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Effects Of Missing Atom Defect On The Mechanical Properties Of Black Phosphorene Nanotube

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ABSTRACT: We investigate the effect of missing atom defect to the mechanical properties of black phosphorene nanotube (BPNT) through molecular dynamics finite element method with Stillinger-Weber potential.We found that effect of the defect on Young's modulus of phosphorene tube is insignificant. In contrast to, fracture stress and facture strain of defective tube reduce up to 14% and 57%, respectively, compared with the pristine one. Simulation results will help to design and use BPNT for its future applications.
Keywords: Phosphorene, Mechanical properties , Missing atom defect.

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I. INTRODUCTION

Two-dimensional black phosphorous, namely, black phosphorene has been recently synthesis **[1-5]**. Black phosphorene is a semiconductor with a large direct band gap of 1.51 eV **[6]**. Black phosphorene has potential application in nanoelectronics, optoelectronics **[2, 6, 7]**, gas sensors **[8]** and the anode material of Li-ion batteries **[9, 10]**.The pristine and defective armchair (0, 10) black phosphorene nanotube (BPNT) isstudied. Defect is assumed to locate at tube's center.

The mechanical properties of pristine black phosphorene nanotube have been investigated clearly bydensity functional theory (DFT) calculations **[11-14],** density functional theory based finite element model (DFT-FEM)**[15]**, density functional tight-binding (DFT-TB)**[16]**, molecular dynamics simulations (MD)**[17-21]**, molecular dynamics finite element method (MDFEM)**[22-24]**. However, effects of missing atom defect on the mechanical properties of black phosphorene nanotube have a little study. Liu et al.**[25, 26]** showed that missing atoms could reduce significantly the tensile performance of BPNTs. The fracture strength and strain of black phosphorene were reported to reduce about 23-50% and 40-66%,respectivelyby MD simulation**[25]**.

The present work studies through molecular dynamics finite element method (MDFEM) the effect of a missing atom defect to the mechanical properties BPNTsunder uniaxial tension. Since, the zigzag BPNT was found to have poorer stability than the armchair BPNT **[27]**. Hence, only the armchair BPNT is considered in this study.

II. Framework for analysis

Stillinger-Weber potential is here used to model the P-P interatomic interactions[28].The potential energy E of the atomic structure is the total of the bond stretching energy E_r and bond angle bending energy E_θ:

$$E = E_r + E_\theta \quad (1)$$

$$E_r = \sum_{e=1}^{M} V_2, \qquad E_\theta = \sum_{e=1}^{N} V_3 \quad (2)$$

$$V_2 = Ae^{\left[\rho/(r_{ij}-r_{\max ij})\right]}\left(B/r_{ij}^4 - 1\right) \quad (3)$$

$$V_3 = Ke^{\left[\rho_{ij}/(r_{ij}-r_{\max ij})+\rho_{ik}/(r_{ik}-r_{\max ik})\right]}\left(\cos\theta_{ijk} - \cos\theta_o\right)^2 \quad (4)$$

WhereV_2corresponds to the bond-stretching và V_3associates with the angle-bending. M and N denote the total numbers of bond-stretching and angle-bending element, respectively (Fig. 1). Cutoffs $r_{\max ij}, r_{\max ik}$ are geometrically determined by the material's structure. A, Kare energy parameters. ρ, B, ρ_{ij}, ρ_{ik}, $\theta_o$are five geometrical parameters. r_{ij}, r_{ik} are length ofij andik. θ_{ijk} is angle between bondij and ik.

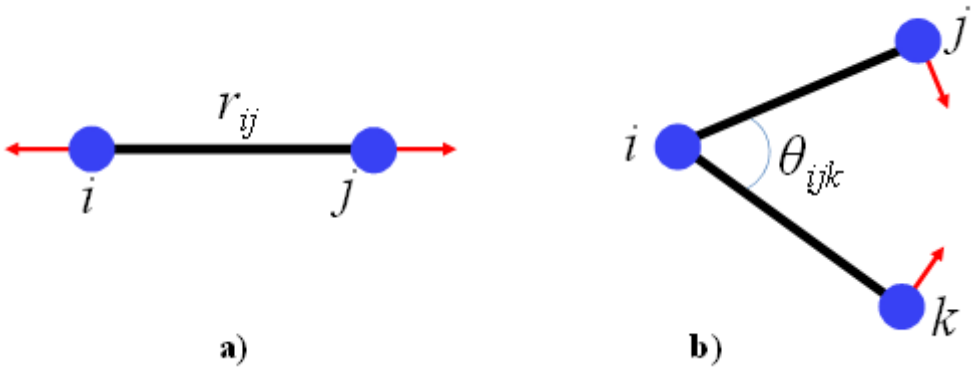

Fig. 1. Two element types used in MDFEM with Stillinger-Weber potential: a) Two-body (bond-stretching) element; and b) Three-body (angle-bending) element.

Stillinger-Weber potential parameters are taken from **[28]** for P-P interaction in black phosphorene and tabulated in table 1 and 2.

Table 1 Two-body (bond-stretching) Stillinger-Weber potential parameters

	A, nN.Å	ρ, Å	B, $Å^4$	r_o, Å	r_{maxij}, Å
P – P	5.7962	0.809	14.287	2.224	2.790

Table 2 Three-body (angle-bending) Stillinger-Weber potential parameters. P_t and P_b indicate the phosphorus atoms belonging to inner and outer tube diameter, respectively.

Types	K, nN.Å	θ_o, degree	ρ_{ij}, Å	ρ_{ik}, Å	r_{maxij}, Å	r_{maxik}, Å	r_{maxjk}, Å
P_t – P_t – P_t	57.068	96.359	0.8099	0.809	2.790	2.790	3.89
P_b – P_b – P_b	57.068	96.359	0.8099	0.809	2.790	2.790	3.89
P_t – P_t – P_b	51.162	102.094	0.8099	0.809	2.790	2.790	3.89
P_b – P_b – P_t	51.162	102.094	0.8099	0.809	2.790	2.790	3.89

While density functional theory (DFT) calculations and molecular dynamics (MD) simulations are time-consuming, molecular dynamic finite element methods (MDFEM), sometime known as atomic-scale finite element methods or atomistic finite element methods, have been developed to analyze nanostructured materials in a computationally efficient way, see e. g. **[29, 30]**. To achieve the atomic positions of the BPNT under specific boundary conditions, molecular dynamic finite element method (MDFEM) is here adopted. In MDFEM, atoms and atomic displacements are considered as nodes and translational degrees of freedom (nodal displacements), respectively. Both first and second derivatives of system energy are used in the energy minimization computation, hence it is faster than the standard conjugate gradient method which uses only the first order derivative of system energy as discussed in **[29]**. The stiffness matrices of these elements are established based upon interatomic potentials. Similar to conventional finite element method, global stiffness matrix is assembled from element stiffness matrices. Hence, relations between atomic displacement and force can be derived by solving a system of equations.Molecular dynamics finite element method (MDFEM)with Stillinger-Weber potential is used to simulate the uniaxial compression and tension of BPNT**[22-24]**. σ and ε are the nominal axial stress (engineering stress) and nominal axial strain (engineering strain), respectively. Young's modulus Y is determined from the first derivative of the stress-strain curve at strain ε=0. Due to an ambiguous value of the tube's thickness t, we use the product Yt and σt to denote 2D Young's modulus and 2D stress, respectively. Pristine and defective (0, 10) armchairBPNT is considered.

III. RESULTS AND DISCUSSION

Fig.2 shows the stress-strain curves of pristine and defective (0, 10)armchair BPNT under

uniaxial tension. The axial stress increases monotonously with the rising of the axial strain up to a peak value, then the stress drops suddenly as shown in Fig. 2. Hence, maximal axial stress and strain at maximal stress refer to fracture stress and fracture strain, respectively.

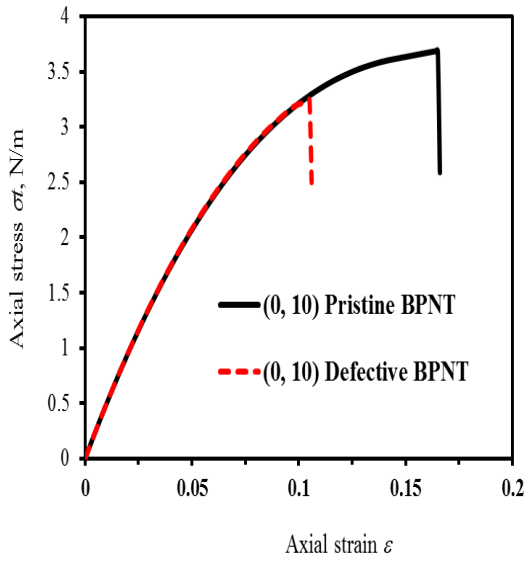

Fig. 2. The stress-strain curves of pristine and defective (0, 10) armchair BPNT under uniaxial tension

Table 3 showsthe Young's modulus, fracture stress and fracture strain of pristine and defective (0, 10) armchair BPNT under uniaxial tension.

Table 3 Mechanical properties of pristine and defective (0, 10) armchair BPNT under uniaxial tension

Armchair nanotube	Young's modulus Yt, N/m	Fracture stress σt, N/m	Fracture strain ε, %
(0, 10) pristine	51.68	3.689	16.5
(0, 10) defective	51.93	3.243	10.5

The results show that the defective tube exhibit almost the same Young's modulus as the pristine one as indicated in Table 3. Therefore, the defect has almost no effect on Young's moduli of phosphorene tube. In contrast, the defectaffectssignificantly on the fracture stress and strain. Due to a single defect in the tube's center, the fracture stress and facture strain of defective tube reduce up to 14% and 57%, respectively, compared with the pristine one. Our results are in good agreement with those from MD simulations[25]. Fig. 3 shows snapshots of defective (0, 10) armchair BPNT under uniaxial tension.

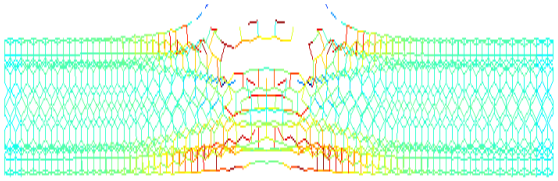

Fig. 3. shows snapshots of defective (0, 10) armchair BPNT under uniaxial tension.

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