



# A density-functional-theory-based finite element model to study the mechanical properties of zigzag phosphorene nanotubes

R. Ansari<sup>a</sup>, A. Shahnazari<sup>a</sup>, S. Rouhi<sup>b,\*</sup>

<sup>a</sup> Department of Mechanical Engineering, University of Guilan, P.O. Box 3756, Rasht, Iran

<sup>b</sup> Young Researchers and Elite Club, Langarud Branch, Islamic Azad University, Langarud, Guilan, Iran

## ARTICLE INFO

### Keywords:

Density functional theory  
Finite element method  
Zigzag phosphorene nanotube  
Elastic modulus

## ABSTRACT

In this paper, the density functional theory calculations are used to obtain the elastic properties of zigzag phosphorene nanotubes. Besides, based on the similarity between phosphorene nanotubes and a space-frame structure, a three-dimensional finite element model is proposed in which the atomic bonds are simulated by beam elements. The results of density functional theory are employed to compute the properties of the beam elements. Finally, using the proposed finite element model, the elastic modulus of the zigzag phosphorene nanotubes is computed. It is shown that phosphorene nanotubes with larger radii have larger Young's modulus. Comparing the results of finite element model with those of density functional theory, it is concluded that the proposed model can predict the elastic modulus of phosphorene nanotubes with a good accuracy.

## 1. Introduction

The great physical properties of graphene and carbon nanotubes (CNTs) have led to motivating the research community to search for other nanomaterials with the attractive properties. Phosphorene which recently has been synthesized from the layered black phosphorus bulk materials [1–3] has found extensive applications in different fields such as in nanodetectors [4,5], batteries [6–9], gas sensing [10], water splitting photocatalyst [11] and transistors [12]. Therefore, different research works have been performed to clearly describe the mechanical [13–25], electronic [26–34,44–48], thermal [35–43], optical [44–48] and magnetic properties [49] of phosphorene nanosheets and nanotubes.

Ding et al. [13] used first-principles calculations to study the mechanical and electronic behavior of phosphorene nanosheets. It was represented that the phosphorene nanosheets exhibit a significant anisotropic elastic behavior along the armchair direction versus the zigzag direction. The mechanical properties of monolayer and bilayer phosphorene nanosheets were investigated by Hu et al. [14]. It was shown that under a sufficiently large tensile isotropic strain, decreasing the distance between two inner sublayers of the bilayer phosphorene could result in their bonding.

Wei et al. [15] showed that the armchair and zigzag phosphorene monolayer nanosheets can tolerate the tensile strains upto 27% and 30%, respectively. The anisotropic electro-mechanical properties of phosphorene nanosheets were also investigated by Wang et al. [16].

Wang et al. [17] represented that due to having a structural flexibility along the armchair direction, they can have large curvatures. Wang et al. [18] investigated the effect of mechanical strain on single-layer black phosphorus nanoresonators at different temperatures. They reported that the resonant frequencies of the phosphorene nanosheets are also anisotropic. Investigating the effect of temperature on the mechanical properties of the phosphorene nanosheets, it was shown that the fracture strength and strain depend on the environmental temperature [19].

They also showed that a 2% concentration of randomly distributed mono-vacancies can reduce fracture strength by about 40% [20]. Liu et al. [21] showed that the fracture of the armchair phosphorene nanosheets occurs due to the interlayer bond angles. However, the breakage of both the intra-layer angles and bonds is the reason of the fracture of the zigzag phosphorene. DFT simulations were used by Sorkin and Zhang [22] to investigate the elastic properties of defect-free phosphorene nanoribbons (PNRs) by using DFT simulations. It was shown that the armchair PNRs possess smaller failure stress than the zigzag ones. However, its failure strain is larger [23]. Investigation the mechanical properties of phosphorene nanotubes (PNTs) by Sorkin and Zhang [24] showed a strong anisotropic deformation and failure behavior. MD simulations were employed by Liao et al. [25] to study the structural stability and mechanical properties of PNTs.

In this paper, DFT calculations are used to propose a finite element (FE) model which can predict the mechanical properties of zigzag PNTs. To this end, the similarity between molecular and structural

\* Corresponding author.

E-mail address: [s\\_rouhi@iaul.ac.ir](mailto:s_rouhi@iaul.ac.ir) (S. Rouhi).

mechanics is used. Employing the proposed model, the effect of PNT geometrical properties on its Young's modulus is investigated.

## 2. Methodology

### 2.1. Molecular structural model

The total potential energy of a molecular system can be expressed as [50,51]:

$$U_{total} = \sum U_r + \sum U_\theta + \sum U_\phi + \sum U_\omega + \sum U_{vdW} \quad (1)$$

where  $U_r$ ,  $U_\theta$ ,  $U_\phi$ ,  $U_\omega$  and  $U_{vdW}$  as the bonding, bond stretching, bond angle bending, dihedral angle torsion, out-of plane torsion and non-bonding van der Waals energies. Here, the third and fourth terms which are associated with the torsions of the bonds are merged in a single term. Besides, the harmonic forms are used to express the bonding energies. Therefore [52,53]:

$$U_r = \frac{1}{2} k_r (r - r_0)^2 = \frac{1}{2} k_r (\Delta r)^2 \quad (2)$$

$$U_\theta = \frac{1}{2} k_\theta (\theta - \theta_0)^2 = \frac{1}{2} k_\theta (\Delta \theta)^2 \quad (3)$$

$$U_\tau = U_\phi + U_\omega = \frac{1}{2} k_\tau (\Delta \phi)^2 \quad (4)$$

where  $k_r$ ,  $k_\theta$  and  $k_\tau$  are the force constants of the bond stretching, bending, and out-of-plane torsion. Moreover,  $\Delta r$ ,  $\Delta \theta$  and  $\Delta \phi$  are changes of the bond length, the bond angle, and the dihedral angle from the initial position, respectively.

Simulating the bonds by beam elements, the strain energies of the beam due to pure tension  $N$ , pure bending moment  $M$  and torque  $T$ , which are named as  $U_A$ ,  $U_M$  and  $U_T$ , respectively, are expressed as [54,55]:

$$U_A = \frac{1}{2} \int_0^L \frac{N^2}{EA} dL = \frac{1}{2} \frac{N^2 L}{EA} = \frac{1}{2} \frac{EA}{L} (\Delta L)^2 \quad (5)$$

$$U_M = \frac{1}{2} \int_0^L \frac{M^2}{EI} dL = \frac{2EI}{L} \alpha^2 = \frac{1}{2} \frac{EI}{L} (2\alpha)^2 \quad (6)$$

$$U_T = \frac{1}{2} \int_0^L \frac{T^2}{GJ} dL = \frac{1}{2} \frac{T^2 L}{GJ} = \frac{1}{2} \frac{GJ}{L} (\Delta \beta)^2 \quad (7)$$

In the above equations,  $E$ ,  $L$ ,  $A$ ,  $I$ ,  $J$  and  $G$  are Young's modulus, length, cross-sectional area, moment of inertia, polar moment of inertia and shear modulus of beam elements. Besides,  $\Delta L$ ,  $\alpha$  and  $\Delta \beta$  are length variation, bending angle and torsion angle, respectively. Comparing the corresponding energies from Eqs.(2)–(4) to Eqs. (5)–(7) one could have:

$$\frac{EA}{L} = k_r \quad (8)$$

$$\frac{EI}{L} = k_\theta$$

$$\frac{GJ}{L} = k_\tau$$

If the  $A$ ,  $I$  and  $J$  are substituted as  $A = \pi d^2/4$ ,  $I = \pi d^4/64$  and  $J = \pi d^4/32$  in the Eq. (8), the mechanical properties of beam elements are obtained as functions of the bond stiffnesses as [54,55]:

$$d = 4 \sqrt{\frac{k_\theta}{k_r}}, \quad E = \frac{k_r^2 L}{4\pi k_\theta}, \quad G = \frac{k_r^2 k_\tau L}{8\pi k_\theta^2} \quad (9)$$

To obtain the stiffnesses, the following relations can be used [56–58]:

$$Y_S = \frac{8\sqrt{3} k_r}{\frac{k_r r_1^2}{k_\theta} + 18} \quad (10)$$

$$\nu = \frac{\frac{k_r r_1^2}{k_\theta} - 6}{\frac{k_r r_1^2}{k_\theta} + 18} \quad (11)$$

$$k_\tau = 24D \quad (12)$$

where in which  $Y_S$ ,  $\nu$  and  $D$  are surface Young's modulus, Poisson's ratio and flexural rigidity of the nanostructures. Besides,  $r_1$  is the bond length of the equilibrated structure.

### 2.2. DFT details

All of the DFT calculations are performed by using the SIESTA code (Spanish Initiative for Electronic Simulations with Thousands of Atoms) [59,60]. To evaluate the interaction of the nuclei and core electrons with the valence electrons, the Troullier–Martin pseudopotentials [61] is utilized. A double-zeta polarized basis set (DZP) is utilized as the wave functions. Moreover, to evaluate the exchange–correlation functional, the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) flavor [62] is employed. The atomic nuclei positions are optimized by using the conjugate gradient (CG) method. The Hellman–Feynman theorem [63] including the Pulay correction [64] is employed to record the force. The mesh cutoff is chosen as 475 Ry and a  $1 \times 1 \times 20$  Monkhorst–Pack grid is used for  $k$ -point sampling of the Brillouin zone.

## 3. Results and discussion

### 3.1. Results of DFT simulations

Table 1 shows the radii and unit cell constants of the optimized nanotubes (see Fig. 1). The inner and outer diameters of the simulated phosphorene nanotubes, which are represented schematically in Fig. 1, are given in Table 2. Some of the considered zigzag PNTs are shown from the side and front view in Fig. 2. To compute the Young's modulus of the zigzag PNTs, they are loaded by the strain between –6% and 6% with the step of 1%. The strain energy should be evaluated at each step. A sample nanotube with the axial loading is represented in Fig. 3. Surface Young's modulus of the PNTs is stated as:

$$Y_s = Yt \quad (13)$$

where  $Y$  is the bulk Young's modulus and  $t$  is the thickness of the nanostructure. The bulk modulus is expressed as:

$$Y = \frac{1}{V_0} \frac{\partial^2 E_s}{\partial \epsilon_{axial}^2} \quad (14)$$

Substituting  $V_0 = A_0 t$  in Eq. (14) and then using Eq. (13), surface Young's modulus is obtained as [65]:

$$Y_s = \frac{1}{A_0} \frac{\partial^2 E_s}{\partial \epsilon_{axial}^2} \quad (15)$$

where  $\epsilon_{axial} = \frac{\Delta c}{c}$  and  $E_s$  are the uniaxial strain and strain energy which is

**Table 1**

The radius and unit cell constants of the considered PNTs.

Chirality	Average radius (Å)	$a=b$ (Å)	$c$ (Å)
(14,0)	8.1867	24.9826	4.4200
(16,0)	9.1563	27.1229	4.5141
(18,0)	10.1692	29.2633	4.5593
(20,0)	11.1694	31.4037	4.6044
(24,0)	13.1827	35.6844	4.6504

Download English Version:

<https://daneshyari.com/en/article/5450229>

Download Persian Version:

<https://daneshyari.com/article/5450229>

[Daneshyari.com](https://daneshyari.com)