Effect of aspects ratio on Young’s modulus of boron nitride nanotubes: A molecular dynamics study

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Abstract
As the first of its kind, this study reports the effect of aspect ratio (L/D) on Young’s modulus of Boron nitride nanotubes (BNNTs) within the framework of molecular dynamics simulations using a Tersoff force field. The variation in the length of BNNTs may influence their elastic properties; therefore, the values of L/D of BNNTs were varied as 5, 10, 15, 20 and 25. Our results reveal that Young’s modulus of a BNNT increases as its aspect ratio increases and the values become stable at L/D ~ 15. The current fundamental study highlights the important role of aspect ratio of BNNTs to determine their mechanical behaviours as fillers in multifunctional nanocomposites.

1. Introduction
In the past decades, the discovery of the superior mechanical and other physical properties of carbon nanotubes (CNTs) have triggered great interest in other type of nanotubes. Later on, BNNTs exhibited its extraordinary mechanical [11], thermal [2] and electromechanical properties [3]. The structure of CNTs and BNNTs are same in which carbon atoms are substituted by alternating boron (B) and nitrogen (N) atoms. BNNTs were theoretically predicted in 1994 [4] and synthesized in 1995 [5]. Theoretical and experimental studies showed that BNNTs have a large band gap (5.5 eV) regardless of the tube chirality and its morphology [6]. BNNTs are thermally and chemically more sophisticated than the CNTs. On the other hand, BNNTs demonstrated comparable mechanical properties to CNTs [7]. Such outstanding properties make BNNTs a suitable material for many applications such as composite material [8,9], hydrogen storage [10,11], transistors and optoelectronics [12,13].

Due to the rapid use of BNNTs in the aforementioned applications, it becomes essential to investigate mechanical properties of BNNTs. Many researchers studied mechanical properties of BNNTs, analytically as well as several simulation techniques. A very few of these techniques are molecular mechanics [14], tight-binding [15], ab-initio [16], continuum modelling [17] and classical molecular dynamics (MD) simulation, [18–20]. These studies mainly focused on the effect of nanotube diameter and chirality of BNNTs. Suryavanshi et al. [21] measured the 722 GPa effective elastic modulus of BNNTs using electric-field-induced resonance method inside a transmission electron microscope. Li and Chou [22] and Verma et al. [18], found the significant effect of nanotube diameter and chirality on their elastic properties. They found that as the nanotube diameter increased the value of Young’s modulus decreased and armchair BNNTs show less value than zigzag ones.

To the best of the current author’s knowledge, in determining BNNTs mechanical properties in the variation of aspect ratio (L/D) for different chirality have not been reported. This indeed provided us with the motivation for the current study. In this work, MD simulations were performed to investigate the influence of aspect ratio on Young’s modulus as well as the deformation behavior of BNNTs.

2. Modeling
MD simulations trace the trajectory of thousands, millions, and even billions of particles over millions of time steps, enabling materials science research at the atomistic level. In the present study, all MD simulations were performed using open source software, LAMMPS [23], and molecular interactions were modelled in...
terms of three-body Tersoff-type potential force field [24]. First, the optimized BNNT structures were obtained by minimizing the energy of the structure, using conjugate gradient algorithm. After that, found locally energy minimized structure of the BNNTs was relaxed under room temperature (300 K) for 30 ps to reach its equilibrium state. It is worthwhile to point out that, to maintain the constant simulation temperature of 300 K, the canonical (NVT) ensemble together with the Nosé-Hoover thermostat algorithm was employed in the simulations. The velocity Verlet algorithm with a time step of 0.0005 ps to integrate the Hamiltonian equations of motion determined by Newton’s second law [19, 25]. MD simulations were used to determine Young’s modulus of BNNTs under uniaxial tension loading conditions shown in Fig. 1(a) and 1(b), respectively for (10, 10) armchair and (0, 17) zigzag BNNTs.

The comprehensive deformation of the BNNTs under the uniaxial tension loading can be obtained using elasticity theory. Therefore, Young’s modulus can be expressed based on their conventional definitions by considering BNNT as a hollow cylinder. Young’s modulus was calculated from the initial slope of the stress-strain curve and deformation energy density-elastic constants relations. The axial stress was determined by assuming a uniform tensile stress distribution over the cross-sectional area of the BNNT and expressed as follows:

$$\sigma = \frac{1}{V} \frac{dE}{d\varepsilon}$$  \hspace{1cm} (1)

where $\sigma$ is the longitudinal stress, $\varepsilon$ is the axial strain, $V$ is the volume of a BNNT, and $E$ is the stored strain energy in a BNNT. Accordingly, the strain energy density of a BNNT can be expressed as

$$U = \frac{1}{2} \frac{\Delta E}{A}$$  \hspace{1cm} (2)

in which $U$ is the strain energy per unit volume and is given by,

$$U = \frac{\Delta E}{A\Delta l}$$  \hspace{1cm} (3)

Equating both these energy equations Eq. (2) and Eq. (3)

$$E = \frac{\varepsilon}{\Delta l}$$  \hspace{1cm} (4)

where $\Delta E$ is the change in the potential energy, $A$ is the cross-sectional area ($\pi (D_o^2 - D_i^2) l/4$) of a BNNT, $\varepsilon = \Delta l/l$ is the axial strain of a BNNT, and $\Delta l$ is the increment length of a BNNT. Where $D_o$ and $D_i$ are the outer and inner diameters, and $l$ is the length of a BNNT. Its effective wall thickness $(t)$ as 3.4 Å [19].

3. Result and discussion

First, we performed MD simulations on BNNTs under the axial loading until they fractured. In this study, we focused BNNTs having aspect ratios of 5, 10, 15, 20 and 25. Variation of PE with an axial strain of BNNTs under uniaxial tension is shown in Figs. 3 and 4. It is observed that higher aspect ratios BNNTs show higher PE than lower ones. This is attributed to the fact that the higher aspect ratios BNNTs have more volume which eventually stores more PE. It may also be observed that the zigzag BNNTs store slightly less PE than armchair BNNTs.

Figs. 5 and 6 shows stress-strain curves of BNNTs. It can be seen from Figs. 5 and 6 that trend for various aspect ratio is almost the same up to fracture point. It may be observed that for aspect ratio (AR) ~25, maximum stress reached 97.02 GPa at strain value of about 0.50 and 99.07 GPa at strain value about 0.52, respectively for (10, 10) and (17, 0) BNNTs. The energy-strain and stress-strain curves obtained in the current study are found to be in good agreement with previous results.

**Fig. 1.** Loading conditions imposed on BNNTs (a) Armchair, (b) Zigzag.

**Fig. 2.** Geometrical parameter of BNNTs.
agreement with those obtained for BNNTs in the existing MD studies [19].

To evaluate the influence of the aspect ratio, Young’s modulus of BNNTs calculated within the elastic limit and the obtained values were collected in the Table 1. The inset Figs. 4 and 5, show the linear stress-strain curves within an elastic limit from which Young’s moduli were obtained. As shown in Tables 1 and 2, values of Young’s modulus for (10, 10) armchair and (17, 0) is 1.0534 and 1.0658 TPa were close to the results investigated by Verma et al. [18], which was in good agreement with the results in our work. It can be observed from Table 1 that the value of Young’s modulus (E) increases with the increase in aspect ratio and its maximum values are obtained around 1.0534 and 1.0658 TPa for (10, 10) and (17, 0) BNNTs, respectively, when the aspect ratio (AR) is >15. The value Young’s modulus is found to stable for aspect ratio more than >15.

This study reports Young’s modulus of BNNTs and investigates the effects of the aspect ratio on their Young’ modulus within the framework of MD simulations. Our results disclose that Young’s modulus of BNNTs largely affect by its aspect ratio and increase with an aspect ratio up to 15 then it becomes stable. Zigzag BNNTs displays the higher value of Young’s modulus compares to armchair BNNTs for different aspect ratio. Also, deformation behaviours of the BNNTs under axial tensile loading is explained via MD simulations.

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References


Table 1

<table>
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<tr>
<th>S.N.</th>
<th>Aspect Ratio (L/D)</th>
<th>E (TPa)</th>
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<tbody>
<tr>
<td></td>
<td>(10, 10) BNNTs</td>
<td>(17, 0) BNNTs</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>0.8125</td>
</tr>
<tr>
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<td>10</td>
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