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Original Research Article

Vibrational analysis of armchair phosphorene nanotubes by a DFT-based finite element model

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ABSTRACT

A finite element model based upon the density functional theory is developed to investigate the vibrational characteristics of armchair phosphorene nanotubes. To this end, the P–P bonds are simulated by beam elements whose elastic properties are obtained from the analogy of molecular and structural mechanics. The effects of nanotube length, diameter and boundary conditions on the frequencies of armchair phosphorene nanotubes are evaluated. It is shown that the effect of nanotube radius on its natural frequency is weakened by increasing the nanotube aspect ratio. Comparing the first ten frequencies of armchair phosphorene nanotubes with different diameters, it is observed that the effect of diameter on the vibrational behavior of phosphorene nanotubes is more pronounced at higher modes.

1. Introduction

Recently, phosphorene synthesized from the layered black phosphorus bulk materials [1–3] has attracted the attention of research community due to its applications in different fields [4–8]. To take the advantages of this material, its physical properties should be clearly identified. In this regard, the mechanical characteristics of phosphorene nanosheets and nanotubes have been investigated in several papers.

First-principles calculations were employed by Hu et al. [9] to examine the mechanical and electronic properties of monolayer and bilayer phosphorene nanosheets. When a uniaxial tensile strain was applied along a zigzag direction, they obtained a specific negative Poisson's ratio for the pucker distance of each layer in the bilayer phosphorene. The sustainable tensile strains of armchair and zigzag monolayer phosphorene nanosheets were respectively computed as 27% and 30% by Wei and Peng [10]. Employing first-principles calculations, Ding et al. [11] investigated the mechanical and electronic behaviors of phosphorene nanosheets. They observed prominent anisotropic elastic characteristics with a large elastic strain limit of 0.31 for armchair nanosheet and 0.22 for zigzag ones. Sorkin and Zhang [12] studied the deformation and failure behavior of phosphorene nanoribbons under uniaxial tensile strain. Employing the uniaxial stress along an arbitrary direction, the anisotropic electro-mechanical properties of phosphorene nanosheets were observed by Wang et al. [13]. Molecular dynamics (MD) simulations were employed by Wang et al. [14] to study the effect of mechanical strain on single-layer black phosphorus nanoresonators at different temperatures. Based on their results, the intrinsic

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Nomenclature

Y_S	surface Young's modulus of the nanostructure
υ	Poisson's ratio of the nanostructure
D	flexural rigidity of the nanostructure
d	diameter of the beam element
E	Young's modulus of the beam element
G	shear modulus of the beam element
L	length of the beam element
A	cross-sectional area of the beam element
I	moment of inertia of the beam element
J	polar moment of inertia of the beam element
k_τ	force constant of bonds against out-of-plane torsion
k_θ	force constant of bonds against bending
k_r	force constant of bonds against stretching
a, b, c	unit cell constants

puckered configuration of phosphorene nanosheets leads to a highly anisotropic behavior for their resonant frequencies. Sha et al. [15] studied the effect of temperature on the mechanical properties of the phosphorene nanosheets. They indicated that the mechanical properties of the zigzag phosphorenes are more sensitive to the temperature change than their armchair counterparts. Investigating the effect of atomic vacancy on the mechanical properties of the phosphorene showed that 2% concentration of randomly distributed mono-vacancies can lead to decreasing fracture strength by about 40% [16]. A large structural flexibility along the armchair direction was observed for the phosphorene nanosheets allowing them to have large curvatures [17]. Liu et al. [18] used MD simulations to study the fracture mechanism and energy release rate of phosphorene nanosheets. It was shown that the energy release rate is not affected by the strain rate significantly. Studying the mechanical properties of phosphorene nanotubes (PNTs), Sorkin and Zhang [19] revealed that as the phosphorene nanosheet, a strong anisotropic behavior is observed for the PNTs. Using DFT simulations, Sorkin and Zhang [20] studied the elastic properties of defect-free phosphorene nanoribbons. The influence of intrinsic strain on the structural stability and mechanical properties of PNTs was evaluated by Liao et al. [21] using MD simulations.

In this paper, a DFT-based FE method is used to study the vibrational behavior of armchair PNTs. To accomplish this aim, beam elements are used to simulate the structure of armchair PNTs. The effects of diameter and aspect ratio (length/diameter) of PNTs on their natural frequencies are studied. Besides, the nanotubes are considered under different boundary conditions.

2. Methodology

2.1. Molecular structural model

The total potential energy of a molecular system is stated as [22]:

$$U_{total} = \sum U_r + \sum U_\theta + \sum U_\phi + \sum U_\omega + \sum U_{vdW} \tag{1}$$

where U_r, U_θ, U_ϕ, U_ω and U_{vdW} are the bonding, bond stretching, bond angle bending, dihedral angle torsion, out-of plane torsion and nonbonding van der Waals energies, respectively. By merging the torsional terms, third and fourth terms, into a single term and accepting the harmonic form of the bonding energies, one can write [23,24]:

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

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

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

wwhere k_r, k_θ and k_τ are the force constants of the bond stretching, bending, and out-of-plane torsion, respectively. Moreover, Δr, $\Delta\theta$ and $\Delta\phi$ are changes of the bond length, the bond angle, and the dihedral angle from the initial position, respectively. If the bonds are substituted by beam elements in the structural mechanics, the corresponding strain energies are expressed as:

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

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

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

where U_A, U_M and U_T are strain energies of beam due to pure tension N, pure bending moment M and torque T. 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, ΔL, α and $\Delta\beta$ are length variation, bending angle and torsion angle, respectively. The following relations are obtained by comparing the equivalent energy terms in Eqs. (2)–(4) and Eqs. (5)–(7):

$$\begin{aligned}\frac{EA}{L} &= k_r\\ \frac{EI}{L} &= k_\theta\\ \frac{GJ}{L} &= k_\tau\end{aligned} \tag{8}$$

To obtain the diameter, d, Young's modulus, E, and shear modulus, G of the beam elements, the cross section of the beams are considered as circle ($A = \pi d^2/4$, $I = \pi d^4/64$ and $J = \pi d^4/32$). Therefore [25,26],

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

Considering Y_S, υ and D as Young's modulus, Poisson's ratio and flexural rigidity of the nanostructures,