MOLECULAR MECHANICS STUDY ON SIZE-DEPENDENT ELECTRO-MECHANICAL PROPERTIES OF BORON NITRIDE NANOTUBES

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Summary We present an analytical study on the electro-mechanical properties of single-walled boron nitride nanotubes via a molecular mechanics model. Closed-form expressions for Young's modulus, Poisson's ratio and surface shear modulus are derived as functions of the nanotube diameter and chiral angle. Furthermore, the electric-field-induced deformation of boron nitride nanotubes is studied by this model. We predict large, size- and chirality-dependent electric-field-induced deformation, comparable to the density functional theory calculations.

INTRODUCTION

Boron nitride nanotubes (BNNTs) have been studied intensively recent years and show exceptional mechanical and electronic properties. Its great Young's modulus and stiffness could provide potentially important applications in synthesis of highly resistant composite materials. BNNTs are also interesting materials for their unique electronic properties. Unlike carbon nanotubes, BNNTs are all semiconductors; furthermore, there is a constant wide band gap (5.5 eV) in the nanotube when the diameter is greater than 9.5 Å, independent of chirality, while small nanotubes show interesting size-dependent electronic and magnetic properties. On the other hand, due to the ionicity of B-N bonds, the structure of the nanotube is buckled. This buckling, which is absent in CNTs, could produce an effect on the mechanical properties of BNNTs.

Chang and Gao [1-4] established a stick-spiral model based on molecular mechanics method and for the first time derived closed-form expressions for the elastic properties of single-walled carbon nanotubes. By giving explicit solutions to the problems considered, analytical methods are especially useful in linking theories at different length scales, which is in fact a very important subject in solid mechanics, because the mechanical properties at different length scales of nanotubes can be directly connected by the closed-form expressions.

To extend this analytical method to composite nanostructures formed by two or more elements, we present in this paper an improved model to investigate the elastic properties of boron nitride nanotubes. Our aim is to show that mechanical properties of composite nanotubes are possible to be described and qualified by analytical methods based on molecular mechanics, and they have essential dissimilarities compared to carbon nanotubes.

MODEL

In the framework of molecular mechanics, the total potential energy, E_{t}, of a SWNT at small strains can be expressed as a sum of energies associated with the variance of bond length, U_ρ, and bond angle, U_θ, in the form of Hooke's law,

$$E_{\mathrm{t}} = U_\rho + U_\theta = \sum_i \frac{1}{2} K_\rho (\mathrm{d}r_i)^2 + \sum_j \frac{1}{2} K_\theta (\mathrm{d}r_j)^2$$

where $\mathrm{d}r_i$ is the bond elongation of bond *i* and $\mathrm{d}r_j$ is the variance of bond angle *j*, and K_ρ and K_θ are the related force constants. In our model, we use an elastic stick with an axial stiffness of *K* and an infinite bending stiffness to model the force-stretch relationship of a boron-nitrogen bond. For angle variation, we have to employ two spiral springs with different angular stiffness coefficients of C_{N} and C_{B} to model the twisting moments resulting from angle bending on boron and nitrogen atoms, respectively.

Size-dependent elastic properties of A- and Z-SWBNNTs

First we derive expressions for equivalent Young's modulus and poisson's ratio of both armchair BNNTs,

$$Ys_{\mathrm{A}} = \frac{K}{\sin\left(\frac{\alpha}{2}\right)\left[1+\cos\left(\frac{\alpha}{2}\right)\right]\left[1+\frac{Kb^2}{C_{\mathrm{N}}\lambda_{\mathrm{N}}+C_{\mathrm{B}}\lambda_{\mathrm{B}}}\cot^2(\frac{\alpha}{2})\right]}$$

$$\nu_{\mathrm{A}} = \frac{\left[\frac{Kb^2}{C_{\mathrm{N}}\lambda_{\mathrm{N}}+C_{\mathrm{B}}\lambda_{\mathrm{B}}}-1\right]\cos(\frac{\alpha}{2})}{\left[1+\cos\left(\frac{\alpha}{2}\right)\right]\left[1+\frac{Kb^2}{C_{\mathrm{N}}\lambda_{\mathrm{N}}+C_{\mathrm{B}}\lambda_{\mathrm{B}}}\cot^2(\frac{\alpha}{2})\right]}$$

and zigzag BNNTs,

$$Ys_{\mathrm{Z}} = \frac{(\cos\zeta-\cos\beta')K}{\sin\beta'\left[2\cos^2\zeta+\cos^2\beta'+\frac{Kb^2}{C_{\mathrm{N}}\lambda_{\mathrm{N}}+C_{\mathrm{B}}\lambda_{\mathrm{B}}}\sin^2\beta'\right]}$$

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$$\nu_{\mathrm{Z}} = \frac{\left[1 - \dfrac{Ka^2}{C_{\mathrm{N}}\lambda_{\mathrm{N}} + C_{\mathrm{B}}\lambda_{\mathrm{B}}}\right]\cos\beta'\,(\cos\zeta - \cos\beta')}{2\cos^2\zeta + \cos^2\beta' + \dfrac{Kb^2}{C_{\mathrm{N}}\lambda_{\mathrm{N}} + C_{\mathrm{B}}\lambda_{\mathrm{B}}}\sin^2\beta'}$$

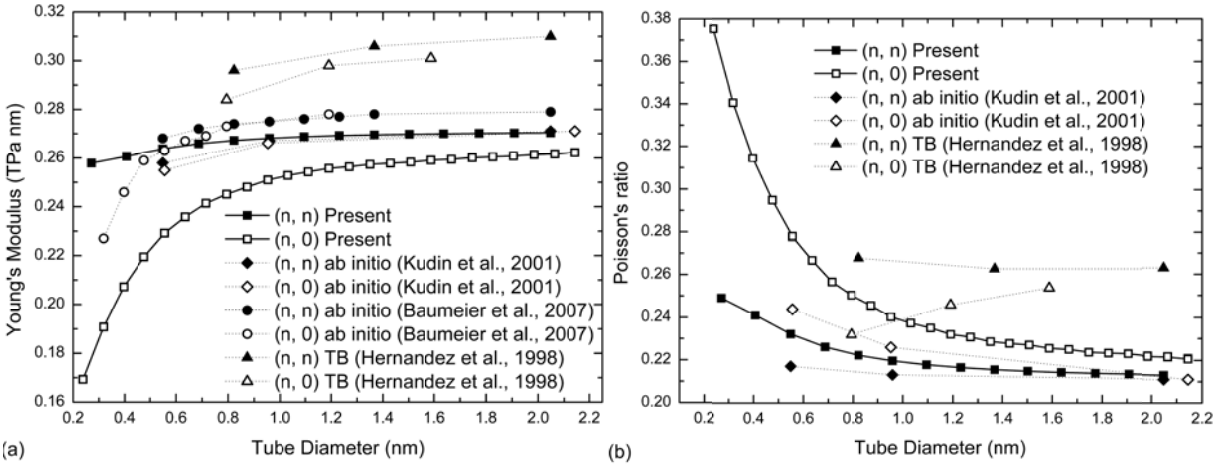

Fig.1 Comparison on (a) Young's modulus and (b) Poisson's ratio between the present model and other existing results. Solid symbols are for armchair tubes and open ones for zigzag tubes.

Surface shear modulus is also derived in the same way.

Size-dependent elastic properties of chiral SWBNNTs

For chiral SWBNNTs, geometry becomes much more complex, because the geometry of buckling changes a lot as the chiral angle changes. But the equilibrium conditions of local structure of both boron and nitrogen atom sites are similar to the armchair and zigzag situations.

We also find the size-dependent and chiral-angle-dependent elastic modulus for chiral BNNTs. The smaller the tube diameter, the stronger the dependence of the elastic properties on the tube size and chirality. For same tube diameter, Young's modulus decreases, and Poisson's ratio increases as chiral angle increases.

Electric-field-induced deformation of SWBNNTs

Using present stick-spiral model, the deformation of a boron nitride nanotube under the electric field can be analysed. It is found that BNNTs have very large electric-field-induced deformation, which is found to arise from both the converse piezoelectric effect and the electrostrictive effect of BNNTs.

CONCLUSIONS

In this paper a stick-spiral molecular mechanics model is adopted to study the electro-mechanical properties of single-walled boron nitride nanotubes. We derived expressions for Young's modulus, Poisson's ratio and surface shear modulus as functions of the nanotube diameter and chiral angle. Furthermore, the electric-field-induced deformation of boron nitride nanotubes is studied by this model. We predict large, size- and chirality-dependent electric-field-induced deformation, comparable to the density functional theory calculations.

References

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