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Prediction of chirality- and size-dependent elastic properties of single-walled boron nitride nanotubes based on an accurate molecular mechanics model

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ABSTRACT

Molecular mechanics theory has been widely used to investigate the mechanical properties of nanostructures analytically. However, there is a limited number of research in which molecular mechanics model is utilized to predict the elastic properties of boron nitride nanotubes (BNNTs). In the current study, the mechanical properties of chiral single-walled BNNTs are predicted analytically based on an accurate molecular mechanics model. For this purpose, based upon the density functional theory (DFT) within the framework of the generalized gradient approximation (GGA), the exchange correlation of Perdew–Burke–Ernzerhof is adopted to evaluate force constants used in the molecular mechanics model. Afterwards, based on the principle of molecular mechanics, explicit expressions are given to calculate surface Young's modulus and Poisson's ratio of the single-walled BNNTs for different values of tube diameter and types of chirality. Moreover, the values of surface Young's modulus, Poisson's ratio and bending stiffness of boron nitride sheets are obtained via the DFT as byproducts. The results predicted by the present model are in reasonable agreement with those reported by other models in the literature.

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1. Introduction

The landmark research about carbon nanotubes (CNTs) carried out by Iijima [1] made the possibility to develop other types of tubular nanostructures with non-carbon atoms which has been attracted much attention lately. Through the astonishing properties of BNNTs such as high sound velocity and thermal conductivity, they have become ideal candidates for multifarious applications in different fields of nanoscience and nanotechnology. So, various investigations have been conducted about the properties of BNNTs, both theoretically and experimentally.

Menon and Srivastava [2] used a generalized molecular dynamics (MD) simulation to investigate the structure of BNNTs. They indicated that the three different morphologies of the nanotubes as flat, conical and amorphous ends are directly related to the nanotube chiralities. Tang and his coworkers [3] synthesized multi-walled BNNTs using a carbon-free chemical vapor deposition process. They found that opposed to the CNTs, bending of BNNTs typically results in fracture at their concave side. Based on *ab initio* simulations of bundled single-walled zigzag and armchair BNNTs, Kunstmann and Quandt [4] studied the detailed atomic structures of BNNTs. They observed new forms of the radially constricted nanotubes which were energetically superior to the previous isomers ones. Nirmala and Kolandaivel [5] investigated the structure and electronic properties of armchair BNNTs as a function of tube diameter using density functional theory (DFT). To represent the interactions inside the nanotubes, they used NBO partitioning scheme.

Study on the mechanical properties and strength of nanotubes have been the subject of several researches [6–18]. Using the electric-field-induced resonance method, Suryavanshi et al. [8] measured the average effective elastic modulus of BNNTs equal to 722 GPa. In [11–13], it was shown that nonlinearity and defects could affect the elastic properties and strength of nanotubes. Fang et al. [14] calculated surface Young's moduli of single-walled CNTs with dissimilar diameters as well as chiral angles using molecular mechanics simulation. Verma et al. [15] calculated the elastic properties of BNNTs for different chiralities and diameter values by means of the Tersoff–Brenner potential. The elastic properties of BNNTs were studied by Griebel and Hamaekers [16] in which the nanotubes were embedded in amorphous silicon-boron-nitride ceramics. The analysis was performed on the basis of MD simulations. Moreover, they examined the influence of the nanotube/matrix ratio on the elastic modulus of the composite. They demonstrated that the extended rule-of-mixtures predicts Young's modulus of the composite with a good estimation. Based on the molecular mechanics, Santosh et al. [17] studied Young's modulus and shear modulus of BNNTs. A finite element model of single-walled CNTs based on molecular mechanics theory was proposed by Rossi and Meo [18] to evaluate Young's modulus, ultimate strength and strain of single-walled CNTs.

Compared to the numerical methods, analytical solutions have the capability to give explicit expressions for the related problem which make it possible to incorporate directly the properties of the nanostructures at different length-scales into the obtained expressions. Molecular mechanics model is considered as a powerful tool to investigate the mechanical responses of nanostructures analytically. This model has been widely used by different researchers [7,9,10,14,17–19].

In this work, to predict the elastic properties of chiral single-walled BNNTs, closed-form analytical solution is used. To this end, the elastic properties of a boron nitride (BN) sheet are first calculated on the basis of DFT which leads to obtain force constants of the molecular mechanics theory. Then, based on a molecular mechanics model, explicit formulas are employed to obtain the values of surface Young's modulus and Poisson's ratio as functions of tube diameter and chirality. The results are compared to the ones available in the literature to show the reliability of the present methodology.

2. Molecular mechanics model

For the current study, bond stretching and angle variation energy terms are expected to be the most important in the total molecular potential energy of the system and the remaining contributions are negligible [7]. Thus, based upon Hooke's law, the total potential energy of the system can be written as

$$E_t = \sum \frac{1}{2} K_{\rho_i} (dr_i)^2 + \sum \frac{1}{2} C_{\theta_j} (d\theta_j)^2 \tag{1}$$