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Electromechanical properties of Boron Nitride Nanotube: Atomistic bond potential and equivalent mechanical energy approach

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ABSTRACT

We present a molecular mechanics-based approach to model the isolated zigzag BNNTs bonds by an (energy-) equivalent piezoelectric beam element. The harmonic DREIDING force field is employed for bonded and non-bonded interatomic interactions. To investigate the effectiveness of the proposed method we predict the elastic modulus and piezoelectric coefficients of BNNTs and demonstrate good accuracy compared to quantum mechanics predictions. Subsequently, we study the influence of some input parameters such as the tube diameter, aspect ratio and chirality. Finally, our approach is validated by comparison to data from the literature.

1. Introduction

Boron Nitride Nanotubes (BNNTs) are one-dimensional nanostructures with unique mechanical, electrical and thermal characteristics. They have been synthesized in the 1990s and have been the interest of research in various research communities [1,2]. The importance of BNNTs emanate from their outstanding strength, lightweight, high heat resistance, radiation shield and piezoelectric properties making them excellent candidates in industries like energy, health, aerospace, defense, and security. BNNTs are also smart materials being frequently used in micro/nanoelectromechanical devices (MEMS/NEMS) [3]. They show potential in fire-retardant products, drug delivery, water desalination, hydrogen storage, energy harvesters and power generation [4–6]. The structure of BNNT is similar to hexagonal Carbon Nanotube (CNT). However, BNNTs do not only possess 95% of the CNT's elastic modulus but they also show superior characteristics like high thermal stability and piezoelectricity [7,8].

Research of BNNT materials has focused on the prediction of effective properties such as elastic and shear modulus, piezoelectric and dielectric coefficients. Since it is sometimes difficult to extract those parameters experimentally, computational modeling has become a complementary and good alternative. A wide range of approaches from quantum mechanics (QM) and molecular dynamics (MD) to continuum mechanics (CM) including multiscale modeling have been developed and employed for this purpose. For instance, QM simulations [9] based and density functional theory (DFT) [10] solve the Schrödinger equation, while MD [11] and Monte Carlo (MC) methods are based on the numerical solution of the equation of motion.

QM-based models are usually very accurate, but they are computationally expensive and cannot be used for large systems. Force field methods such as molecular mechanics (MMs) are based on energy minimization. These methods reduce the computational cost. However, they require also more input parameters such as the aspect ratio, length, chirality, volume fraction, aligned direction, number of tube layer and composite contents [12]. The total potential energy in the harmonic force field for example is the sum of the bonded and non-bonded potential energies. The bonded potential energy is based on two, three and four atoms body interactions which are referred to as the axial, bending and torsion energies. The non-bonded potential energy includes the electrostatic and Van-der-Waals energies related to each bond. These energies can also be formulated in so-called equivalent elements, in which the spring, rod and beam elements have been used to model the atomistic structure in multi-scale analysis [13–15].

Xiang et al. [16] predicted the piezoelectric properties of zigzag BNNTs with a hybrid density functional (B3LYP) method. They found that the piezoelectric properties of BNNTs are higher compared to those of most polymers. Nakhmanson et al. [9] studied the spontaneous polarization and predicted piezoelectric properties of a zigzag BNNT by ab initio simulations and the polarization theory of Berry phases or Wannier functions. The results revealed the spontaneous polarization coupling with lattice symmetry breaking leading to the piezoelectric behavior of BNNT. The results also implied that the zigzag BNNT

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piezoelectric properties are lower than the inorganic piezoceramic contents such as PZT, BTO and STO materials, but higher than those in the piezopolymer categories like PVDF. Sai and Mele [17] used ab initio and a tight-binding (TB) approach to predict the piezoelectric properties of a BNNT. The zigzag and armchair tubes are induced by uniaxial and torsional strains yielding different piezoelectric behavior. While the zigzag tubes only respond to the uniaxial strain, the armchair nanotubes have a linear electric dipole moment related to torsion. Zhang and Meguid [18] investigated the effect of the number of tube layers on the piezoelectric properties of a multi-wall BNNT employing MD simulations and a CM model. The MD simulation for the zigzag single-walled BNNT resulted in $e_{11} = 0.24\ C/m^2$ while CM modeling gave a similar value of $e_{11} = 0.25\ C/m^2$. Also, both approaches for the armchair counterpart led to an equal torsional piezoelectric coefficient of $e_{14} = 0.25\ C/m^2$. The piezoelectric coefficient is positive/negative for the odd/even layers number and decreased by increasing the number of layers. The MD results were replicated well by the CM model. Yamakov et al. [19] presented a strain-dependent dipole energy term in their MD model to investigate the piezoelectric properties of a BNNT for all chiral angles under axial and torsional loading showing the dependency of the piezoelectric properties on both chiral angle and nanotube radius.

Jaffari et al. [20] studied the effective elastic and piezoelectric characteristics of a thin film made of BNNT reinforced polymers exploiting the finite element method (FEM) and representative volume elements (RVEs). They considered several volume fractions, aspect ratios and compared their predictions to three analytic approaches (Voigt, Reuss, and Mori–Tanaka). They showed that the effective elastic and piezoelectric properties improved with increasing the BNNT volume fraction, while the dielectric properties decreased slightly. Jaffari et al. [21] predicted the Young's and shear modulus as well as the axial and torsional piezoelectric constants of zigzag BNNTs. Therefore, they employed a structural element accounting for chemical bonds and interactions. The results showed that the axial piezoelectric coefficients fluctuated depending on the diameters of the nanotubes and then approach a value of $0.2\ C/m^2$ while the Young's modulus increased with increasing tube diameter and converged to a maximum value of 1 TPa. Several studies have revealed that the average elastic module range is from 0.5 TPa up to 1.22 ± 0.24 TP [23–25]. Also, the torsional piezoelectric coefficients are varying around a value of $5 \times 10^{-6}\ C/m^2$.

In this study, we present a beam element accounting for the coupled multi-physics problem at nanoscale. In order to simultaneously capture the bonded and non-bonded interatomic interactions, the chemical bond is considered in the structural beam element formulation-including the coupled electrical and mechanical properties – for the first-time. The formulation is based on the piezoelectric element enthalpy energy density and chemical bond potential energy to set up an equivalency between chemical and structural nature.

2. Modeling method

BNNT atoms are constrained by covalent bonds [25]. Symmetry breaking of the hexagonal atomic structure of BNNTs, changing the atomic coordinate of Boron (B), and Nitride (N) cause polarization of the nanotube. In other words, it results in piezoelectric properties of BNNTs. The BNNTs generate a coupled electric dipole dependent on their chirality and the loading type. The armchair nanotube generates a coupled electric dipole when subjected to a torsional excitation while the zigzag nanotube responds to axial extension. We believe that the latter loading has more practical relevance. Nonetheless, it is still possible to extend/modify this formulation to armchair nanotubes [26]. The DREIDING force field is employed since it is ideally suited for predicting structures, relative energies, rotational barriers, and dynamics of organic, biological and inorganic molecules. The total potential energy in this force field can be additively decomposed as [27]

$$U = U_a + U_\theta + U\varphi + U_\omega + U_{vdw} + U_{el} \tag{1}$$

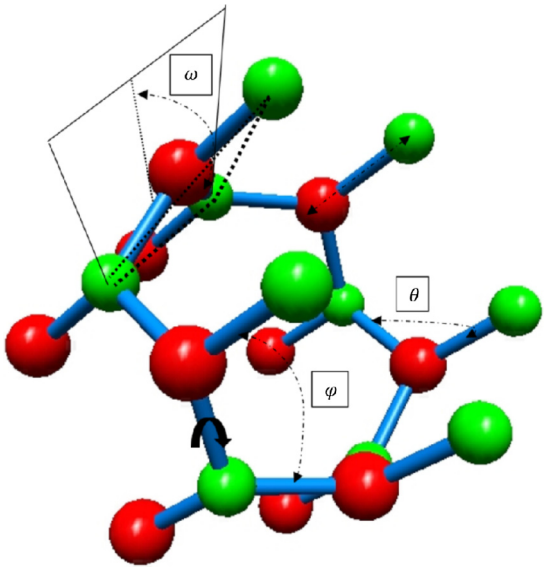

Fig. 1. Atomic structure of zigzag BNNT.

Where U_a,U_θ,U_φ and U_ω denote the potential energy due to axial stretching, bending, torsion and inversion; the latter one stems from three bonds in the same plane; U_{vdw} and U_{el} are the non-bonded potential energies that determine the van der Waals and electrostatic terms, respectively. The subscripts a, θ, φ, ω, vdw and el indicate bond length, bond angle, dihedral angle, inversion angle, van der Waals and electrostatic, respectively. Fig. 1 shows the atomic structure of the zigzag nanotube. We assume small strain theory accounting for the electrostatic nonbonded energy to model the piezoelectric behavior. Only the van der Waals nonbonded energy is neglected in the calculation. The DREIDING force field describes the total energy terms for one single bond [29]. They need to be related to the energy terms expressed as:

$$U_a = \frac{1}{2}K_a(a-a_0)^2 \tag{2}$$

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

$$U_\varphi = \frac{1}{2}K_\varphi\{1-\cos[2(\varphi-\varphi_0)]\} \tag{4}$$

$$U_\omega = \frac{1}{2}K_\omega(\omega-\omega_0)^2 \tag{5}$$

where K_a, K_θ, K_φ, and K_ω are the force field coefficient for the bond axial stretching, bending, dihedral torsion, and inversion, respectively. The subscript "0" refers to the equilibrium position.

According to [30], the harmonic expression appropriately describes the potential energies. In order to simplify the calculation, the total bond potential energy in the DREIDING force field is modified by combining the dihedral angle, torsion and inversion. This compound energy is considered as an equivalent torsion energy in the harmonic form. Eqs. (4) and (5) then becomes:

$$U_\varnothing = U_\varphi + U_\omega = \frac{1}{2}K_\varnothing(\varphi-\varphi_0)^2 \tag{6}$$

in which, the B—N bond axial stretching and bending energy coefficients are given in the DREIDING force field [29], such that; $K_a = 700\ [\frac{kcal/mol}{Å^2}]$, $K_\theta = 100\ [\frac{kcal/mol}{rad^2}]$ and $K_\varnothing$ is the modified torsion energy coefficient [30] that is predicted as $K_\varnothing = 90\ [\frac{kcal/mol}{rad^2}]$.

One can write the last term of Eq. (1) as [31]:

$$U_{el} = \frac{q^2}{4\pi\varepsilon_0 a} \tag{7}$$