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EFFECT OF VACANCY DEFECT ON ELASTIC PROPERTIES OF BORON NITRIDE NANOTUBES USING MD SIMULATIONS

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Abstract

Molecular dynamics (MD) simulations with a three-body Tersoff potential force fields were conducted to determine the elastic properties of pristine and defective boron nitride nanotubes (BNNTs). The simulation results show that the value of Young's moduli are independent of the tube length, but decreases significantly with increasing tube radius. The value of axial Young's moduli and poison's ratio of smaller diameter BNNTs than the larger ones decrease by 9% and 15% and 7% and 19% for 1% and 2% vacancy concentrations, respectively. The current fundamental study highlights the important role played by vacancy defected BNNTs in determining their mechanical behaviors in multifunctional nanocomposites. Index Terms – Component, formatting, style, styling, insert.

I. INTRODUCTION

Among the Non-carbon-based nanostructures, boron nitride is one of them. BN (Boron nitride) nanostructures, which consecutively substitute of boron and nitrogen atom, are similar structural analogues of graphene nanostructures [1]. Crystallographic parameters of hexagonal layered BN sheets are similar to those of graphene sheet [2]. BNNTs be situated theoretically Predicted in 1994 [3] and synthesized in 1995 [4]. (BNNTs) have attracted more attention due to their attractive mechanical, electrical and thermal properties [5]. Single-walled boron nitride nanotubes (SBNNTs) are semiconductors, with a large band gap 5.5 eV [6]. BNNTs are expected as semiconductors regardless of the chirality or the number of walls of the tube. The BNNTs shows high thermal stability and relative chemical inertness also distinguish from their carbon counterpart [7]. These distinctive properties of BNNTs particularly useful for nanoscale electronic devices, hydrogen storage, and seawater desalination[8].

There have been several studies conducted to explore the mechanical properties of BNNTs subjected to uniaxial tension loadings using various techniques such as ab-into tight-binding

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approach [9], molecular dynamics (MD) simulations [10], and molecular mechanics [11]. Li and Chou [12], and Santosh et al. [13] used molecular mechanics approach to study the torsional properties of BNNTs. Krishnan and Ghosh [14] studied the chirality dependent elastic properties of BNNTs under uniaxial and torsional loadings. For the first time in literature, vacancy defects were observed by Schmidt et al. [15] in BNNTs. A further study carried out by Li et al. [16] Showed that vacancy defects affect the reactivity of BNNTs and play a critical role in their electronic structures. A MD study by Wang et al. [24] studied the stiffness, intrinsic strength and failure strain of TSW and single vacancy defective CNTs. Their results revealed that vacancy defects significantly affect the mechanical properties of CNTs compared to that of TSW defects.

II. MODELING

Molecular dynamics is a computational simulation technique where time evolution of a set of an interacting atom is integrated by their equation of motion. MD is based on classical Newtonian mechanics. The apparent advantage of MD over classical models is that it provides a route to dynamical properties of the system: transport coefficients, time-dependent responses to perturbations, rheological properties and spectra, thermo-mechanical properties, and many more unique characteristics. Therefore, MD simulations were shown in the current study to determine the elastic properties of BNNTs at the atomic scale.

First we build a boron nitride nanotube, then simulation performed with minimize energy by using conjugate gradient method to attained an optimized atomic structures of BNNTs. Simulation performed in the constant volume and constant temperature (NVT) ensemble with a time step of 0.5 fs with a total time of 50 ps to equilibrate the BNNT structures. Velocity Verlet algorithm was used to integrate Newton's classical equations of motion. The defects play a vital role in BNNTs

The vacancy defect's in the BNNTs were introduced by removing an equal number of boron and nitrogen atoms from the pristine BNNTs. Note that taking advantage of the possibility to create a controlled vacancy concentration in BNNTs by electron or ion irradiation process [2], one can alter their mechanical properties. The vacancy concentration is defined to express the number of incorporated defects as follows:

$$\rho = \frac{number\ of\ removed\ atoms}{total\ atoms\ in\ a\ BNNT} \times 100 \quad (1)[2]$$

To create a vacancy defect, the same number of boron and nitrogen atoms from the middle segment of BNNTs were removed as shown in figure

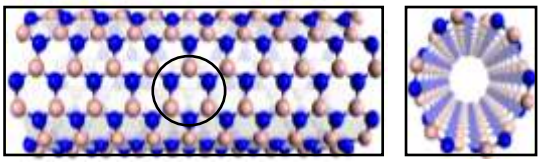

Figure 1: Schematics of different atom vacancies in (10, 10) BNNT

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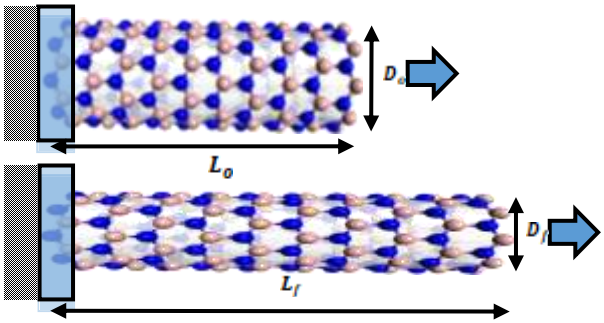

Figure 2: BNNTs deformation when applying a tensile load

Axial Young's moduli (E_1):

The Young's Moduli of BNNTs were calculated from the initial slope of the stress-strain curve and deformation by the 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; as follows

$$\sigma = \frac{1}{V}\frac{dE}{d\varepsilon} \qquad (2)[2]$$

where σ axial longitudinal stress, ε axial strain, V volume of a BNNT,

$$V = Al = \frac{\pi(R_1^2 - R_0^2)t}{4} \times L \qquad (3)[2]$$

Where A is the cross-sectional area of a BNNT, t thickness of BNNTs 3.34Å and E is the stored strain energy in a BNNT.

Accordingly, the strain energy density of a BNNT can be expressed as

$$U = \frac{1}{2}E_1\bar{\varepsilon}^2 \qquad (4)[2]$$

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

$$U = \frac{\Delta E}{Al} \qquad (5)[2]$$

Where ΔE is the increment of the potential energy, A is the cross-sectional area of a BNNT,
Equating equation 4 and 5 then we get Young's module (E_1)

$$E_1 = \frac{2\times\Delta E}{A\times\Delta L\times\bar{\varepsilon}} \qquad (6)[2]$$

$\bar{\varepsilon} = \Delta l/l$ is the axial strain of a BNNT, and Δl is the increment of a BNNT length.
Using the following definition, the major Poisson's ratio (v12) of a BNNT can be obtained,

$$\vartheta_{12} = -\frac{\frac{\Delta R}{R_o}}{\frac{\Delta L}{L_o}} \qquad (7)[2]$$

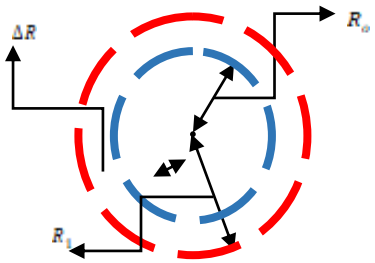

Figure 3: Top view of Nanotube

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III. RESULT AND DISCUSSION

In this work, determine only two independent elastic properties Young's Moduli and Poisson's ratio of BNNTs under only uniaxial tension were investigated by using MD simulation for armchair structure of BNNTs. The necessary simulation were performed parallel software, LAMMPS (Large-scale atomic molecular massively parallel simulator).

The MD modeling procedure detailed section is adopted to determine the elastic coefficients of pristine and defective BNNTs. Figure 4 and 5 shows stress-strain curves of armchair (10, 10) and (15, 15) BNNTs with maximum stress being 93.02 GPa at strain 0.50-0.58. The sets of energy-strain and stress-strain curves obtained in the current study are found to be in good covenant with those obtained for pristine BNNTs in the existing MD studies {Formatting Citation}. It may be observed from Figure 4 and 5 that the defected BNNTs were fractured at lower strain levels than pristine BNNTs [2]. As expected, larger vacancy concentration (2%) significantly affects the mechanical behaviour of BNNTs. Although it is not shown here, the trends of Poisson's ratios are found to be same as those shown in Fig. 4 and 5.

Table 1 showing Youngs Moduli for armchair BNNTs

Chirality (m, n)	BNNTs Diameter(Å)	E_1 (TPa)	E_1 (TPa)	E_1 (TPa)
		ρ = 0%	ρ = 1%	ρ = 2%
(5,5)	6.9549	0.9921	0.88499	0.85328
(10,10)	13.8336	1.06349	0.94834	0.91397
(15,15)	20.7293	1.08762	0.9737	0.94345
(20,20)	27.6292	1.10135	0.98975	0.95436

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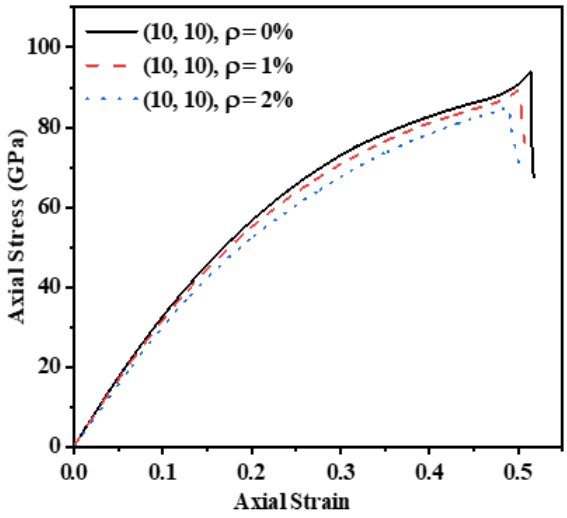

Figure 4 Stress-strain curves for pristine and vacancy defected armchair BNNTs, (10, 10)

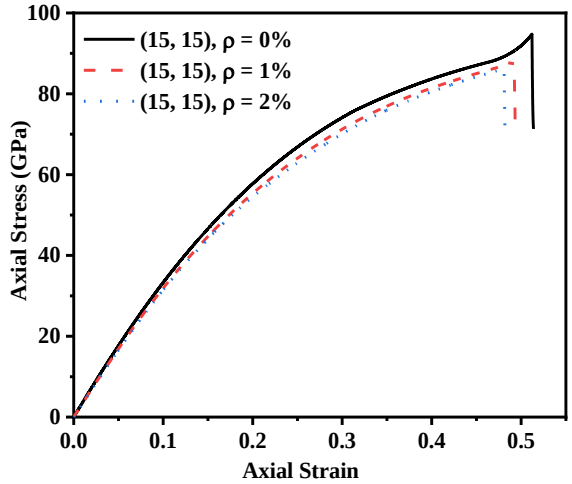

Figure 5 Stress-strain curves for pristine and vacancy defected armchair BNNTs, (15, 15)

Table 1 and 2 demonstrates the influence of vacancies on 1% and 2% for the axial Young's moduli and Poisons ratio of armchair BNNTs.

Table 2 showing Poisons ratio for armchair BNNTs

Chirality (m, n)	BNNTs Diameter (Å)	υ_{12}	υ_{12}	υ_{12}
		ρ = 0%	ρ = 1%	ρ = 2%
(5,5)	6.9549	0.21051	0.19392	0.17163
(10,10)	13.8336	0.19938	0.18268	0.16073

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(15,15)	20.7293	0.16227	0.1506	0.12828
(20,20)	27.6292	0.15646	0.1394	0.11717

The variation of potential energy increases with increase in axial strain is graphically shown in figure 6, and it seen that the PE (eV) increases with size of BNNTs. It may also be observed that both types of BNNTs show almost similar trends till they were fractured. The marginal differences were attributed to the variation in their diameters and chirality.

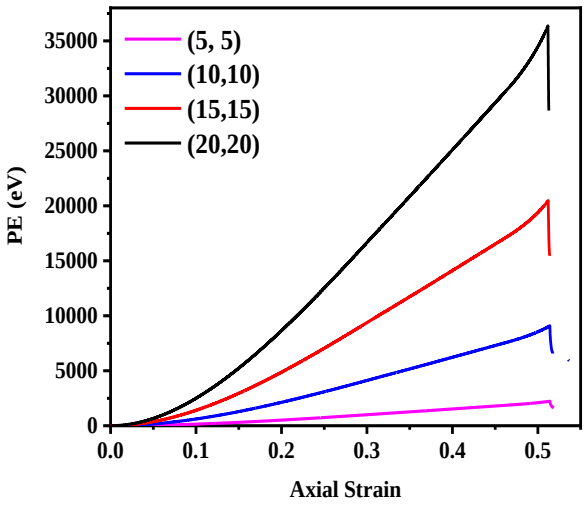

Figure 6: The variation of the PE (eV) & axial strain of armchair BNNTs

The armchair nanotube (10, 10) and (15, 15), which possess the dissimilar diameter, were selected and explain the difference between the elastic properties (Young's Moduli and poison's ratio), of the armchair BNNTs. To verify the validity of current MD simulations, the two elastic constants: Young's moduli and Poisson's ratio of pristine (10, 10) BNNTs were compared with existing results [18] and the comparison was found to be in good agreement. The value of young's moduli and poisons ratio of armchair BNNTs increases when diameter 15 Å, after that the value of both elastic constant value decreases. Table 1 & 2 shows the value of armchair BNNTs for both elastic constant.

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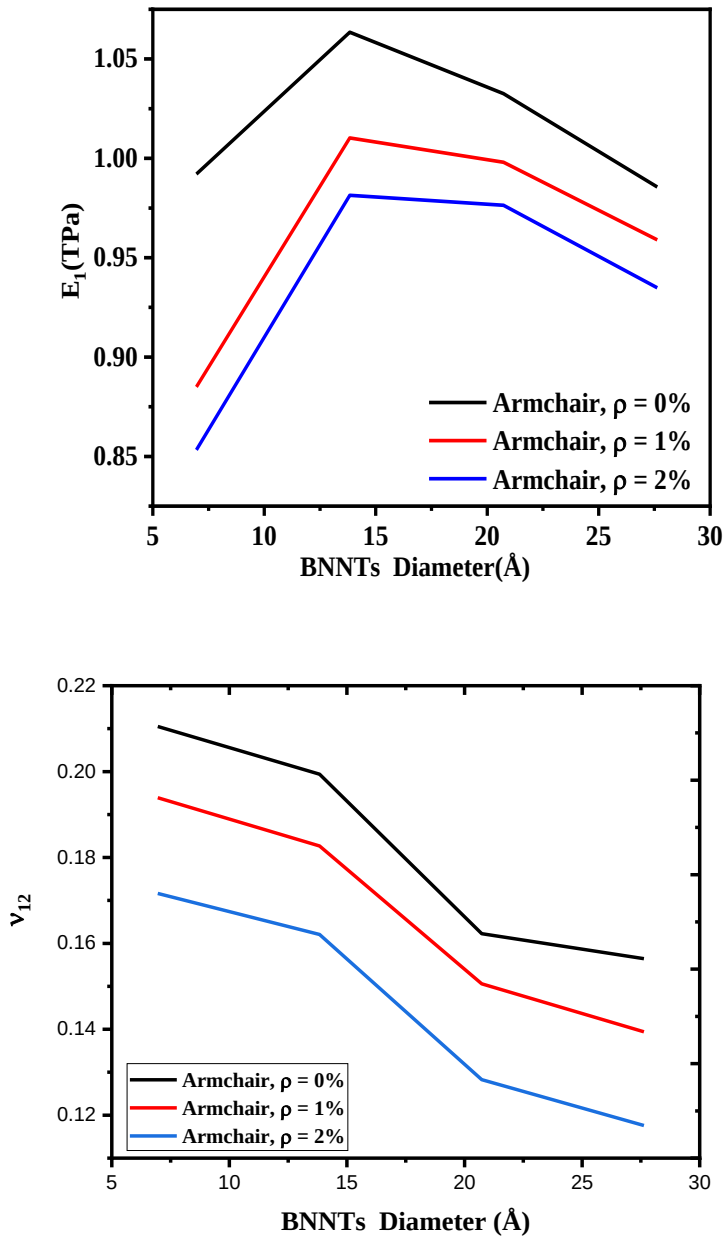

Figure 7 Effect of vacancy defects on the Young's moduli and major Poisson's ratios of different armchair BNNTs

IV. CONCLUSION

As the first of its kind, this study reports the elastic properties of pristine and vacancy defective Boron Nitride nanotubes (BNNTs) were simulated based on classical molecular dynamics (MD) method. The relationship between the mechanical properties of BNNTs and tube diameter or

chirality armchair has been analyzed. Effects of vacancy defects on the properties of BNNTs were discussed. The main results are summarized as follows:

I. The elastic constant (Young's moduli and poison's ratio) of BNNTs decrease with the increase of the nanotube diameter and strength and failure strain was relatively stable corresponding to different diameter or chirality.

II. The elastic constant of vacancy defective in BNNTs reduced with vacancy concentration and their influence becomes more prominent for the smaller diameter.

III. Figure (4), demonstrates the variation of PE of the armchair BNNTs subjected to axial strain. As expected that when the diameter BNNTs more than 10 its shows higher PE energy than smaller ones. It may also be observed that both types of BNNTs show almost similar trends until they were fractured.

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