The Young’s Modulus of Single-Walled Carbon Nanotubes

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Introduction
Carbon nanotubes (CNTs) were discovered in 1952, but their exciting properties have been brought to the attention of the scientific community only recently. CNTs, which can be thought of as rolled up sheets of graphene, can be classified into three categories based on the edge pattern: armchair, zigzag, and chiral.

Many unique properties are demonstrated by CNTs, including variable conductivity and extreme stiffness. These and other properties have led to a host of proposed applications, but problems with the production and characterization of CNTs are preventing many from coming to fruition.

Ambiguity of Young’s Modulus in Nanomaterials
Young’s modulus $Y$ characterizes the strain response $\varepsilon$ of a material to the applied stress $\sigma$ along an axis of symmetry. $Y = \sigma/\varepsilon$. Unfortunately, the definition of Young’s modulus in nanomaterials is ambiguous. This ambiguity lies in the definition of applied stress. In a continuous solid, $\sigma = \frac{F_{\text{applied}}}{A_{\text{cross section}}}$. For CNTs, the cross-sectional area over which the force is applied cannot be uniquely defined. The resulting uncertainty is a major hindrance to the advancement of many CNT applications.

Results and Analysis

To check the reliability of the simulation and to validate the new method, estimated values of Young’s modulus are also derived using the traditional definition. Both the estimated values and the calculated values (which were calculated using the new internal elastic strain energy density method) are relatively insensitive to CNT diameter over the diameter range 0.678-0.705 nm that was explored.

Discussion
The resulting Young’s moduli calculated with the new method, using data from the simulations, correlate closely with the estimated values. This confirms the accuracy of the results for SWCNTs. The results are also in agreement with the experimental data, which sets the estimated Young’s modulus of any given SWCNT around 1 TPa.

These results validate the script used to simulate the CNTs, which was developed to generate SWCNT structures of arbitrary size and to explore the mechanical strength of these structures using a unique definition of Young’s modulus. In the future, this extensible XMD script could be used as a base for many other simulations involving SWCNTs.

The results also validate the new method of calculating Young’s modulus of CNTs. This new method has the potential to uniquely define Young’s Modulus, which would remove one of the major obstacles that are preventing the use of CNTs in many practical applications.

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References