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Molecular Dynamics Simulations of Single-wall GaN Nanotubes

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We have investigated the structural properties and the thermal behavior of single-wall GaN nanotubes using atomistic simulations based on the Tersoff-type potential. The Tersoff potential for GaN has effectively described the properties of GaN nanotubes. The caloric curves of single-wall GaN nanotubes were divided into three regions corresponding to nanotube, disintegrating range and vapor. Since the stability or the stiffness of the tube decreased with increasing curving strain energy of sheet-to-tube, the disintegration temperatures of GaN nanotubes were closely related to the curving strain energy of sheet-to-tube.

Keywords: Single-wall gallium nitride nanotubes; Atomistic simulations; Carbon nanotubes; Tersoff-type potential

PACS numbers: 61.46. + w; 68.90. + g; 83.10.Rs

INTRODUCTION

Carbon nanotubes (CNTs) have excited a considerable interest in the condensed-matter and materials research communities in the last ten years, due to their extraordinary properties and their potential for nanotechnology applications [1,2]. Recently, synthesis of nanotubes having other chemical compositions has been reported in several cases. Examples are $B_xC_yN_z$ composite nanotubes [3–6], Mo and W chalcogenide tubes [7–9], vanadium oxide nanotubes [10], NiCl cage structures and nanotubes [11], NiCl₂ nanotubes [12], H₂Ti₃O₃ nanotubes [13], TiO₂ nanotubes [10], Y₂O₃:Eu nanotubes [14] and rare earth oxide nanotubes [15]. Theoretical GaN [16],

GaSe [17], P [18], Cu [19], Bi [20], B₂O and BeB₂ [21] nanotubes have been reported in the literature.

Among the III–V nitrides, gallium nitride (GaN) is technologically the most interesting compound and has attracted extensive interest because of its importance in science and technology for optoelectronic applications in the short-wave length range as well for high-temperature, high-power and high-frequency electronic devices. In particular, GaN is a basic material for the realization of light-emitting diodes [22], lasers in the blue and ultraviolet range of the spectrum [23,24], optical-pumping structure [25], photodetectors [26] and heterostructure field-effect [27].

Under ambient conditions, the stable configuration of GaN is the wurtzite structure with mainly covalent, partially ionic tetrahedral bonding and a direct electronic gap of 3.5 eV at the Γ point [23]. Lee *et al.* [16] thought that the existence of BN nanotubes suggests the possibility of other III–V nitride nanotubes, and then proposed the novel forms of GaN nanotubes. They have shown that the rolling strain energies, the energy costs to wrap up graphite-like GaN sheets into nanotubes, are comparable with those of CNTs. They have also presented that the zigzag GaN nanotubes are semiconductors with a direct band gap, whereas armchair GaN nanotubes have an indirect band gap. The band gap of zigzag GaN nanotubes decreased with decreasing tube diameter, whereas that of armchair GaN nanotubes was almost constant over a wide range of the diameter, which was contrary to the case of CNTs. They have shown that nanoscale optoelectronic

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devices for a wide range of wavelengths may be realized using GaN nanotubes.

Although studies of GaN nanotubes have been performed, the current knowledge of the properties of GaN nanotubes is still quite limited. Atomistic simulations have played important roles in scaling down to nanometer scales and can help in the elucidation of their properties and in the development of methods for their fabrications and applications. Computational materials science also provides detailed microscopic informations on the physical properties of GaN nanotubes. In this paper, we have investigated the single-wall free-standing GaN nanotubes for various diameters using a classical molecular dynamics (MD) simulation. Since we investigated the proposed GaN nanotubes, which are not prepared at the present time, we would like to emphasize that results obtained in this investigation cannot be compared with the experimental results. Nevertheless, since many nanotubes have been recently synthesized using a template such as porous alumina and carbon nanotubes, it has been anticipated that before long, GaN nanotubes can be prepared. Quite recently, the single-crystal GaN nanotubes have been synthesised by using GaN chemical vapor deposition and the templates of ZnO nanowires [28]. Therefore, this investigation will show the structural properties and the thermal behaviors of single-wall GaN nanotubes using atomistic simulations based on the Tersoff-type potential.

EMPIRICAL POTENTIAL

We have used a many-body empirical potential, the Tersoff-type potential. Tersoff potential function has been widely used to develop the empirical potential function for several elements and compound materials. This potential has been applied to the static structural analysis of solids of group-VI elements and multicomponents [29–31], III–V compounds [32–34], Si-B-N [35], P[36], SiO₂ [37], Al₂O₃ [38], Si-H [39], Cu_xAg_{1-x}I, [40], CuCl and CuBr [41] etc. Recently, the Tersoff-type potentials for GaN have been developed by Benkabou *et al.* [42] and Nord *et al.* [43].

It is clear that the Tersoff-type potential has a limited ability to describe the differences in chemical reactivity but it describes well the chemical differences of valence *s* and *p* electron properties. The Tersoff-type potential has good transferability and has been an effective tool for evaluating new materials.

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

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

$$f_c(r_{ij}) = \begin{cases} 1, & r \leq R - D \\ \frac{1}{2} - \frac{1}{2} \sin\left[\frac{\pi}{2} \left(\frac{r-R}{D}\right)\right], & R - D < r \leq R + D \\ 0, & r > R + D \end{cases} \quad (2)$$

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* and has the forms as follows

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

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

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

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

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

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. Values of λ_2 and α are set equal to zero. This work uses the parameters fitted by Benkabou *et al.* [42], which are summarized in Table I. Benkabou *et al.* pointed out that their parameter fitting of the Tersoff potential was reasonable for covalent materials formed by sp^3 hybridized orbitals of nearest neighbors. Since the Tersoff-type potential has good transferability for bond orbitals, the parameters fitted to sp^3 hybridization have been applied to nanotube material with the sp^2 hybridization. Table II summarizes the comparison between the experimental and the calculated results for cubic GaN. The calculated equilibrium lattice constants for cubic GaN is identical to the experimental result and the values of bulk modulus are in agreement with the experimental result. The calculated elastic constants, except for C_{44} , are also in good agreement with

TABLE I The Tersoff parameters for GaN

<i>A</i>	2975.4
<i>B</i>	540.31
λ_1	3.3718
λ_2	2.22
β	1.5724×10^{-7}
<i>n</i>	0.72751
<i>c</i>	38049
<i>d</i>	4.384
<i>h</i>	− 0.57058
<i>R</i>	2.4
<i>D</i>	0.2

TABLE II Comparison between the calculated and the experimental results. The equilibrium lattice constants a , the bulk moduli B , the pressure derivatives B' , the cohesive energy E_{coh} and the elastic constants C_{ij} of GaN in the zinc-blende structure

	<i>Tersoff potential</i>	<i>Experiment</i>
a (Å)	4.501	4.5*
B (Mbar)	1.897	1.90 [†]
B' (Mbar)	4.607	—
E_{coh} (eV)	4.320	4.45 [‡]
C_{11} (Mbar)	2.59	2.64 [¶]
C_{12} (Mbar)	1.551	1.53 [¶]
C_{44} (Mbar)	1.894	0.68 [†]

* Ref. [49]. [†] Ref. [50]. [‡] Ref. [51]. [¶] Ref. [52].

the experimental elastic constants. The C_{44} obtained from the Tersoff potential is three times higher than experimental value.

SIMULATION RESULTS AND DISCUSSION

Structures

Optimal atomic configurations of GaN nanotubes were obtained using the steepest descent (SD) method, which is the simplest of the gradient methods, from the atomic configurations of BN nanotubes having B–N bond length, 1.42 Å. The choice of direction was determined by where the force exerted by inter-atomic interaction decreased the fastest, which was in the direction opposite to ∇E_i , where E_i is the potential energy of i th atom. In this work, the SD method was applied to the atomic positions, and the next atomic position vector (\mathbf{r}'_i) was obtained by a small displacement of the existing atomic position vector (\mathbf{r}_i) along a chosen direction under the condition, $|\mathbf{r}'_i - \mathbf{r}_i|/|\nabla E_i| = 0.001$. We investigated the $(n, 0)$ and (n, n) GaN nanotubes for $n = 5$ –30 composed of 32 unit cells.

Figure 1 shows the axial strain energy as a function of small axial strain for (n, n) GaN nanotubes. Axial strain energy of GaN nanotubes is the second order function of axial strain and this is in concordance with the classical mechanical theory. Young's moduli of the GaN nanotubes can be directly evaluated from Fig. 1 as 796 GPa. In the optimal structure, the lattice constant of (n, n) GaN nanotubes is 3.214025 Å. Table III shows the values obtained from the Tersoff potential and the density functional calculation [16] for GaN nanotubes. Optimal Ga–N bond length obtained from the Tersoff potential is 0.11 Å higher than that obtained from the density functional calculation [16]. In the case of the optimal structures of the armchair (5, 5) and zigzag (9, 0) GaN nanotubes, the optimal diameters, 8.98493 and 9.25846 Å, based on the Tersoff potential are similar to those of the density functional calculation, 8.47 and 8.81 Å, respectively. However, since the bond length obtained from the Tersoff potential is slightly higher

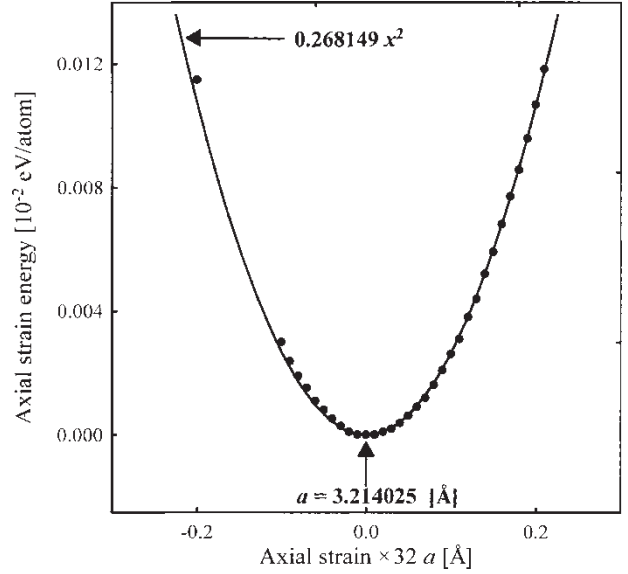


FIGURE 1 Axial strain energy as a function of small axial strain for (n, n) GaN nanotubes.

than that obtained from the density functional calculation, the diameters and the circumferential N–N distances of armchair and zigzag GaN nanotubes obtained from the Tersoff potential are slightly greater than those obtained from the density functional calculation as shown in Table III.

We also calculated the strain energy per atom required to be rolled up a graphite-like sheet of GaN into a tube. The potential energy per atom of the graphite-like sheet for GaN is 0.053 eV/atom higher than those for the cubic GaN structures. The cohesive energy of the nanotubes for the studied GaN materials are below 98.8% of the bulk materials. Comparing with CNTs that have been around 99% of the cohesive energy that they would have in perfect crystalline, we have a clear understanding of the possibility of producing GaN nanotubes. This value obtained from the density functional calculation was around 94% [16]. Figure 2 shows that the strain energy decreases with the increasing tube diameter. Generally, the curving strain energy of sheet-to-cylinder of all nanotubes follows the classical elasticity theory stating that the strain

TABLE III Comparison between values obtained from the Tersoff potential and the density functional calculation [16] for GaN nanotubes. $d_{\text{N-N}}$ is the circumferential N–N distance in GaN nanotubes

	<i>Tersoff potential</i> (Å)	<i>Density functional calculation</i> (Å)
Bond length	1.864	1.755
Diameter of (5, 5)	8.95	8.47
Diameter of (9, 0)	9.26	8.81
$d_{\text{N-N}}$ for (n, n)	2.79	2.66
$d_{\text{N-N}}$ for $(n, 0)$	3.22	3.07

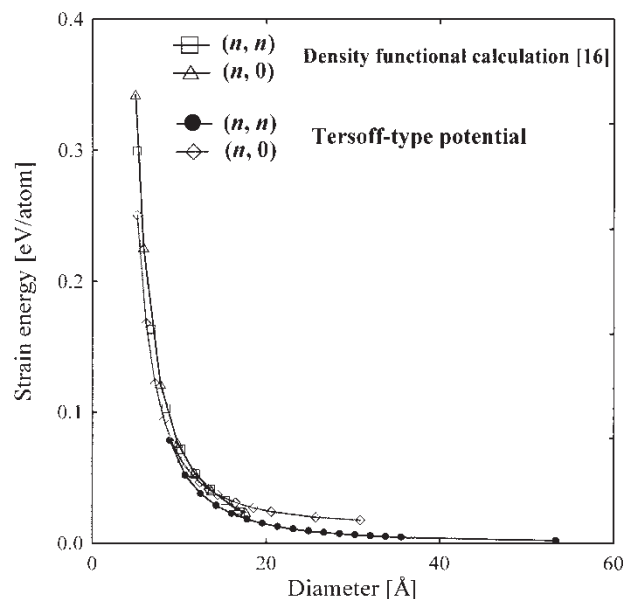


FIGURE 2 Curving strain energy of sheet-to-cylinder of GaN nanotubes.

energy is proportional to the inverse square of the tube diameter. Lee *et al.* have concluded that the low strain energies of GaN nanotubes as much as that of CNTs reveal that GaN nanotubes are stable as CNTs and can be formed at some extreme conditions [16]. The strain energy obtained from the Tersoff potential is in good agreement with that obtained from the density functional calculation. Therefore, the strain energy (E_s) can be expressed as follows

$$E_s(d) = \frac{c}{d^2} \quad (8)$$

where d is the diameter of GaN nanotubes and c is a fitting constant, $7 \text{ eV}\text{\AA}^2$.

Some errors in bond length and cohesive energy are induced so that this work models the hypothetical nanotubes sp^2 hybridization using the Tersoff-type potential that was optimized for the sp^3 hybridization. However, the results of GaN nanotubes using the Tersoff potential are, on the whole, in agreement with those using the density functional calculation, and the Tersoff potential can be efficiently applied to the investigation of GaN nanotubes.

Disintegration of GaN Nanotubes

In addition to the structural study, we have also studied the thermal behavior of these nanotubes using MD simulations. On heating the single-wall GaN nanotubes, the kinetic temperature increased from 100 K by 50 K interval. At each temperature, MD runs of 2×10^5 steps were made with a time step of 0.5 fs (total 100 ps) and the statistical data were obtained from the last 10^3 steps.

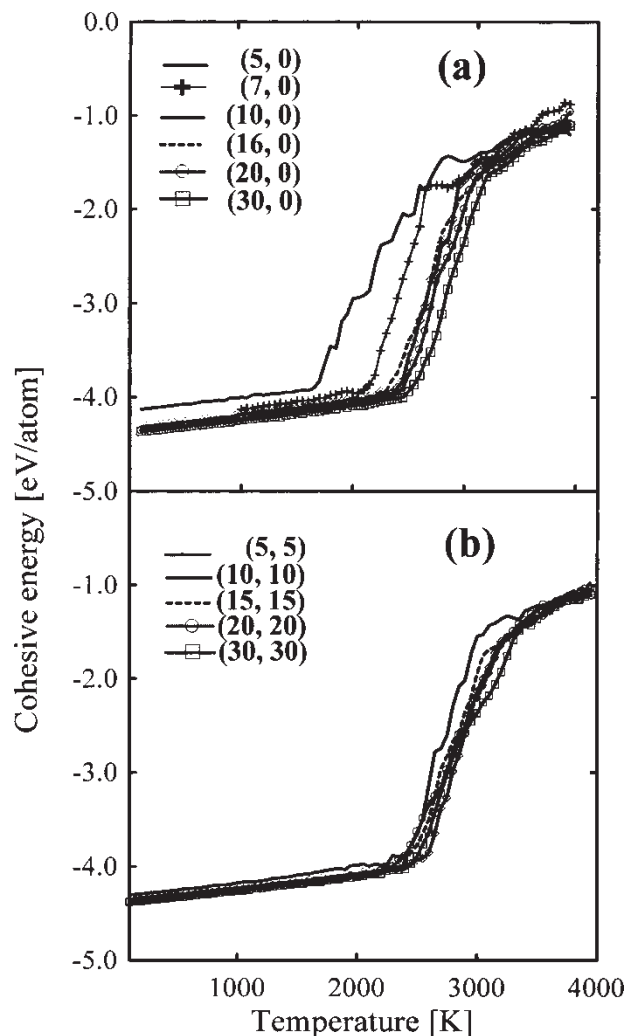


FIGURE 3 Selected caloric curves of single-wall GaN nanotubes.

Our MD simulations used the same MD method as in our previous works [44–47]. The MD code used the velocity Verlet algorithm, a Gunsteren–Berendsen thermostat to maintain constant temperature, a periodic boundary condition (PBC) and neighbor lists to improve the computing performance.

Figure 3 shows the selected caloric curves of single-wall GaN nanotubes. The caloric curves of bulk materials generally fall into five regions corresponding to solid, solid–liquid transition, liquid, liquid–vapor transition and vapor. However, the caloric curves of single-wall GaN nanotubes fall into three regions corresponding to an ordered structure as nanotube, disintegrating region and vapor, as shown in Fig. 3. In the first region, the GaN nanotubes maintain their initial tube structures, and the slope corresponds to the Dulong–Petit specific heat. In the second region, the caloric curve exhibits an upward curvature where the specific heat is pronouncedly increased by the beginning of

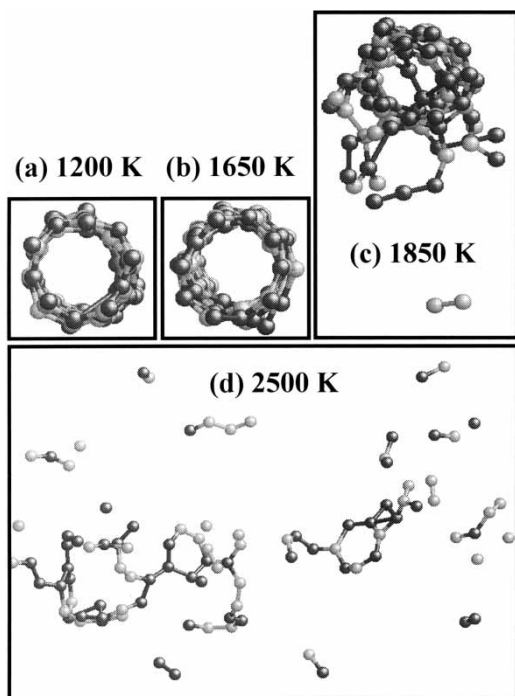


FIGURE 4 Disintegration process for (5, 0) GaN nanotubes at different temperature.

disintegration. For bulk materials, the second region corresponds to the melting point of material. However, in the second region, GaN nanotubes are disintegrated by a kind of explosion of its original structure, as can be observed in Fig. 4. Therefore, the third region in the caloric curves of GaN nanotubes becomes the vapor-like phase. Figure 4 shows the disintegration process for (5, 0) GaN nanotube at different temperature. Figure 4(a),(b) shows the structure of (5, 0) GaN nanotube below the disintegration temperature and at the disintegration temperature, respectively. Figure 4(c) shows the structure of the GaN nanotube during the disintegration process, the second region in the caloric curve, and Fig. 4(d) shows the structure after the disintegration process, the third region in the caloric curve. Thus the disintegration process for GaN nanotubes is similar to that for CNTs. Fagan *et al.* [48] have shown the disintegration process of CNT using the Monte Carlo method and the Tersoff potential and the integration temperature of CNTs was above 4500 K. Carbon, in its disintegration process, preferred to predominate only coordination numbers 3 (sp^2) or smaller than 3 during all the process, in a kind of explosion of its original structure. Their results showed the early stage of the disintegration process of CNT but did not show the stage after the disintegration process of CNT.

Figure 5 shows the disintegration temperature of GaN nanotubes. In our results, the disintegration temperatures (T_d) of GaN nanotubes gradually

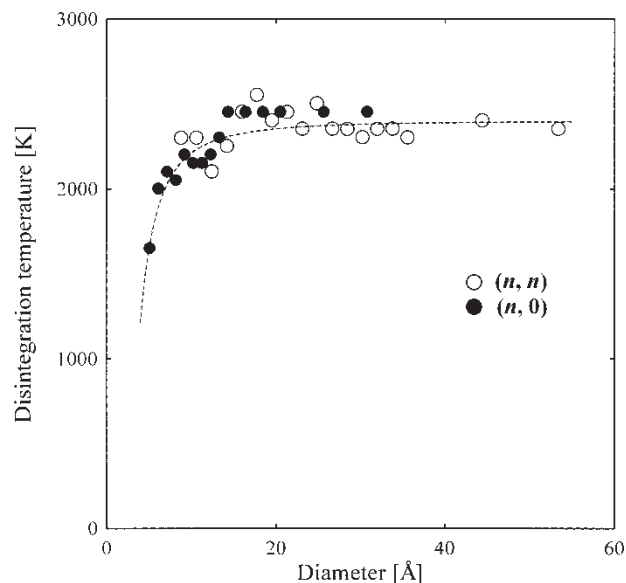


FIGURE 5 Disintegration temperature of GaN nanotubes as a function of the diameter of GaN nanotubes.

increase and saturate as their diameters increase, and this relation can be expressed as follows

$$T_d(d) = T_0 - \frac{k}{d^2}, \quad (9)$$

where d is the diameter of GaN nanotube, T_0 is the saturated disintegration temperature, 2400 K, in this work, and k is a fitting constant, $19,000 \text{ K} \cdot \text{\AA}^2$. Equation (9) is the dashed line in Fig. 5. When we compare Eq. (8) with Eq. (9), it is clear that the disintegration temperatures of GaN nanotubes are closely related to the curving strain energy of sheet-to-cylinder. As the curving strain energy of sheet-to-cylinder increases, the stability or the stiffness of cylinder decreases. Therefore, the integration temperature is inversely proportional to the reciprocal of the square of the tube diameter.

SUMMARY

We have investigated the structural properties and the thermal behavior of single-wall GaN nanotubes using atomistic simulations and the Tersoff-type potential. The Tersoff potential for GaN has been effective in describing the properties of GaN nanotubes, such as the bond length, the diameter, the curving strain energy of sheet-to-tube, and the disintegration temperature. The caloric curves of single-wall GaN nanotubes were divided into three regions corresponding to nanotube, disintegrating

range and vapor. Since the stability or the stiffness of cylinder decreases with the increase of the curving strain energy of sheet-to-cylinder, the disintegration temperatures of GaN nanotubes were closely related to the curving strain energy of sheet-to-cylinder.

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