The Young's Modulus of Single-Walled Carbon Nanotubes

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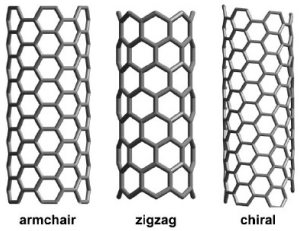
Introduction

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.

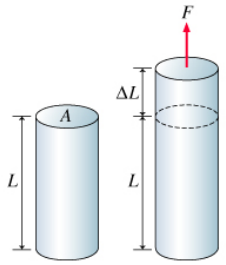
Many unique properties are demonstrated by CNTs, including variable conductibility and extreme stiffness. These and other properties have led to a host of proposed applications, but problems with the production and characterization of CNTs are preventing many from coming to fruition.



The 3 different types of CNTs

Ambiguity of Young's Modulus in Nanomaterials

Young's modulus Y characterizes the strain response ε of a material to the applied stress σ 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, $\sigma = F_{applied}/A_{cross\text{-}sectional}$. 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.



The traditional method of defining Young's modulus for continuous materials is $Y = (F/A)/(\Delta L/L)$

Project Goals

- Find a new method for calculating the Young's modulus of CNTs which avoids the ambiguities that have plagued the traditional method
- Simulate various single-walled CNTs (SWCNTs) experiencing strain with this method
- Calculate the Young's modulus of these SWCNTs with data from the simulations

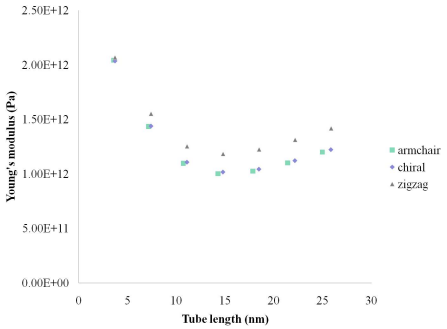
Method

- The internal elastic strain energy density of a CNT under linear-elastic strain can be written as $V = \frac{1}{2} Y \varepsilon^2$. Young's modulus Y can be obtained by taking its second derivative with respect to strain ε.[1]
- The classical molecular dynamics code, XMD,[2] is used to simulate a variety of CNT structures experiencing axial strain.
- Finite sized scaling analysis is performed on the data in order to efficiently produce reliable results.
- The Young's moduli calculated from the data with the new method are compared with an estimate calculated using the traditional method, as well as with existing experimental data.

Results and Analysis

	Armchair CNTs	Zigzag CNTs	Chiral CNTs
Calculated Y in TPa (new method)	0.954 ± 0.048	1.123 ± 0.062	0.968 ± 0.049
Estimated Y in TPa (traditional method)	0.959 ± 0.049	1.146 ± 0.046	0.987 ± 0.035

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.



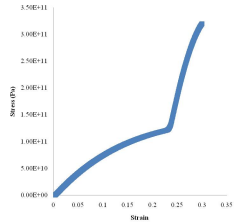
Young's moduli for three CNTs at variable lengths. The finite sized scaling analysis concludes that data from CNTs which are shorter than 14 nm are unreliable.

Discussion

The resulting Young's moduli calculated with the new method, using data from the simulations, correlates 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.



The estimated stress-strain curve of a zigzag SWCNT. Strains greater than .04 are considered outside the linear regime.

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References

[1] V. N. Popov & V. E. Van Doren, Phys. Rev. B **61**, 4 (2000).

[2] J. Rifkin. *XMD - Molecular Dynamics for Metals and Ceramics*. <http://xmd.sourceforge.net/>