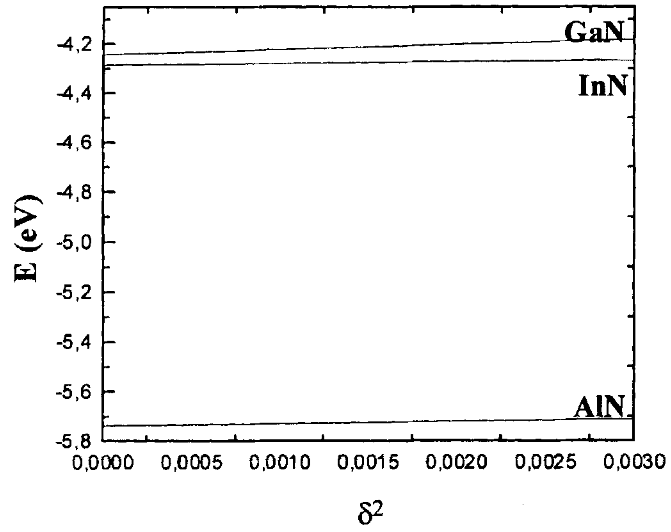

FIGURE 3 Energy as a function of the square of the orthorhombic strain (10).

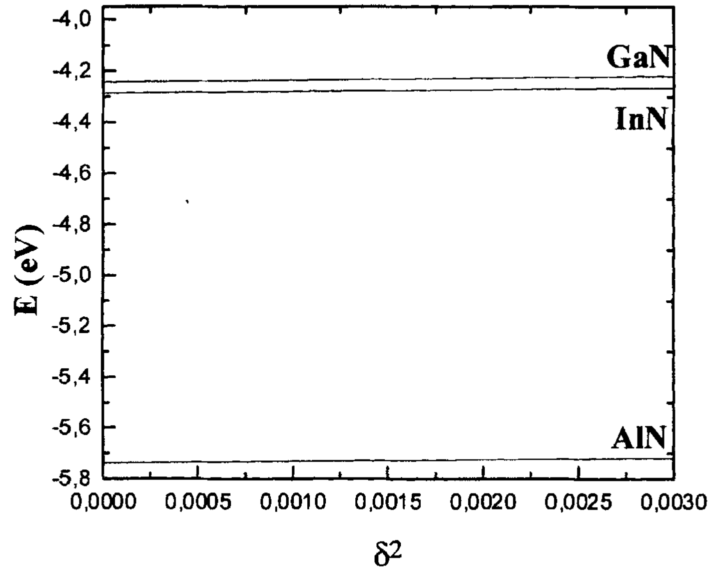

FIGURE 4 Energy as a function of the square of the monoclinic strain (12).

TABLE IV The Calculated and experimental elastic constants C_{ij} (Mbar) of GaN, AlN and InN in the zinc-blende structure

	GaN	*AlN*	*InN*
Present.	2.59	3.02	1.896
C_{11} Calc.	2.93[a], 2.96[b,c], 2.61[d]	3.04[a], 3.48[e], 3.04[b,c], 3.01[d]	1.87[a], 1.84[b,c], 2.14[d]
Exp.	2.64[f]	–	–
Present.	1.551	1.63	1.196
C_{12} Calc.	1.59[a], 1.54[b,c], 1.27[d]	1.60[a], 1.68[e], 1.52[b,c], 1.62[d]	1.25[a], 1.16[b,c], 1.37[d]
Exp.	1.53[f]	–	–
Present.	1.894	1.92	1.478
C_{44} Calc.	1.55[a], 2.06[b,c]	1.93[a], 1.35[e], 1.99[b,c]	0.86[a], 1.77[b,c]
Exp.	0.68[f]	–	–

[a]Ref. [32]; [b]Ref. [33]; [c]Ref. [34]; [d]Ref. [35]; [e]Ref. [38]; [f]Ref. [37].

4. DYNAMIC PROPERTIES

4.1. Mean Square Displacements

The mean square displacement of atoms in a simulation can be easily computed by its definitions

$$\mathrm{MSD} = \langle r(t) - r(0) \rangle \tag{16}$$

Where $\langle \cdots \rangle$ denotes here averaging over all the atoms (or all the atoms in a given subclass). The mean square displacement (MSD) of GaN, AlN

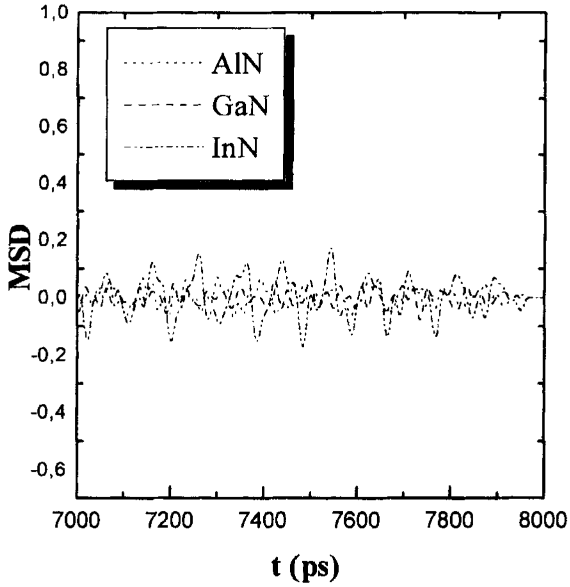

FIGURE 5 Mean displacements of GaN (a), AlN (b) and InN (c) at 300 K.

and InN as function of time is shown in Figure 5, which shows that GaN, AlN and InN has a lattice stability at 300 K while at 1200 K will migrate slightly far due to the diffusion effects. This is due that the MSD contains information on the atomic diffusely. If the system is solid, MSD saturates to a finite value, while if the system is liquid, MSD grows linearly with time. In this case it is useful to characterize the system behavior in terms of the slope, which is the diffusion coefficient D,

$$D = \langle |r(t) - r(0)| \rangle / 6(t_2 - t_1) \tag{17}$$

Where $r(t)$ means the position vector of GaN, AlN and InN at time t. By using the Einstein relation (17) we deduce the diffusing constant at 300 K to be $(0.414, 0.493, 0.454)10^{-8}\,\mathrm{cm}^2/\mathrm{s}$. At 1200 K, we found that the diffusion coefficient is $(0.78, 0.798, 0.707)10^{-8}\,\mathrm{cm}^2/\mathrm{s}$ higher than the values at 300 K.

5. THERMODYNAMIC PROPERTIES

The thermal expansion coefficient α measures how the lattice constant responds to an isometric change in temperature,

$$\alpha = \frac{1}{a}\left(\frac{\partial a}{\partial T}\right)_p \tag{18}$$

The thermal expansion coefficient at room-temperature is then computed from the temperature derivative of these lattice constants. At temperatures below the Debye temperature, quantum effects are important in determining thermal expansion. Above the Debye temperature, quantum effects become unimportant and thermal expansion may be determined from classical calculations, such as molecular dynamics (MD). Thermal expansion is due to anharmonic terms in the cohesive energy for small displacements of the atom about its equilibrium position at 0 K. The thermal expansion of GaN, AlN and InN has been studied in the temperature range from 300 K to 1200 K.

Figure 6 shows the variations of the lattice parameter of GaN, AlN and InN with temperature. The collected data can be fitted to polynomial functions of temperature as:

$$a_{\mathrm{GaN}} = 4.489 + 6.10^{-5}T \tag{19}$$

$$a_{\mathrm{AlN}} = 4.384 + 3.10^{-5}T \tag{20}$$

$$a_{\mathrm{InN}} = 4.954 + 4.10^{-5}T \tag{21}$$

The linear temperature coefficients determined from Eq. (19) to Eq. (21) are $(1.32, 0.68, 0.80)10^{-5}\mathrm{K}^{-1}$ of GaN, AlN and InN, respectively.

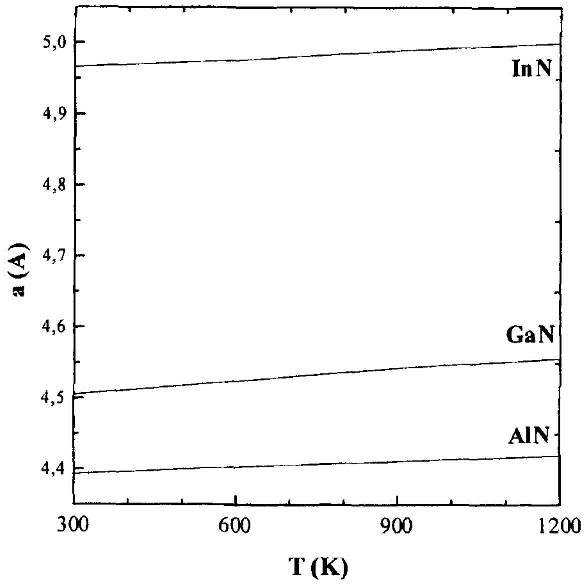

FIGURE 6 The lattice constant as function of GaN, AlN and InN temperature for in the zinc-blende structure.

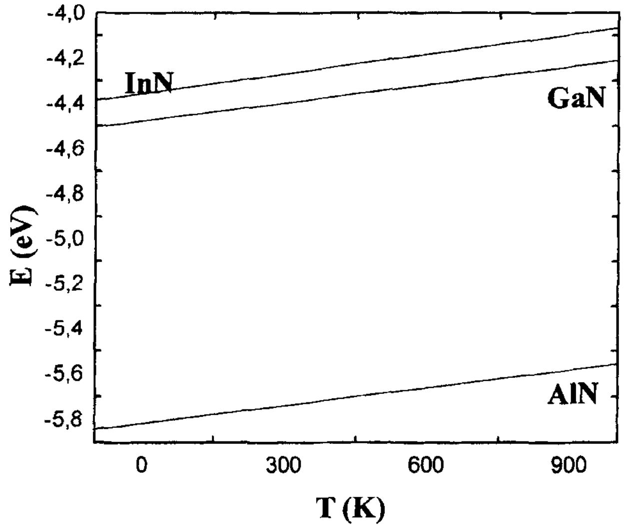

FIGURE 7 The total energy of the system as function of temperature.

The results are in good order of many other semiconductors with zincblende structure, indicating that the average anharmonicity of the interactions in the Tersoff potential is reasonable.

The specific heat of GaN, AlN and InN at constant volume (C_v) is also calculated using the Tersoff potential. The constant-volume heat capacity measures how the internal energy responds to an isometric change in temperature,

$$C_v = \left(\frac{\partial E}{\partial T}\right)_V \tag{22}$$

From Figure 7 we determine the specific heat GaN, AlN and InN, which is estimate to be $C_v = 5.98$; 5.98 and 6.67 cal/K · mol, respectively. This result is certainly in agreement with experiment at high temperature, where the value of is close to 3R, where R is the universal gas constant (R $\approx$ 2 cal/K · mol) for GaN, AlN and InN. This range usually includes room temperature. The fact that is nearly equal to 3R at high temperatures regardless of the substance described is called the Dulong-Petit law.

6. CONCLUSION

We have proposed empirical parameters for Tersoff potentials for GaN, AlN and InN. We have tested the validity of our parameters by calculating elastic constants for nitride-compound semiconductors, lattice parameters, bulk modulus, thermal expansion coefficient and specific heat. The result of the thermal and dynamical properties of GaN, AlN and InN are in the same order of many other semiconductors with zinc-blende structure. The diffusion coefficient of GaN, AlN and InN evaluated from the relation between the mean square displacement and time is predicted. Under temperature effects, the migration, behavior of GaN, AlN and InN solid is observed.

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