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Effects of in-plane electric field and temperature change on Young's modulus of hexagonal boron nitride nanosheets with different chiralities

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ABSTRACT

In the current investigation, the influences of in-plane electric field and temperature change on Young's modulus of boron nitride nanosheets (BNNs) are studied for both armchair and zigzag chiralities. To this end, the density functional theory (DFT) and quasi-harmonic approximation (QHA) are applied to calculate the total energy of the system. It is found that in the presence of temperature change, by applying the electric field along the zigzag and armchair directions, Young's modulus of BNNs decreases and increases, respectively. Moreover, it is revealed that the range of variation in Young's modulus of zigzag BNNs corresponding to different values of electric field is generally lower than that of armchair ones, but the slope of this variation with temperature for zigzag BNNs is more than Armchair ones. Also, it is observed that the rate of variation of Young's modulus with temperature at lower values is sharper than that at higher temperatures. This behavior can be useful in designing electro-thermo-mechanical nanosensors.

1. Introduction

Nano- and micro-electromechanical systems (NEMS and MEMS) have been the subject of intense research in recent years [1–4]. Carbon nanotubes and graphene sheets are the commonly used nano-

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structures in NEMS and MEMS. Recently, nanostructures with non-carbon atoms such as boron nitride nanotubes (BNNTs) and boron nitride nanosheets (BNNs) have attracted a lot of interest from the research community for the use in NEMS and MEMS. BNNs are two-dimensional crystals including boron and nitrogen atoms covalently bonded as honeycomb-like networks which have demonstrated exceptional mechanical and physical properties. It has been observed that there is a very close structural analogy between BNNs and graphene. Recent rise of various applications of graphene has led to intensive attention from the scientific community in order to investigate the stability and mechanical characteristics of its BNN counterpart.

Synthesis of pure boron nitride nanotubes (BNNTs) by the arc discharge method was first achieved by Chopra et al. [5]. In contrast to carbon nanotubes (CNTs) which are with zero band gap and possess unstable electrical properties changing from metallic to semiconducting [6,7], BNNTs have a large band gap and are always semiconducting. The stable behavior and also their relative chemical inertness make them different from their carbon counterparts leading to their applications in a wide variety of electronic and photonic nanodevices. These superb properties and the potential applications of BNNT demonstrate its unique scientific and technical importance and have recently attracted industrial and academic attention. So far, a number of researchers have given the reports on the mechanical properties of BNNTs [8–23]. Among these properties, Young's modulus, which is a useful parameter to measure the resistance of a material to the deformation in a special direction, has been evaluated for BNNTs by Chopra and Zettl [8], Kudin et al. [11], Demczyk et al. [12], Akdim et al. [14], Suryavanash et al. [15], and Song et al. [18].

Electric field and temperature change can affect the characteristics of nanostructures. For example, Zhou et al. [24] used density functional theory to show that an applied electric field can substantially improve the hydrogen storage properties of polarizable substrates. Also, Amorim et al. [25] investigated the strain- and electric-field induced modulation of nitride nanomembrances gaps in the framework of density functional theory.

In the current study, an *ab initio* investigation is presented into the influences of in-plane electric field and temperature change on Young's modulus of BNNs for both armchair and zigzag chiralities. To perform this purpose, the density functional theory and quasi-harmonic approximation are applied to calculate the energies of electrons and phonons, respectively, and then to obtain the total energy of system.

2. Methodology

The elastic behavior of BNN based on the strain energy calculations is studied in the range of harmonic deformation. The calculations are performed on the basis of DFT [26,27], in the context of generalized gradient approximation (GGA) and using exchange correlation of Perdew–Burke-–Ernzerhof (PBE) [28,29]. The calculations presented herein are performed via the Quantum-Espresso coding procedure [30]. Based on the previous works in the literature, the change in the results is not significant with increasing the unit cell dimension [31]. Therefore, in the current study, the smallest hexagonal unit cell is utilized in the calculations for more simplicity as shown in Fig. 2. Brillouin zone integration is performed with 20∗20∗1 Monkhorst and Pack k-point mesh [32], and the cut-off energy for plane wave expansion was taken to be 80 Ry. Also, to calculate the phonon energies, the QHA code is employed [33]. It should be noted that the QHA code cannot be implemented for the case of triclinic structures. Thus, the hexagonal unit cell is considered to remain unchanged in shape when temperature increases.

Surface Young's modulus is given by

$$Y_s = \frac{1}{A_0}\frac{\partial^2 E_s}{\partial \varepsilon^2} \tag{1}$$

where A_0 is the cross-sectional area without any strain and E_s denotes the strain energy of structure. Also, ε is the strain which is in the harmonic range from -2% to 2%.

3. Results and discussion

The effects of electric field and temperature change on Young's modulus of BNNs with armchair and zigzag chiralities are investigated in this section. Schematic views of BNN under electric filed in