The stress-strain response of carbon nanotube: A structural mechanics analysis incorporating interatomic potentials

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Introduction

Carbon nanotubes (CNTs) have been the subject of intense research due to their exceptional mechanical, thermal and electrical properties. Experiment methods for measuring the mechanical properties are based mainly on the techniques of transmission electron microscopy (TEM) and atomic force microscopy (AFM) [1,2]. These experiments have contributed to confirming that CNTs have exceptional mechanical properties. Due the experimental error bars, however, it is rather difficult to directly state the effect of the chirality on the strength of CNTs.

This study continues authors' previous work [3], which supplied a very simple method to correctly predict the elastic modulus of SWNTs. Here, we present a theoretical prediction on the stress-strain behavior of carbon nanotubes (CNTs) based on an empirical force-field model combined with a structural mechanics analysis.

Theoretical approach

The carbon atoms in the nanotube structures are considered as individual bodies connected with bond energy. The stretching and bending of chemical bonds are strongly coupled. In small strain condition, harmonic energy functions are commonly used when bond lengths of molecular system are near their equilibrium position. However, this is acceptable as an assumption but is not always valid for chemical bonds. The significant angle distortion can weaken the system and even destabilize bonding which results in complete loss of stretching stiffness. Considering the nonlinearity of the molecular force field under large strain, a nanoscale continuum theory is established to directly incorporate the Morse potential function into a molecular mechanics model of CNT structures. The simplified formulas can be presented for simulating the stress-strain response of SWNTs under axial and twisting loads.

Results and Discussion

Based on the above formulation, we have performed the computer simulation for the (17, 0) zigzag and (10, 10) armchair tubes, which have a nearly equal diameter of 1.33 nm. Figure 1 shows the simulated stress-strain responses for the zigzag and armchair tubes with the same diameter. Slope of the stress-strain curve is defined as the elastic modulus. The elastic modulus of a zigzag tube is the same with that of an armchair tube and is calculated to be 0.94 TPa. The calculated value shows a good agreement with the values found in the literature [4]. As shown in Fig. 1, the stress-strain curves have nonlinear dependence on the tensile strain. The armchair tube is predicted to exhibit larger stress and failure strain than the zigazag tube. According to the calculation, the

zigzag tube is predicted to be the maximum stress of 70 GPa at 11% strain and the armchair tube to be the maximum stress of 86 GPa at 14% strain. Yu et al. [5] measured the strength of SWNT bundles ranged from 11 to 63 GPa and the failure strain of as high as 12%. The maximum stress obtained from the theoretical prediction is much higher than those measured from experiment. One reason is that an atom defective within CNT structures results in the failure at lower strain.

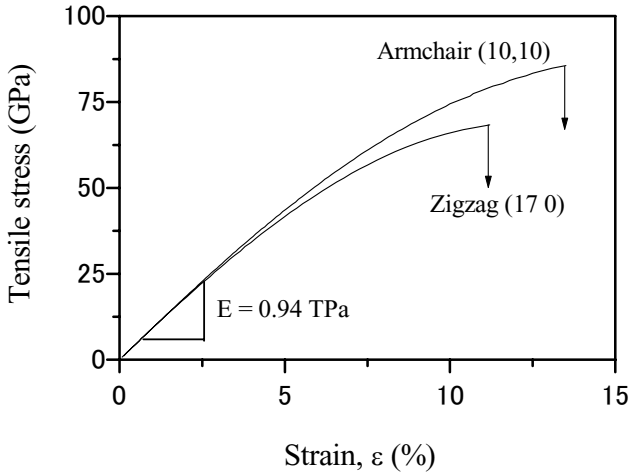

Figure 1. Stress-strain curves for the zigzag and armchair tubes under tensile load

Conclusions

Based on a link between molecular and solid mechanics, a nanoscale continuum theory is established to directly incorporate the Morse potential function into the continuum model of CNT structures. We introduce the procedure of simulating the stress-strain response of CNTs by the molecular structural mechanics approach. The armchair tube exhibits larger stress-strain response than the zigzag tube under the tensile loading.

References

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