Computational Materials Science 156 (2019) 142–147

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Mechanical properties of defective double-walled boron nitride nanotubes for radiation shielding applications: A computational study

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ARTICLE INFO

Keywords:
Boron nitride nanotubes
Young's modulus
Radiation shielding
Vacancy defects
Density functional theory calculations

ABSTRACT

Radiation shielding is of great importance because of the wide-spread use of nuclear radiation in various applications, such as power generation, space industries, nuclear medicine, etc. Current research focuses on developing materials with high shielding efficiency and robust mechanical properties. Boron nitride nanotubes (BNNTs) make good candidate materials for space radiation shielding applications. They are usually mixed with polymer composites to boost their mechanical properties and increase their shielding capability. Shielding can be further enhanced by adding hydrogen to the BNNT lattice, where it binds to atomic sites, or resides in vacancies. These vacancy defects can degrade the mechanical properties of the shielding materials, making them unsuitable for industrial prolonged use. In this work, we study the effect of vacancies on the mechanical properties of double-walled BNNTs (DWBNNTs). Using density functional theory, we calculate Young's modulus of defective DWBNNTs having up to 4 divacancies, in two configurations, armchair and zigzag. We find that defective armchair DWBNNTs suffer a decrease of 5–25% of their Young's moduli, while zigzag DWBNNTs show a lesser decrease of 3–15%, relative to the defect-free DWBNNTs. In addition, the divacancies cause a length contraction in the armchair case, and an ellipsoidal deformation for the zigzag one. Our findings are important for predicting of the tolerance of DWBNNTs to space radiation environment.

1. Introduction

Low dimensional materials have been gaining increased interest over the last decade due to their exotic physical and chemical properties. Structures made from graphene, hexagonal boron nitride, and di-metal chalcogenides, have been studied for various technologies [1–4]. Novel graphene-based materials have been considered for applications in photovoltaics [5,6], nanoelectronics [7,8], chemical separation [9,10], and sensing [11,12]. Two dimensional boron nitride structures are typically insulating, with a large electronic gap of ~ 4 eV [13,14] and superior mechanical properties [14,15], such as boron nitride nanotubes (BNNTs) [16–20]. BN nanostructures have been suggested as templates for various sensors [21–23], and because of their biocompatibility, they have also been considered for biological applications [24,25].

BNNTs have been widely considered for many uses [16,19], including space radiation shielding applications [26]. This is due to their interesting radiation shielding properties as well as their high Young's modulus, which is not significantly altered by their ionization [27–30]. Boron-10, ^{10}B, is known for its high thermal neutron absorption cross section [31]. As such, the boron-based materials are very well suited for neutron shielding applications such as nuclear reactors, as well as mobile reactors and neutron sources. BNNTs are used as nanofillers in polymer-based nanocomposite materials [24,32,33]. This is due to the good shielding properties of polymers [26], which consist mainly of light elements such as hydrogen, carbon, oxygen, and nitrogen. These light elements are very effective in shielding applications, especially for slowing down neutrons. The addition of BNNTs to these polymers enhances their mechanical properties, and makes it possible to utilize them as neutron-shielding materials.

The use of hydrogenated BNNTs enhances the radiation shielding capabilities of composites made from them. This can happen in two ways: (1) atomic hydrogen binds to the B or N sites of the BNNTs, and (2) molecular hydrogen resides in the interior or exterior of the BNNT surface, especially near vacancies. Increasing the H percentage increases the shielding strength of the composite, but may weaken its mechanical properties [34,35]. It has been shown that defects introduced into the BNNTs can increase their ability to adsorb H [36]. For

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https://doi.org/10.1016/j.commatsci.2018.09.040
Received 3 September 2018; Accepted 17 September 2018
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space applications, it is crucial for the hydrogenated structural materials to be as stiff as possible in order to withstand the harsh space environment [26].

Controlling radiation-induced-defects via interfaces is shown to be the key factor in reducing the damage and imparting stability in certain nanomaterials under conditions where bulk materials exhibit void swelling and/or embrittlement [37]. In recent years, effect of radiation on nanomaterials was simulated for diverse materials, irradiation conditions as well as different quantities of interest [38]. As such, different situations arising upon the bombardment of nanostructures by high-energy ions and neutrons were simulated such as: displacement cascades in Ni nanograins or particles with different bombardment energy, radiation stimulated growth of grains in nano Ni for the cascade exited by an impact of a particle with an energy of 5 keV, the behavior of interstitial atoms and Tetrahedral Stacking Fault in damage cascades, evolution of the morphology of nanocrystalline films upon irradiation, the behavior of nanomaterials with bcc and fcc structures upon irradiation, nucleation and growth of vacancy clusters in the cubic modification of silicon carbide, and the behavior of grain boundaries in nanostructures as sinks and sources of defects.

In the meantime, few experimental results for the impact of radiation on BNNT exist. For example, multi-walled boron nitride nanotubes were irradiated with low and medium energy argon and helium ions at room and elevated temperatures [39]. The irradiated samples were characterized by transmission electron microscopy and Raman spectroscopy, and a comparison to the response of carbon nanotubes to irradiation was made. A dose of 2×10^{15} ions/cm^2 was found to give rise to complete amorphization for irradiation with 40 keV Ar ions, while a comparable dose (in terms of displacement per atom) of 1.2×10^{18} ions/cm^2 for 350 keV He caused significantly less damage. Elevated temperatures considerably reduce the amount of damage indicating that efficient annealing of defects occurs in BN nanotubes already at 3000 °C.

In this work, we use density functional theory (DFT) to quantify the effects of BNNT vacancy defects on their mechanical properties, by calculating Young's modulus of the BNNTs. We consider double-walled BNNTs (DWBNNTs), since experiments show that multiwall BNNTs are easier to fabricate [40]. We focus on double vacancy defects (divacancies, DVs), and calculate Young's moduli of DWBNNTs structures with up to four divacancies. Two DWBNNTs are considered; an armchair (5,5)@(10,10), and a zigzag (9,0)@(18,0).

2. Computational methods and structures

DFT calculations were carried out using the Quantum ESPRESSO package [41]. Ultrasoft pseudo-potentials and the PBE generalized gradient approximation have been employed [42]. A kinetic energy cutoff of 50 Ry was used, with a $1 \times 1 \times 6$ Monkhorst Pack k-point grid for geometry optimization and a $1 \times 1 \times 30$ Monkhorst Pack k-point grid for total energy calculations. The unit cells of the non-defective armchair and zigzag DWBNNTs contained 240 and 216 atoms, respectively. A vacuum separation of at least 10 Å was used to prevent image interactions. All systems were structurally relaxed till the total forces were less than 0.002 Ry/Bohr.

3. Results and discussion

The study of vacancies in BNNTs is important for two reasons. First, highly energetic radiation can create vacancies along its path in the material [43]. Second, vacancies increase the hydrogenation capacity of BNNTs, thus boosting their shielding strength [36]. Therefore, it is of great importance to explore the effects of such defects on the mechanical properties of the BNNTs, specially for structural materials used in space applications.

In order to use BNNTs in radiation shielding, they should be included as nanofiller materials into a polymer matrix, thus creating a nanocomposite structure [44]. The proposed defective BNNTs will act even better in the nanocomposite because their active sites (dangling bonds) will strongly bind to the surrounding polymer matrix [45]. Finally, defects may readily exist in BNNTs during the fabrication process.

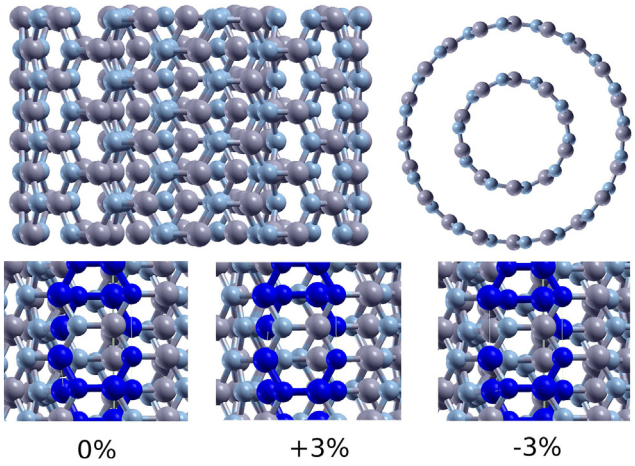

Fig. 1. Defect-free (5,5)@(10,10) DWBNNT. Top: unit cell of the system. Bottom: nanotube segment shown with 0%, +3%, and −3% strain. Dark blue atoms indicate the would-be defect area. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Ab initio calculations have been used to study the stability of the DVs in BN sheets, where it was found that the divacancy formed by removing a B-N pair is the most stable configuration [46,47]. In addition, B-N divacancies were found to be more stable than B and N monovacancies [48].

3.1. Defect-free DWBNNT

To establish a reference system, we first calculate Young's modulus of a (5,5)@(10,10) DWBNNT. The unit cell of the system (Fig. 1) has a length of about 10 Å, with 240 atoms. Structural relaxation yields a B-N distance of 1.46 Å, and radii of $R_{10,10} = 6.96$ Å and $R_{5,5} = 3.48$ Å.

We induce an axial strain, ϵ, ranging from -3% to $+3\%$ of the original unit cell length, in steps of 1%, perform structural relaxation, and compute the total energy E. Young's moduli were then calculated from [49]:

$$Y = \frac{1}{V_0}\left(\frac{\partial^2 E}{\partial\, \epsilon^2}\right)_{\epsilon=0}, \tag{1}$$

where Y is Young's modulus of the structure, V_0 is the volume of the DWBNNT at zero strain, $V_0 = 2\pi(R_o + R_i)(R_o - R_i)$, and R_o and R_i, are the radii of the outer and inner BNNTs, respectively. The shell thickness, $R_o - R_i$, is typically 3.4 Å [50]. We find that Young's modulus of the defect free DWBNNT is $Y_0 = 814$ GPa which is in good agreement with the previous studies [50].

3.2. Defective DWBNNTs

We begin by the case of one DV formed on one side of the outer tube. We form the defect, then structurally relax the system. The applied stress changes the next-nearest-neighbor (n.n.n.) BB, BN and NN bond lengths at the defect site. To quantify these changes we define the fractional parameter η as:

$$\eta_{ij} = \frac{l_{ij} - l_{ij}^{(0)}}{l_{ij}^{(0)}} \tag{2}$$

where $l_{ij}^{(0)}$ is the original (zero stress) length of the ij bond, and $i, j \in \{B,N\}$. Fig. 2 shows the defect site, for maximum positive and negative stress (top), as well as the variation of η with the applied stress. The BB

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