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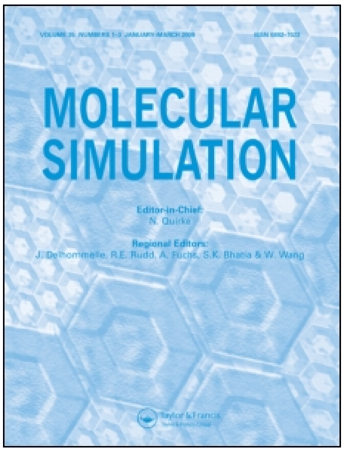

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Elastic Properties of Zinc-blende G a N, A l N and I n N from Molecular Dynamics

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Elastic Properties of Zinc-blende GaN, AlN and InN from Molecular Dynamics

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Molecular dynamics calculations of the adiabatic elastic constants of group III-Nitrides for temperatures ranging from 300 to 900 K have been performed. The results show good agreement with first-principles calculations. The moduli decreased with increasing temperature.

The structural properties of zinc-blende GaN, AlN and InN are reported. Good agreement between the calculated and experimental values of the lattice constant, the cohesion energy, and the bulk modulus and its derivative are obtained.

Keywords: Zinc-blende GaN; AlN; InN; Molecular dynamics

INTRODUCTION

Among the III–V semiconductors the nitrides (GaN, AlN and InN) have attracted both scientific and technological interest in the recent years. This is due to the fascinating mechanical properties of their zinc-blende and/or wurtzite phases, such as hardness, high melting point, high thermal conductivity, large bulk moduli, etc. making them useful for protective coatings. Furthermore, the electronic properties characterized by large band gaps and relatively low dielectric constants indicate potential device applications in ultraviolet optics and high-temperature microelectronics. These outstanding properties are mainly related to the specific role of nitrogen atoms. The smallness of nitrogen atoms gives rise to the formation of short bonds, which leads to significantly smaller lattice constants (by 20–40%) than in other III–V semiconductors.

At ambient conditions, the materials crystallize only in the wurtzite structure (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 [l,2] which are closely lattice matched to β-GaN, also GaAs [3,4] and Si substrates [5] have significant mismatch to β-GaN (cubic form of GaN).

The more ionic compound AlN, is reported to be non polymorphous, it crystallizes at ambient condition in the wurtzite structure [6]. However, several works report the occurrence of a metastable zinc-blende polytype of AlN [7]. Because of the reactivity of AlN, high-purity source material and an oxygen-free environment are required to growth AlN crystals of good quality.

Virtually, all epitaxial AlN, GaN and InN films are expected to contain some amount of residual strain due to differences in the film and substrate lattice constants and in their thermal expansion coefficients. The elastic constants may be needed to calculate the residual strain that may result from thermal expansion coefficient mismatch. This *unintentional* strain can modify the film's electronic structure and accounting of this effect is important when interpreting optical spectra [8,9]. Alternatively, a semiconductor film may be grown *intentionally* strained in order to modify the performance of devices such as laser diodes or light-emitting diodes. Compressive strain, such as, the TE/TM gain ratio in laser diodes are grown from other III–V compounds. Regardless

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of whether strain is introduced intentionally or unintentionally, the effect on electronic properties requires knowledge of the material's elastic properties, specifically the elastic constants which describe the response to an applied macroscopic stress. Nevertheless, these properties are at present poorly known for all these materials. Although several total energy and band structure calculations of the group III nitrides exist, a systematic study of their elastic constants and behavior under temperature effect has been lacking.

The primary objective of this paper is to calculate the adiabatic elastic constants: the elastic constants (C_{11}, C_{12}, C_{44}) and anisotropy constant (A) of GaN, AlN and InN from molecular dynamics (MD). The experiments of the past two decades have shown that MD calculations can provide a valuable tool to investigate nonharmonic effects in solids [10]. We evaluate with this approach the behavior of the elastic constants, bulk modulus, and energies under temperature. In this study, we have used a model of potential developed by Tersoff [11,12], we briefly describe this potential and calculation method in the second section. The results of our calculation are presented and discussed in the third section.

SIMULATION DETAILS

The main ingredient in MD simulations is the choice of the interaction potential between the atoms. For covalently bonded systems, the usual two body potentials cannot be used since they lead to close-packed crystals. Therefore, many-body potentials have to be used which possess angular contributions that prefer certain bonding directions stabilizing covalent crystals. The best known of these potentials are the Stillinger–Weber potential and the Tersoff potentials. This approach is much valid for strongly chemically ordered compounds, such as the case in our study. It has been carried out several stringent tests of Tersoff's potential through static structural analysis of solids of group-VI elements and III–V compounds and examined the chemical properties for C, Si, Ge, BN, CuCl.... It is clear that Tersoff's potential has a limited ability to describe the differences in chemical reactivity between elemental Ge and Si, for example, but well describe the chemical differences of valence *s* and *p* electron properties between elemental C and Si. Tersoff's potential has higher force constants for angular distortions than those in actual systems. We assume that the well-known higher melting points of Tersoff's potential are due to the larger force constants for angular distortions. The calculated elastic constants and Poisson ratios indicate congruity with the experimental values in every element. Tersoff's potential has good transferability and will be an effective tool for evaluating new materials.

The Tersoff potential is based on the bond-order concept [11–13]. The inter-atomic potential energy between two neighboring atoms i and j is written as

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

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

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 [11,12]

$$b_{ij} = \left(1 + \xi_{ij}^{n_i}\right)^{-1/(2n)} \quad (3)$$

with

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

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

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

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

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. We note that λ_3 and α are set equal to zero [11,12]. The nitrides form a specific subgroup of the III–V compounds characterized by high ionicity and very short bond lengths, they share with carbon important physical characteristics including exceptional hardness, high lattice thermal conductivity and a wide band gap [14]. This has prompted us to use carbon's parameters [15] as a starting point for fitting the potential parameter to structural properties of GaN, AlN and InN. To our knowledge, no parameters in the literature have been found for the Tersoff potential which fit crystalline semiconductors of GaN, AlN and InN. The parameters are fitted to polytype energies [16–21]. Our fitted parameters are summarized in Table I.

Computer Simulations

Molecular dynamics is a direct simulation technique at the atomic level. Almost all the physical properties of a material may be determined using molecular

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

	GaN	*AlN*	*InN*
A (eV)	2975.4	1730.0	3297.0
B (eV)	540.310	246.1	280.0
λ_1 (Å^{-1})	3.3718	3.20	3.3
λ_2 (Å^{-1})	2.220	1.853	1.853
β	1.5724×10^{-7}	1.1×10^{-6}	1.1×10^{-6}
n	0.72751	0.72	0.72
c	38049	100390	100390
d	4.384	16.217	16.217
h	− 0.57058	− 0.598	− 0.598
R_0 (Å)	2.40	2.34	2.6405
D (Å)	0.20	0.15	0.15

dynamics. It requires generally an inter-particle potential. Thus, MD computer simulations have been performed to determine the predictions 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 and the atomic structure of solid has been calculated by using a NVT MD 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 time step $\Delta t = 1.86$ fs and an efficient network cube algorithm for nearest-neighbor, details are given elsewhere [22].

After an equilibration period, the histogram of atomic separations is produced in order to compute the pair correlation function [23] $g(r)$, and an other various properties are computed along the trajectory of the system in phase space.

Calculation of the Elastic Moduli

The elastic moduli of a cubic crystal may be divided into two classes, the bulk modulus $B = (C_{11} + 2C_{12})/3$, 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. We begin by making a least squares fit of the computed energies to the form proposed by Birch [24]:

$$\begin{aligned} E(V) = E_0 + \frac{9}{8}B_0V_0[(V_0/V)^{2/3} - 1]^2 + \frac{9}{16}B_0(B'_0 \\ - 4)V_0[(V_0/V)^{2/3} - 1]^3 \\ + \sum_{n=4}^{N} \gamma_n[(V_0/V)^{2/3} - 1]^n \end{aligned} \tag{9}$$

where E_0, V_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 the lattice strain [25]. 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, whereas

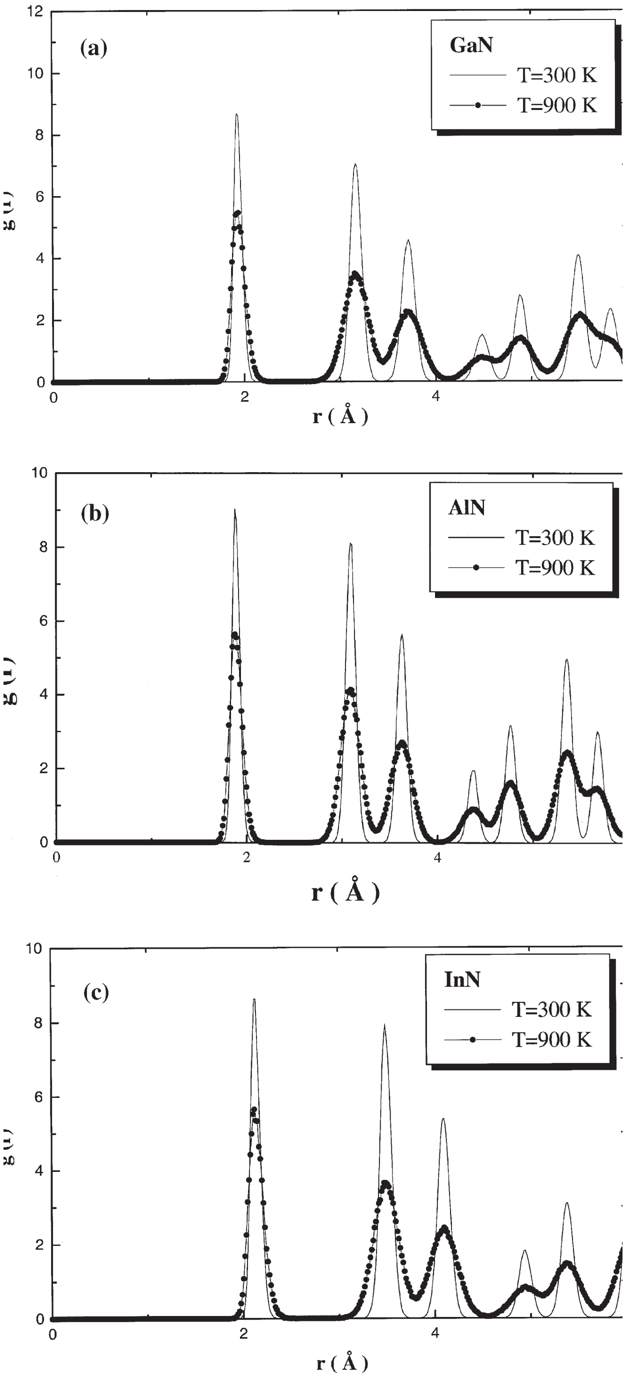

FIGURE 1 Partial pair distribution functions for zinc blende (a) GaN, (b) AlN and (c) InN (solid lines at $T = 300$ K, dotted lines at $T = 900$ K).

TABLE II The values of peak distance and coordination numbers of pairs for (GaN, AlN, InN) in the zinc-blende structure at 300 K

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

Experimental values are in parentheses (from Ref. [26]).

an expansion of the energy in powers of the strain contains no odd powers. Thus, for the calculation of the modulus $C_{11}-C_{12}$, the volume-conserving orthorhombic strain tensor is used

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

undergoing this strain changes of 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}, the volume-conserving monoclinic strain tensor is used

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

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 [26] in either Eqs. (11) and (13) since the strains of Eqs. (10) and (12) are constructed so that $\Delta V = 0$.

The strain Eqs. (10) and (12) can be used for any cubic lattice. Generally, the internal parameters of the lattice must be chosen to minimize the total energy of the strained structure. Fortunately, the discussed lattices fall into a restricted subset of the cubic lattices, where all of the atoms are at inversion sites, even under the reduced symmetry caused by the strains (11) and (13).

For cubic crystal [27] the bulk modulus is given exactly by

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

In true isotropic material the shear modulus is related to the elastic moduli by

$$G = C_{44} = \left(C_{11}^I - C_{12}^I\right)/2 \tag{15}$$

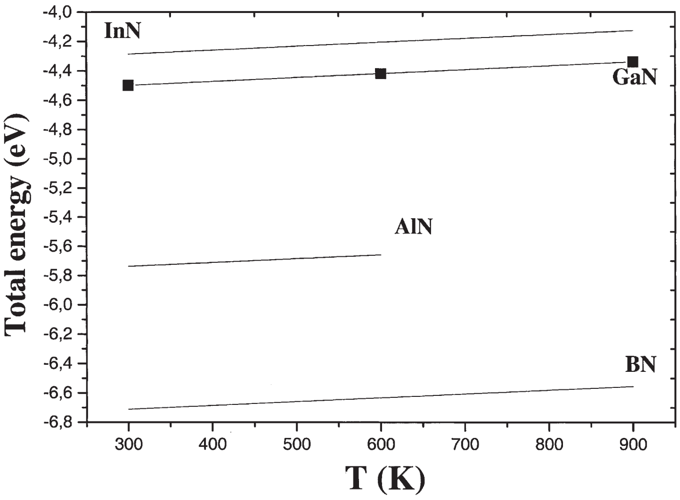

FIGURE 2 The total energy of the system as function of temperature.

but in real crystals the anisotropy constant

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \tag{16}$$

is not unity.

NUMERICAL RESULTS

Partial Pair Distribution Function

The pair correlation function $g(r)$ offers a convenient way to observe and analyze local order in condensed matter systems. In order to test the stability of 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 and 900 K in the zinc-blende structure as shown in Fig. 1. In Table II, the amplitude and peak positions are given.

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

$$\eta = 4\pi\rho_0 \int_0^{R_0} r^2 \rho(r)\,\mathrm{d}r \tag{17}$$

where R_0 denotes the position of the first minima in the $\rho(r)$ and ρ_0 is the density of atoms. It is in good agreement with experimental values [26].

The first peak position of $g(r)$ at 900 K for GaN, AlN and InN is 1.94, 1.87 and 2.12 Å, respectively, which is close to the distance between the first neighbor sites. Fundamentally, it might be said that the structure of group III-Nitrides remains approximately in the zinc-blende structure.

The value of the first and second pair for group III-Nitrides remains approximately at 4 and 12, respectively, for both temperatures 300 and 900 K, which means that GaN, AlN and InN has a stable zinc-blende structure. Figure 1 (doted lines) shows these $g(r)$ near 900 K. The first peak is still present and pronounced for all GaN, AlN and InN and have an oscillatory tail around the value of 1. This behavior is confirmed through the linear behavior of the total energy of the system vs. temperature (Fig. 2).

Structural Properties

Ground state properties of GaN, AlN and InN were calculated within the Tersoff potential model by using MD simulation.

The calculated ground-state energies plotted as functions of the volume for group III-Nitrides are shown in Fig. 3 in zinc-blende phase. The equilibrium parameters from the Birch equation, [24] (E_0, V_0, B_0 and B_0') are listed in Table III.

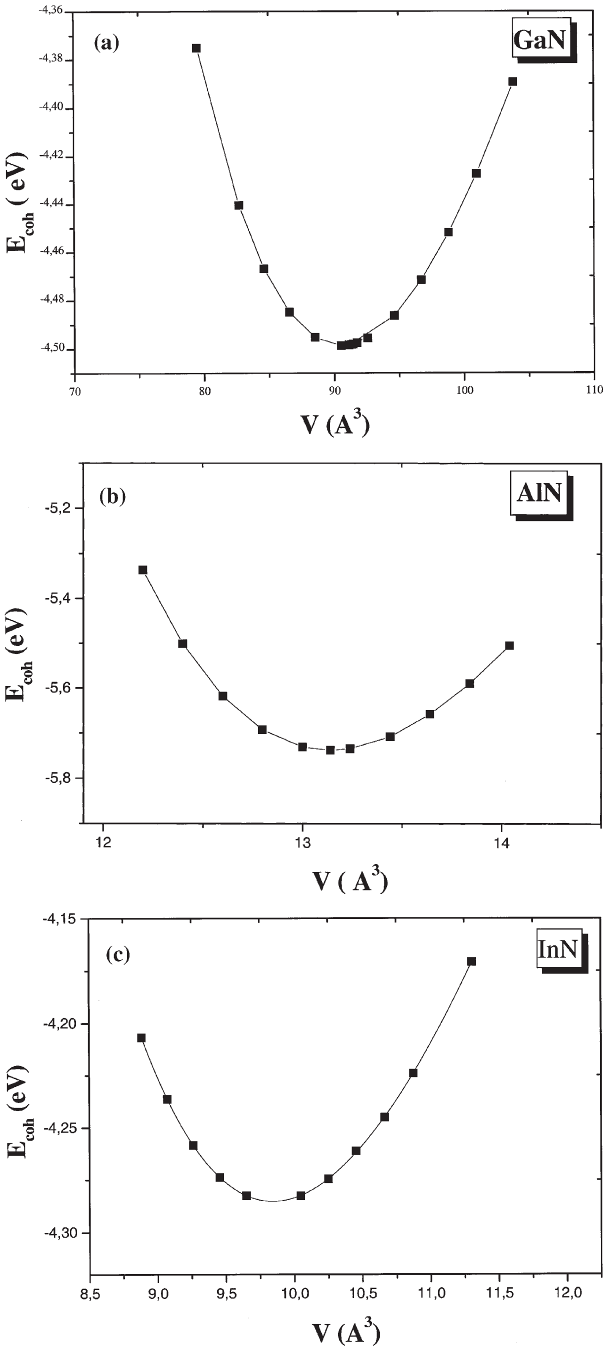

FIGURE 3 The calculated total energies of GaN, AlN and InN in the zinc-blende structure as a function of volume V.

Our calculated equilibrium lattice constants for GaN and AlN are identical to experimental result [16,17] with the discrepancy of 0.6% in InN [18].

Our values of bulk modulus are in agreement with theoretical studies of Christensen *et al.* [28] which use the LMTO method [29] in its scalar-relativistic form in conjunction with the local density approximation (LDA) for zinc-blende type semiconductors to within few percent, our results are also in good agreement with *ab-initio* total energy calculations of Fiorentini *et al.* [30]. The differences between the calculated

TABLE III The calculated equilibrium constants for cubic structures GaN, AlN, and InN, using the $N = 3$ Birch fit [2] of the lattice constant a, the bulk moduli B, the pressure derivatives B', and the cohesive energies E_{coh}

	GaN	*AlN*	*InN*
a (Å)			
Present	4.501	4.379	4.949
Calculated	4.46*, 4.46†, 4.51‡, 4.538¶	4.37*, 4.32†, 4.33‡, 4.394¶	4.95*, 4.92†, 4.97‡, 5.067¶
Experimental	4.5§	4.37‖	4.98#
B (Mbar)			
Present	1.897	2.083	1.429
Calculated	2.01†, 1.84*, 2.00‡	2.03†, 2.15*, 2.04‡	1.39†, 1.37*, 1.49‡
Experimental	1.90**	2.02††	–
B' (Mbar)			
Present	4.607	4.139	4.672
Calculated	3.9†, 4.6*, 4.15‡	3.2†, 4.0*, 4.06‡	4.4†, 4.3*, 4.41‡
Experimental	–	–	–
E_{coh}(eV)			
Present	4.320	5.815	4.363
Calculated	–	–	–
Experimental	4.45††	5.75††	–

*Ref. [28]. †Ref. [32]. ‡Ref. [33]. ¶Ref. [30]. §Ref. [16]. ‖Ref. [17]. #Ref. [18]. **Refs. [19,20]. ††Ref. [21].

Nitrides modulus and those of Christensen *et al.* [28] are within 3.1–4.3% for all the elastic constants. The deviation from the experimental values [18] is smallest by 0.1 and 2.9% for GaN and AlN, however, no experimental data are available for the bulk modulus for InN.

It is interesting to compare our results for B_0 with the values obtained using the Cohen's formula for group-IV elements [31] $B_0 = 1961d^{-3.5}$, where d is the nearest-neighbor distance in angstroms. This relation gives $B_0 = 1.897$, 2.05 and 1.36 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.

Elastics Properties

The elastic moduli of a given system is a first step in understanding its mechanical properties. In addition, the structural stability of a crystal when the system is under no external loading [34] is governed by elastic constants. The comparison of the calculated moduli provides a meaningful test of the interatomic potential function. We have determined the elastic constants at 0 K: C_{11} and C_{12} from Eq. (11) combined with Eq. (14), and C_{44} from Eq. (13).

The energy of GaN, AlN, and InN as a function of orthorhombic strain Eq. (10) for the fixed volume associated with the cubic lattice constant ($a_{GaN} = 4.501$, $a_{AlN} = 4.379$, $a_{InN} = 4.949$) Å is plotted in Fig. 4. Also the energy in terms of the square of the monoclinic strain is plotted in Fig. 5 [12]. The slopes of these curves yield $C_{11}-C_{12}$ and C_{44}. The anisotropy constant A is determined from Eq. (16).

Table IV shows our zinc-blende elastic constants C_{11}, C_{12}, C_{44}, and A together with results from earlier theoretical studies of Wright *et al.* [35] for GaN, AlN, and InN using a method based on density functional–theory calculations (DFT) utilizing

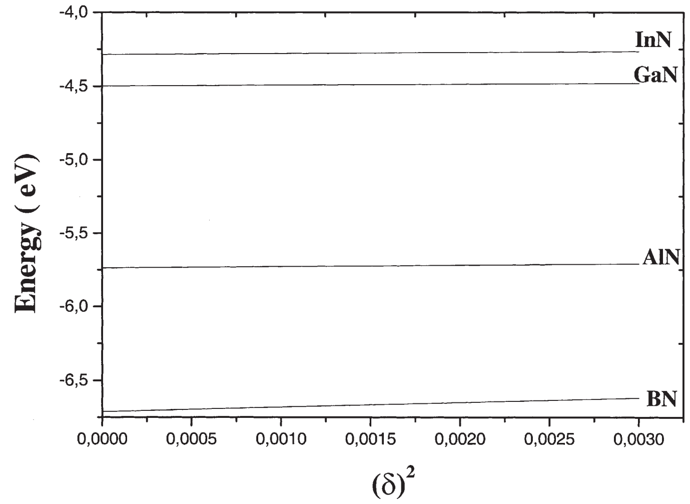

FIGURE 4 The energy as a function of the square of the orthorhombic strain [7].

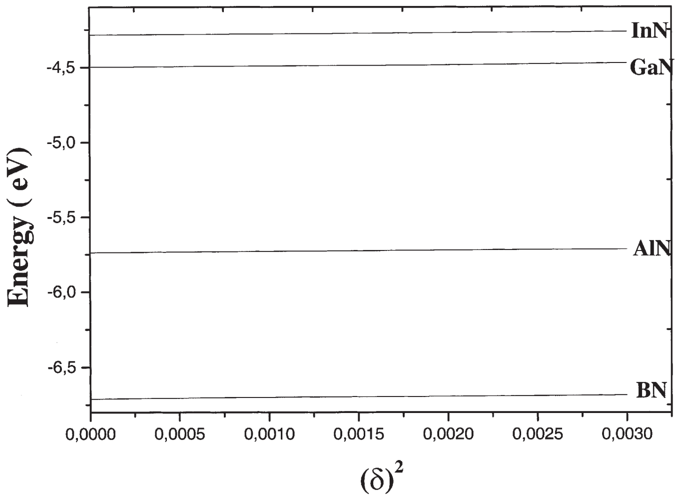

FIGURE 5 The energy as a function of the square of the monoclinic strain [9].

ab-initio pseudopotential and plane wave expansions. We have also compared our results with theoretical studies of Kim *et al.* [36] using DFT implemented via the full potential linear muffin-tin orbitals (FP-LMTOs) method.

Trends

We note several trends among the zinc-blende structure presented above. We find that GaN and AlN are very similar to each other, considerably "harder" compared to InN which is considered "softer". The bulk modulus and elastic constants in particular exhibit this trends. The C_{11} and C_{12} values for GaN and AlN are similar while the corresponding InN values are smaller in magnitude. The C_{44} values decrease in magnitude from AlN to GaN and InN. We also note that the lattice constants and bond lengths of AlN and GaN are close to each other while those of InN are substantially larger than the first two by 10%. This is consistent with the general observation that AlN and GaN are more robust chemically and thermally than InN. These trends are confirmed by the works of Kim *et al.* [36] and Wright *et al.* [35].

In the second part of this work, we have studied the behavior of elastic constants of group III-Nitrides under temperatures variation, we perform MD simulation to calculate C_{11}, C_{12}, C_{44} and B. Figure 6 shows C_{11}, C_{12}, C_{44} and B as a function of temperature. No direct experimental data of elastic constants of group III-Nitrides at elevated temperatures are available in zinc-blende phase. Under temperature effect, all elastic constants show a softening with increasing temperatures very similar to the calculation of polycrystalline β-SiC [39] which has the same properties that the group III-Nitrides. We conclude that the Tersoff potential provides a good description of the mechanical properties of group III-Nitrides at finite stress and elevated temperatures. This decrease in elastic constant was also confirmed by the behavior of bulk modulus and

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

	GaN	*AIN*	*InN*
C_{11}			
Present	2.59	3.02	1.896
Calculated	2.93*, 2.96†	3.04*, 3.48§, 3.04†	1.87*, 1.84†, 2.14‡
–	2.61‡	3.01‡	
Experimental	2.64d	–	–
C_{12}			
Present	1.551	1.63	1.196
Calculated	1.59*, 1.54†,‡, 1.27‡	1.60*, 1.68§, 1.52†	1.25*, 1.16†, 1.37‡
–		1.62‡,	
Experimental	1.53¶	–	–
C_{44}			
Present	1.894	1.92	1.478
Calculated	1.55*, 2.06†	1.93*, 1.35§, 1.99†	0.86*, 1.77†
–			–
Experimental	0.68‖	–	–
A	3.64	2.77	4.22

The last rows lists the anisotropy ratio, *A* [13]. * Ref. [35]. † Ref. [36]. ‡ Ref. [37]. ¶ Ref. [41]. § Ref. [38]. ‖ Refs. [19,20] from Ref. [40].

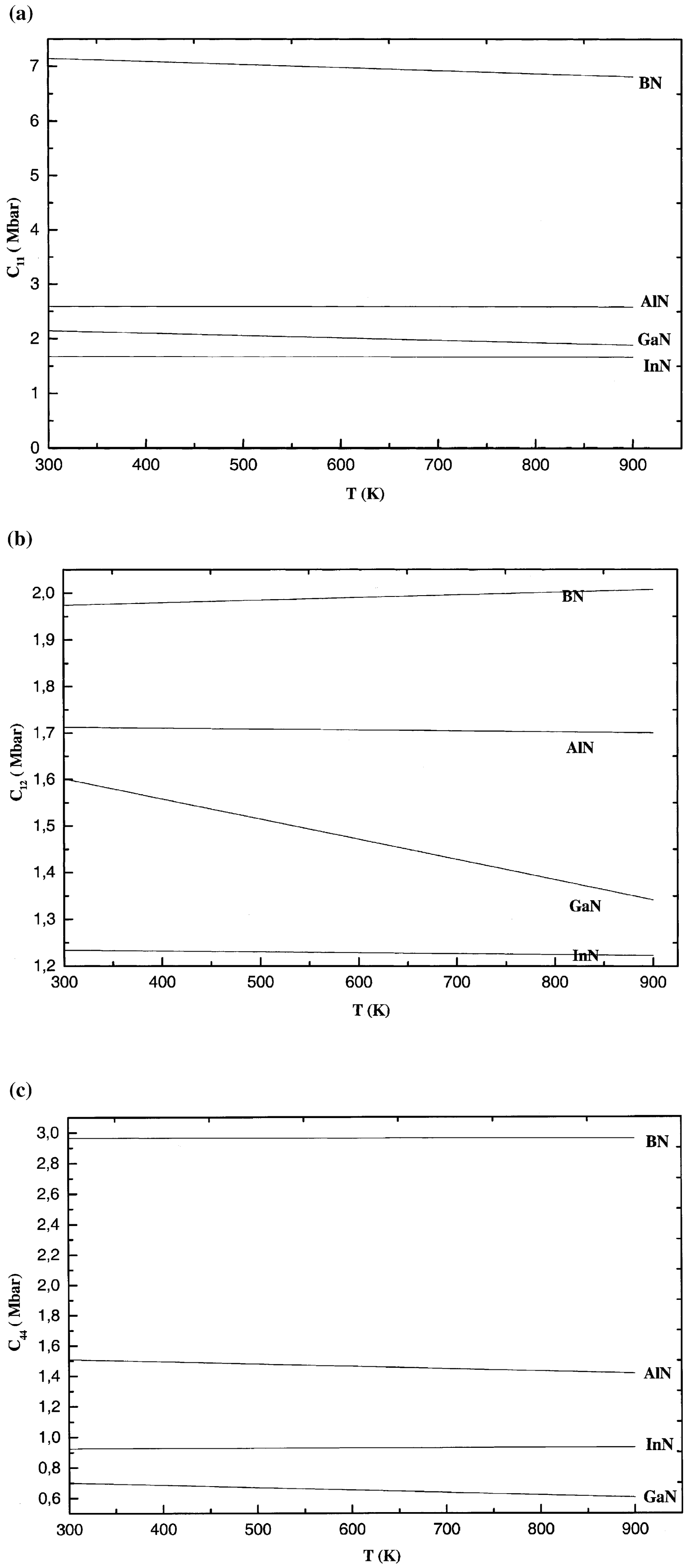

FIGURE 6 The temperature variation of the elastic constants (a) C_{11}, (b) C_{12}, (c) C_{44} and (d) B of group III-Nitrides.

total energy, where both decrease slightly with increasing temperature. Since C_{11}-C_{12} and C_{44} decrease by nearly the same ratio in going from GaN, AlN to InN, and the anisotropy factor A(16) is nearly unchanged.

CONCLUSION

The results of our fitting of parameters potentials of Tersoff exhibit an excellent agreement with available experimental data for structural and elastic properties of group III-Nitrides.

We have also presented a theoretical study of the elastic constants under temperature effect for the group III-Nitrides (GaN, AlN and InN) using the molecular dynamic method. The elastic constants of the zinc-blende structure were obtained directly by fitting the energy vs. volume-conserving orthorhombic strain for the shear modulus ($C_{11}-C_{12}$) and from the volume-conserving monoclinic strain for other shear modulus (C_{44}).

We have calculated the temperature dependence of the elastic moduli for III-Nitrides semiconductor. The computations show that all elastic constants decrease with temperature.

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