



# Mechanical property assessment of black phosphorene nanotube using molecular dynamics simulation



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## ABSTRACT

The study attempts to investigate the mechanical properties of single-walled black phosphorene nanotubes (SW-BPNTs) at atmospheric pressure through molecular dynamics (MD) calculation incorporating with the Nosé-Hoover Langevin (NHL) thermostat. Their dependences on size, chirality and temperature are also addressed. Two typical cross-sectional area definitions, i.e., hollow tube and equivalent solid cylinder, are used in the estimate of the mechanical properties. The predicted results are compared with each other and also with the literature data. The calculation results reveal that the Young's modulus, shear modulus, specific heat and CTE of both armchair and zigzag SW-BPNTs would increase with the tube length and diameter, and additionally, the Young's modulus and shear modulus appear to change significantly with chiral angle. It is also found that the Young's modulus calculated using the hollow tube assumption would increase with the tube diameter while there is an opposite trend for the equivalent solid cylinder assumption. According to the equivalent solid cylinder assumption, the nanoscale SW-BPNTs are not a very stiff material. Moreover, the specific heat and linear coefficient of thermal expansion (CTE) of SW-BPNTs, irrespective of chirality and size, increase with temperature at low temperature and tend to converge to a certain value when temperature is larger than 600 K. Besides, the calculated specific heat of SW-BPNTs closely follows the Debye  $T^3$  law.

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## 1. Introduction

In recent years, there has been great interest in using low dimensional nanostructured material in nano-scale electronic or electromechanical devices and components due to the downsizing trend of integrated circuit (IC) technology [1–5]. Two-dimensional (2D) materials, such as graphene, boron-nitride and transition metal dichalcogenides (TMDCs), have triggered extensive research activities due to their superior optical, electrical and mechanical properties not seen in their counterparts [6–8]. Graphene possesses some extraordinary electrical, mechanical and thermal mechanical properties, such as high carrier mobility and low resistivity. Unfortunately, graphene suffers from relatively high off current and low on/off ratio due to a lack of bandgap. Though having a bandgap and thus achieving a relatively high on/off ratio, TMDCs, such as MoS<sub>2</sub>, yield lower carrier mobility [9]. Recently, monolayer black phosphorus or black phosphorene was successfully exfoliated from black phosphorus by Li et al.

[10]. It has drawn great interest and attention in both academia and industry due to its unique physical properties. For instance, it has carrier mobility up to around  $1000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ , much larger than graphene and MoS<sub>2</sub> [10–12]. Unlike graphene, black phosphorene has a direct bandgap of about 1.5 eV between conduction and valence bands, thereby achieving a relatively high on/off ratio. Besides, several previous reports indicated that the bandgap of black phosphorene can be artificially manipulated by applying external stress or strain [12–14] in order to meet the needs of various nanoelectronic applications. For example, Liu et al. [12] indicated that an in-plane stress can vary the bandgap of black phosphorene from a direct-gap semiconductor to an indirect-gap semiconductor, and even from a semiconductor to a metal. Rodin et al. [13] indicated that strain can remarkably modify the gap size of black phosphorene and induce a semiconductor-metal transition. Because of these advantageous features over graphene and TMDCs, black phosphorene holds tremendous potential for many engineering applications, such as nanoelectronic devices [15], photocatalysts [16] and solar cells [17].

The successful application of black phosphorene in nanoelectronic devices relies on a good understanding of its material behaviors and properties. In literature, there have been many reports on

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the evaluation of the mechanical properties of black phosphorene [18–21]. For example, Sha et al. [18] applied molecular dynamics (MD) simulation to explore the mechanical properties and fracture behaviors of black phosphorene at finite temperatures. Wei and Peng [19] utilized first principles density functional theory calculations to examine the mechanical properties of black phosphorene, including ideal tensile strength and critical strain. They found that monolayer black phosphorus can sustain tensile strain up to 27% and 30% in the zigzag and armchair directions, respectively. Sorkin and Zhang [21] predicted the edge atomic structures and elastic properties of defect-free black phosphorene nanoribbons by way of the tight-binding method. By contrast, the study of mechanical property on single-walled black phosphorene nanotubes (BPNTs) is very limited [22–29]. For example, Seifert and Hernández [22] applied first-principles to calculate the Young's modulus of phosphorus nanotubes. They found that Young's modulus for single-walled BPNTs is around 300 GPa, which slightly depends on the nanotube diameter. Guo et al. [23] utilized first principles study of the electronic properties of phosphorene nanoribbons, phosphorene nanotubes, multilayer phosphorene, and heterobilayers of phosphorene and two-dimensional transition metal dichalcogenide monolayer. They found both armchair or zigzag nanotubes are semiconductors with direct bandgaps. Guan et al. [25] investigated the stability of faceted nanotube by laterally joining nanoribbons or patches of different planar phosphorene phases using *ab initio* density functional calculations. Their calculation results indicated that the faceted nanotube may form very stable, nonplanar joints. Aierken et al. [26] investigated the defect lines influence on electronic property of blue phosphorous. They showed that valence band maximum and conduction band minimum states of the defect-induced faceted PNTs are localized on the defect lines and that these states control the electronic properties of the tubes. Montes and Schwingenschlögl [27] demonstrated structural stability of monolayer zigzag and armchair blue phosphorus nanotubes by MD simulation. Their results also indicated that the nanotubes are found to be semiconductors with a sensitive indirect band gap that allows flexible tuning. Clearly, as compared to carbon nanotubes and even black phosphorene sheets, there is still a great lack of comprehensive knowledge of the material behaviors and properties of SW-BPNTs, not to mention their dependence on size, temperature and chirality. Thus, the study aims at investigating the mechanical properties of various SW-BPNTs by MD simulation using the Nosé-Hoover Langevin (NHL) thermostat method [30], and besides, their relation to size, chirality and temperature. The mechanical properties under investigation are Young's modulus, shear modulus, specific heat and linear coefficient of thermal expansion (CTE). In the calculation of the mechanical properties, both hollow tube and equivalent solid cylinder definitions of the cross-sectional area of the SW-BPNTs are used, and the predicted results are compared with each other. A comparison of the simulation results with the literature data is also made.

## 2. Model and method

The structure of single-layer black phosphorene is shown in Fig. 1, in which the lattice parameters are  $a_1 = 3.31 \text{ \AA}$  and  $a_2 = 4.38 \text{ \AA}$  in the zigzag and armchair directions, respectively. Black phosphorene has a puckered structure with each phosphorus atom bonded with other three atoms. As shown in Figs. 1 and 2, SW-BPNTs can be created by rolling up the single-layer black phosphorene along the vector  $C = na_1 + ma_2$ , where  $n$  and  $m$  are the numbers of the unit cell along  $a_1$  and  $a_2$  directions. In specific, if  $m = 0$ , the nanotube is called a zigzag SW-BPNT, and if  $n = 0$ , the nanotube is called an armchair SW-BPNT. In the study, the covalent bonds between the phosphorus atoms in SW-BPNTs are depicted

using the COMPASS (Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies) force field [31,32], as shown in the following equation,

$$\begin{aligned}
 U_{\text{total}} = & \sum_b [K_2(b - b_0)^2 + K_3(b - b_0)^3 + K_4(b - b_0)^4] \\
 & + \sum_\theta [H_2(\theta - \theta_0)^2 + H_3(\theta - \theta_0)^3 + H_4(\theta - \theta_0)^4] \\
 & + \sum_\phi [V_1[1 - \cos(\phi)] + V_2[1 - \cos(2\phi)] + V_3[1 - \cos(3\phi)]] \\
 & + \sum_x K_x \chi^2 \\
 & + \sum_b \sum_{b'} F_{bb'}(b - b_0)(b' - b'_0) \\
 & + \sum_\theta \sum_{\theta'} F_{\theta\theta'}(\theta - \theta_0)(\theta' - \theta'_0) \\
 & + \sum_\phi \sum_\theta \sum_{\theta'} K_{\phi\theta\theta'} \cos \phi(\theta - \theta_0)(\theta' - \theta'_0) \\
 & + \sum_b \sum_\theta F_{b\theta}(b - b_0)(\theta - \theta_0) \\
 & + \sum_b \sum_\phi (b - b_0)(V_{1b\phi} \cos \phi + V_{2b\phi} \cos 2\phi + V_{3b\phi} \cos 3\phi) \\
 & + \sum_\theta \sum_\phi (\theta - \theta_0)(V_{1\theta\phi} \cos \phi + V_{2\theta\phi} \cos 2\phi + V_{3\theta\phi} \cos 3\phi) \\
 & + \varepsilon_{ij} \left[ 2 \left( \frac{\sigma_{ij}}{r_{ij}} \right)^9 - 3 \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right].
 \end{aligned} \tag{1}$$

The potential describes not only the interactions of phosphorus atoms but also the bond and bond angle of black phosphorene. Basically, the force field can be divided into two main categories, i.e., bonded and non-bonded terms. The bonded terms represent the energy associated with the internal coordinates of bond ( $b$ ), angle ( $\theta$ ), torsion angle ( $\phi$ ) and out-of-plane angle ( $\chi$ ). In addition, the cross-coupling terms are also utilized to represent the combinations of the two or three internal coordinates. The cross-coupling terms are crucial for use in the estimate of vibration frequencies and structural variations in relation to conformational changes. Of these cross-coupling terms given in the equation, the bond-bond, bond-angle and bond-torsion angle are the most frequently used terms. Besides, the non-bonded terms are included for the van der Waals interaction between atoms through Lennard-Jones 9-6 function [33–35].

Fig. 3 illustrates a representation of an SW-BPNT atomistic structure. Based on the continuum mechanics, the Young's modulus of the SW-BPNT in the armchair and zigzag directions (or any other direction) can be derived through an axial tension method, where the atoms at one end of the atomic system are fixed (the red zone in Fig. 3(a)) while those at the other end (the blue zone in Fig. 3(a)) are subjected to an enforced axial (horizontal) displacement. Then, the corresponding strain energy ( $U$ ) under different strains can be computed using an MD model based on the COMPASS force field as the atomic system is in equilibrium state. According to the classical mechanics and the energy method, the axial Young's modulus, it will be abbreviated as Young's modulus ( $E$ ) hereinafter, of the atomic system can be derived from the second derivative of the strain energy density with respect to the axial strain ( $\varepsilon$ ), as

$$E = \frac{1}{V} \frac{\partial^2 U}{\partial \varepsilon^2}, \tag{2}$$

where  $V$  is the volume of the atomic system. Fig. 4 shows the definition of the thickness ( $t$ ) and volume of SW-BPNT, where  $D_1$  and  $D_2$  are inner and outer diameters. The volume of the SW-BPNT can be

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