Atomistic Modeling of the Mechanical Properties of Nanostructured Materials

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Outline

- Introduction
- Objectives
- Computational details
- Results
- Conclusions

Introduction

- CNTs have interesting properties
  - Smaller nanotubes are more chemically reactive
  - Different electrical conductivity depending on the arrangement of carbon atoms around the nanotube axis (chirality)
  - Unique mechanical properties
    - Large Young's modulus in nanotube's axial direction
    - Flexible normal to axial direction

Introduction

- Example applications that make use of the mechanical properties of nanotubes
  - Nanotweezers
  - AFM tips
  - Sensors
  - ……

Need to understand the mechanical behavior of CNTs

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Objectives

- To investigate the tensile and tortional responses of CNTs in molecular dynamics (MD) simulations and explore the effects of
  - Filling with
    - Gas molecules
    - Fullerenes
    - Other nanotubes to form multi-walled nanotubes (MWNTs)
  - Chemical functionalization
  - Temperature

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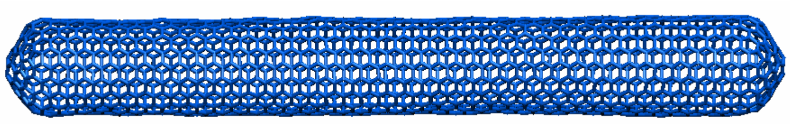
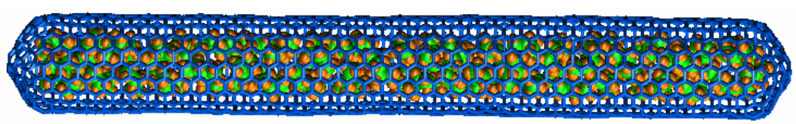
Computational details

- Classical molecular dynamics
- Interaction potential
  - Reactive empirical bond-order (REBO) hydrocarbon potential for covalent interactions
  - Lennard-Jones potential for van der Waals interactions
- Temperature control
  - Velocity-rescaling method
- Method to deform simulation systems
  - Load control method
  - External loads are applied on the simulation systems

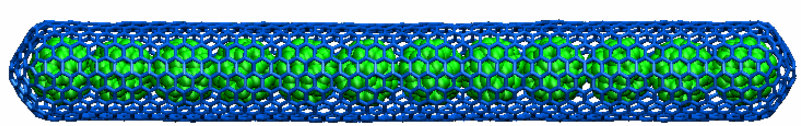
Computational details



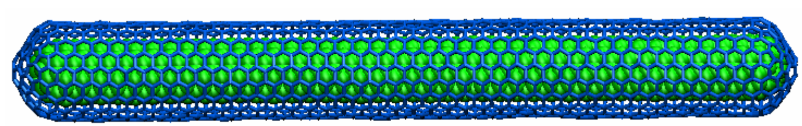
(10,10) SWCNT



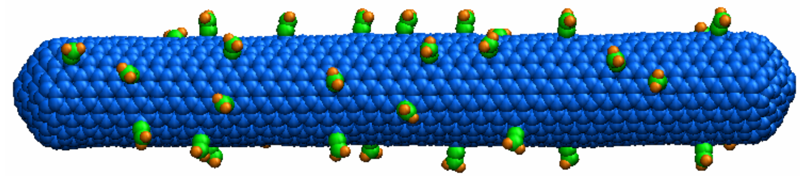
Butane-filled SWCNT



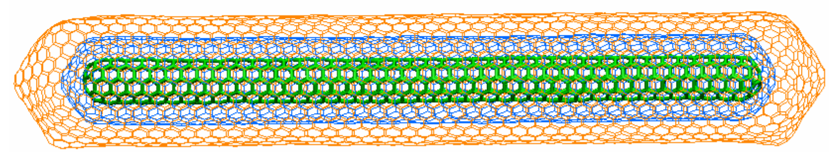
Nanopeapod



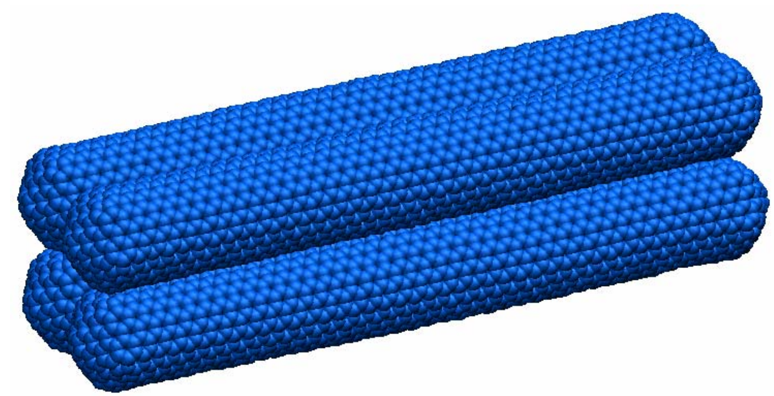
(10,10)@(5,5) DWCNT



Functionalized SWCNT



(15,15)@(10,10)@(5,5) TWCNT



Bundle of four (10,10) SWCNT

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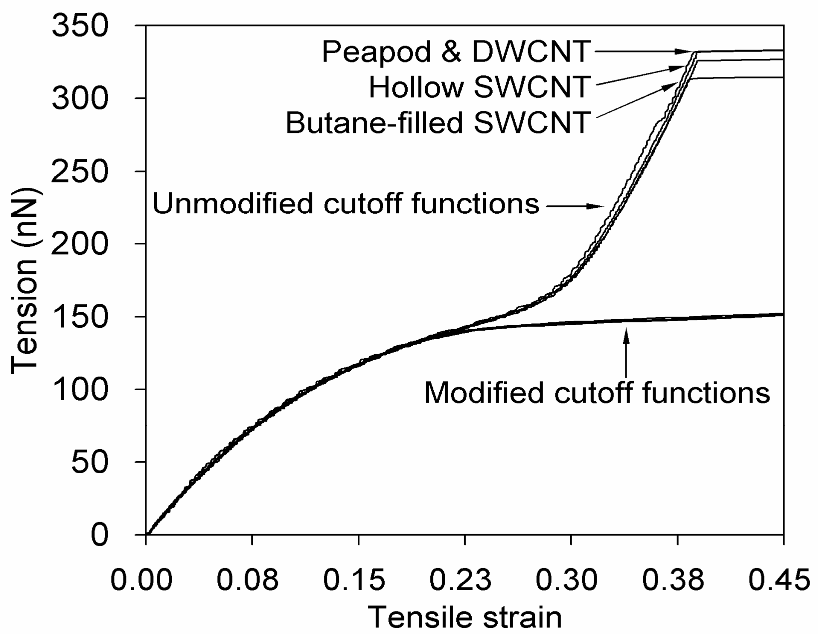
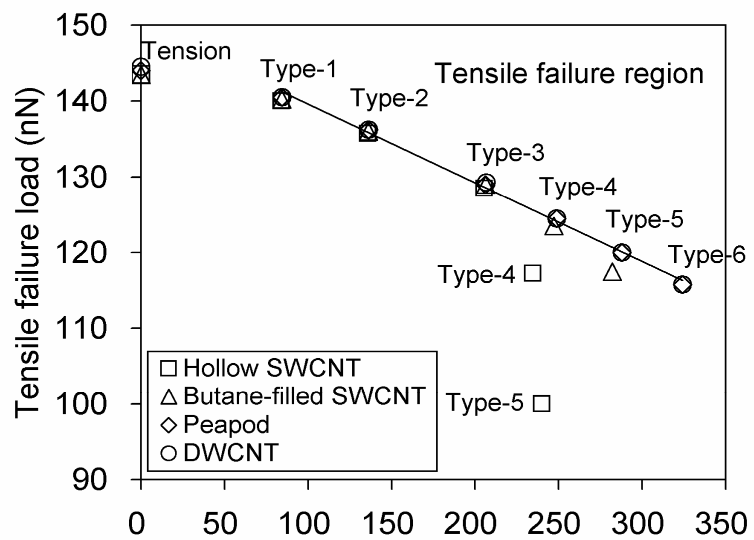
Tensile mechanical responses: Effect of filling

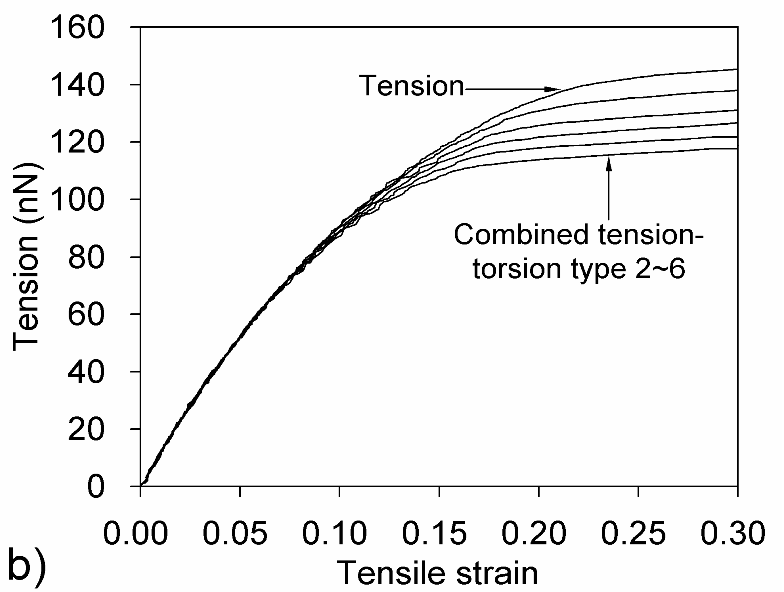


- The tensile failure loads and influence of filling materials are overestimated using the unmodified cutoff functions.
- The tensile failure loads are relatively unaffected by CNT filling.
- The tensile strength is predicted to be 100 GPa.

Tensile mechanical responses: Effect of combined tension-torsion



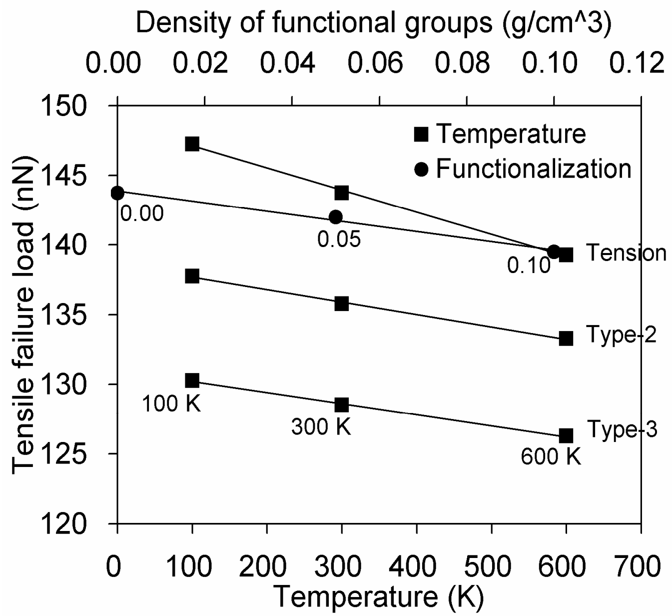
a)



b)

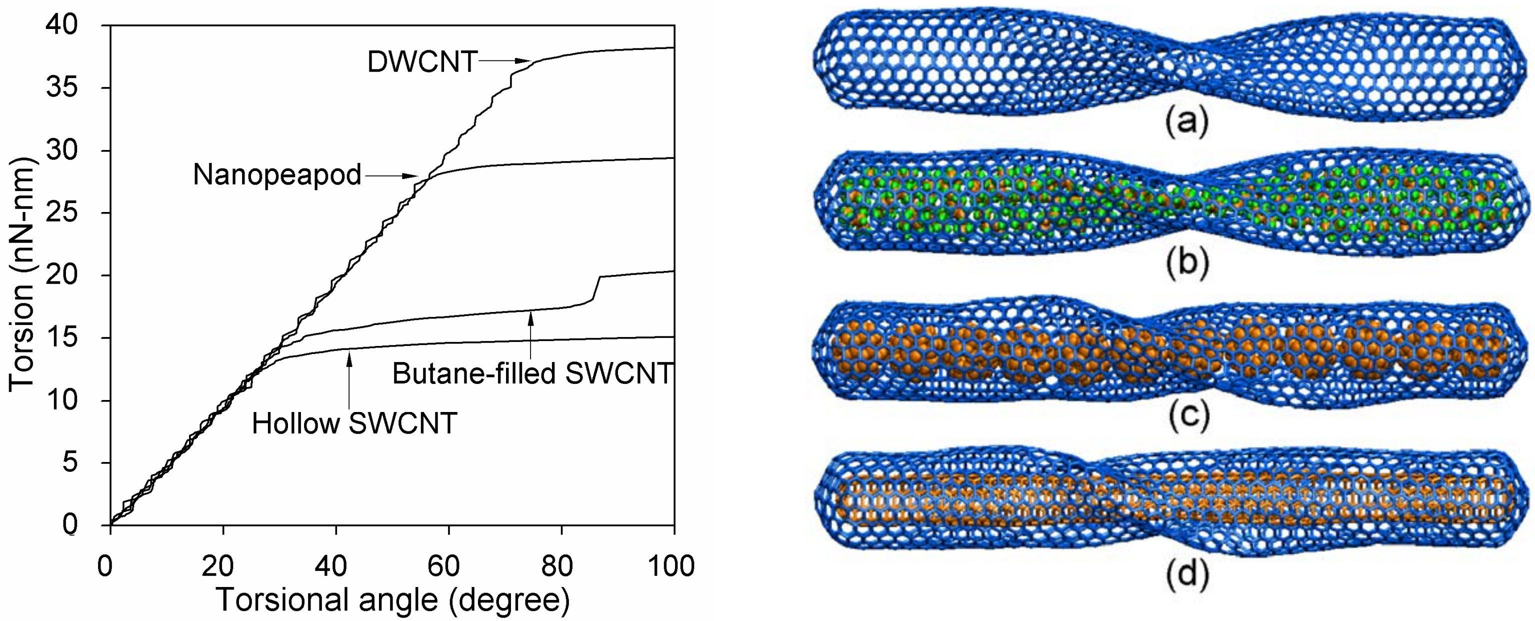
- The tensile strength is decreased by applied torsion
- The tensile strength can be increased by filling CNTs.
- The tensile elastic modulus is unaffected by applied torsion.

Tensile mechanical responses: Effects of temperature and chemical functionalization



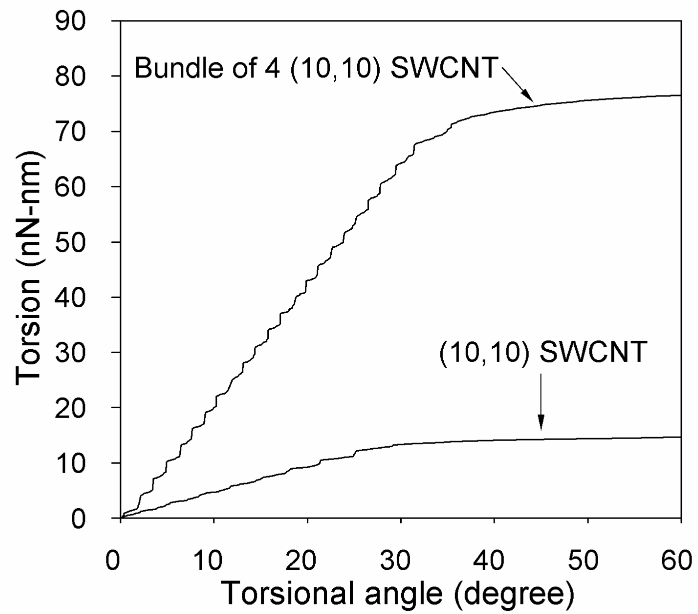
- Chemical functionalization and higher temperatures decrease the tensile failure load.
- Neither chemical functionalization nor temperature affects the CNT tensile elastic modulus.

Torsional mechanical responses: Effect of filling



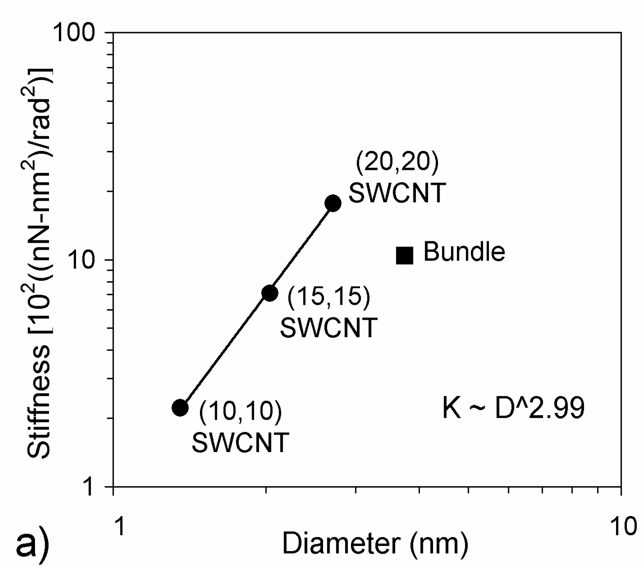
- The critical buckling moment can be increased by the presence of filling materials and the rate of increase is higher than under bending and compression loading.
- The torsional shear modulus is also unaffected by the existence of filling materials.

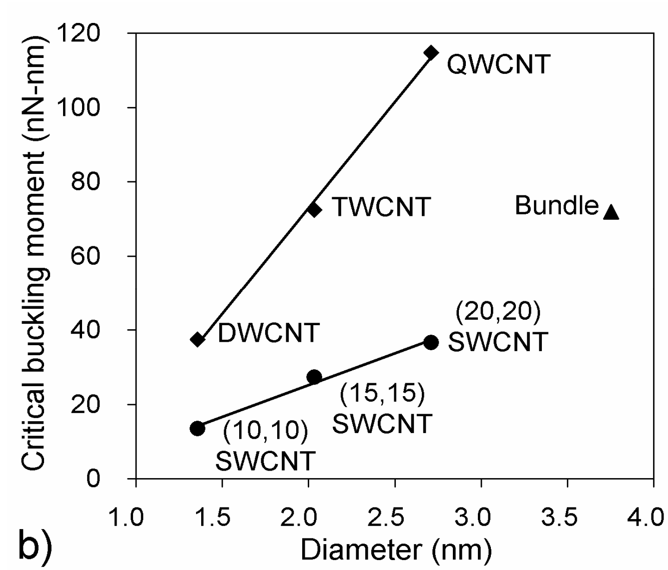
Torsional mechanical responses: Bundle of Nanotubes



- The critical buckling moment of a single carbon nanotube in the bundle is higher than that of the individual carbon nanotubes.
- The twisted form of the bundle is similar to the twisted form of macroscopic ropes.

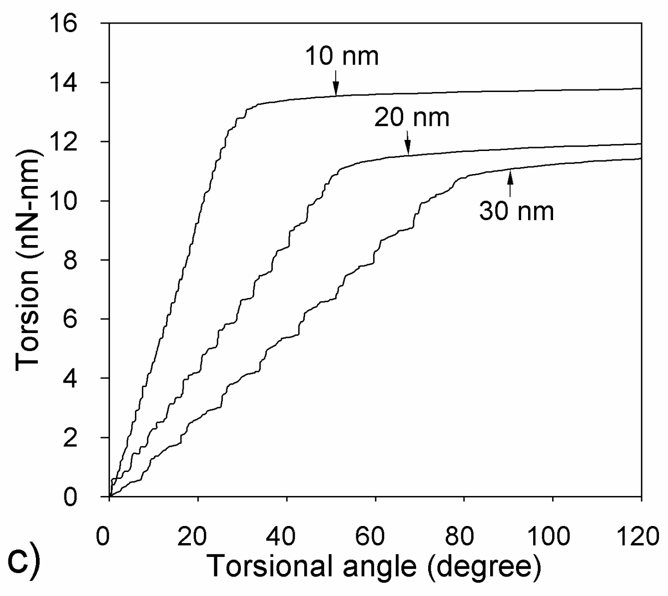
Torsional mechanical responses: Effect of nanotube diameter and number of MWNT shells

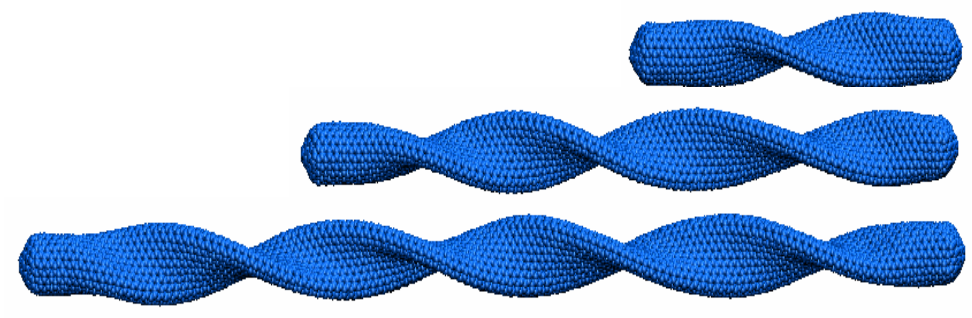




- The dependence of the torsional stiffness on the diameters is found to vary as $K \sim D^{2.99}$ in good agreement with predictions from continuum mechanics theory.
- The torsional shear modulus is predicted to be 350 GPa, and to be relatively independent of the diameter.

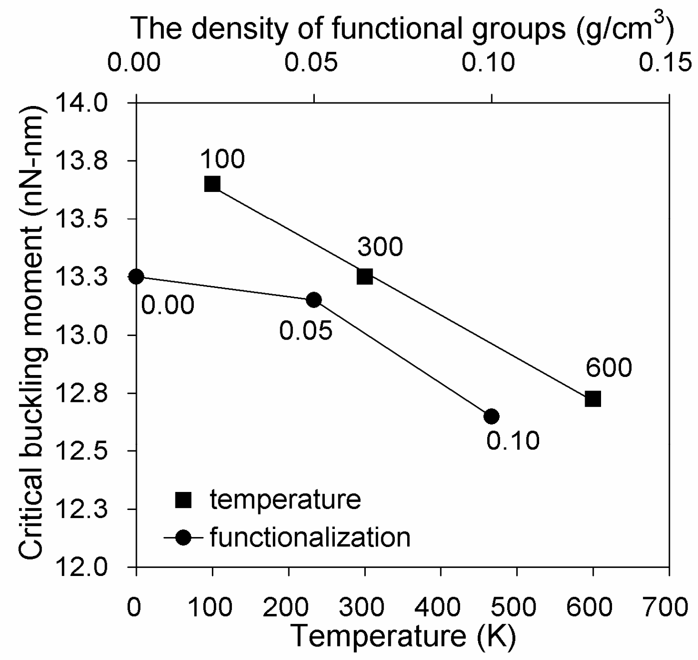
Torsional mechanical responses: Effect of length

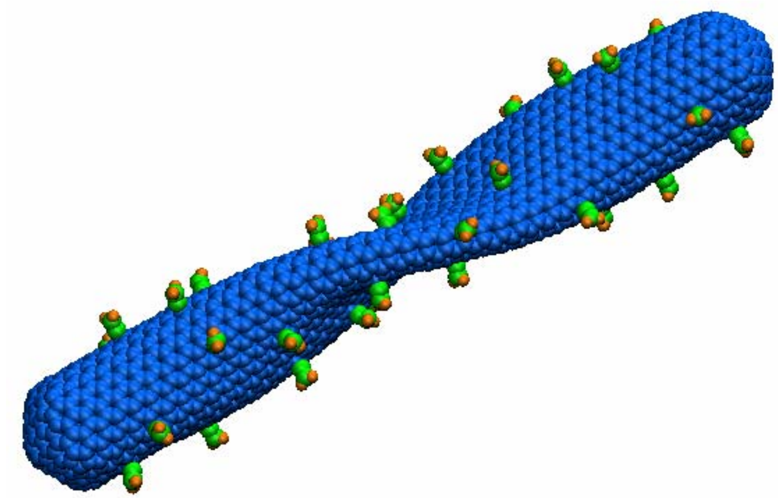




- The dependence of the torsional stiffness per unit length on the length is predicted to vary as $K`\sim L^{-0.99}$.
- The torsional shear modulus is predicted to be 350 GPa, and to be relatively independent of the length

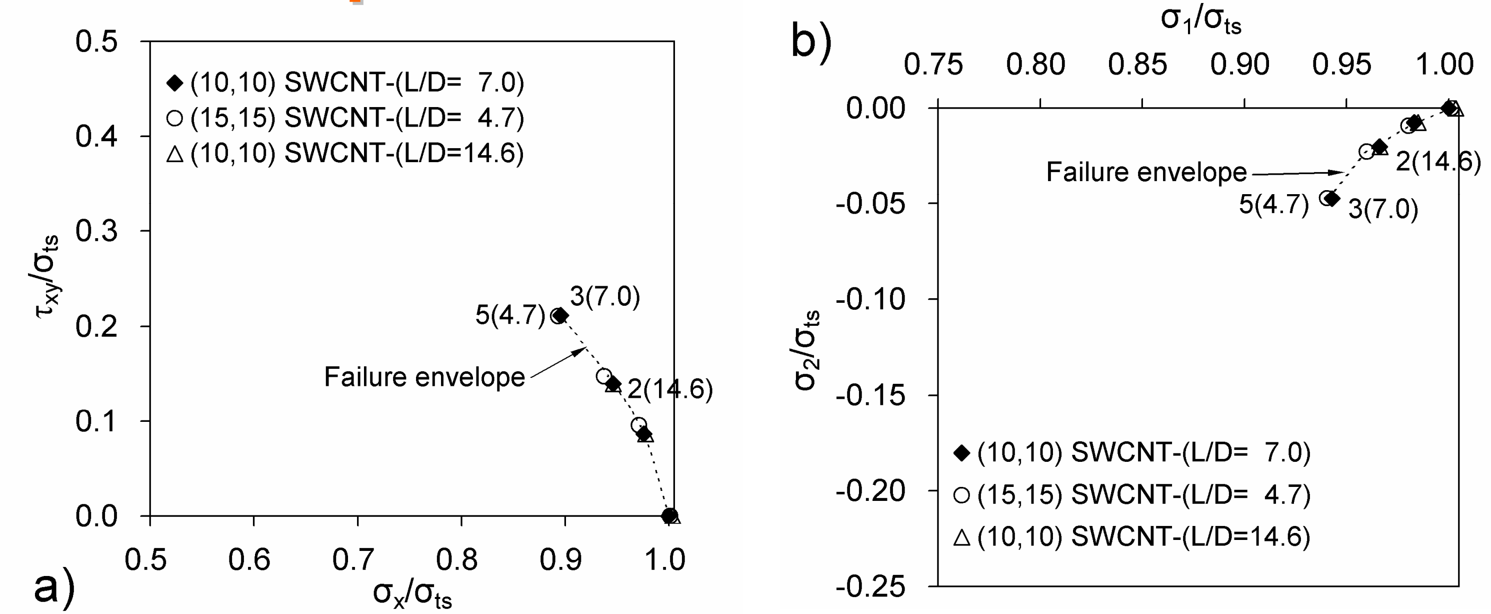
Torsional mechanical responses: Effects of temperature and chemical functionalization





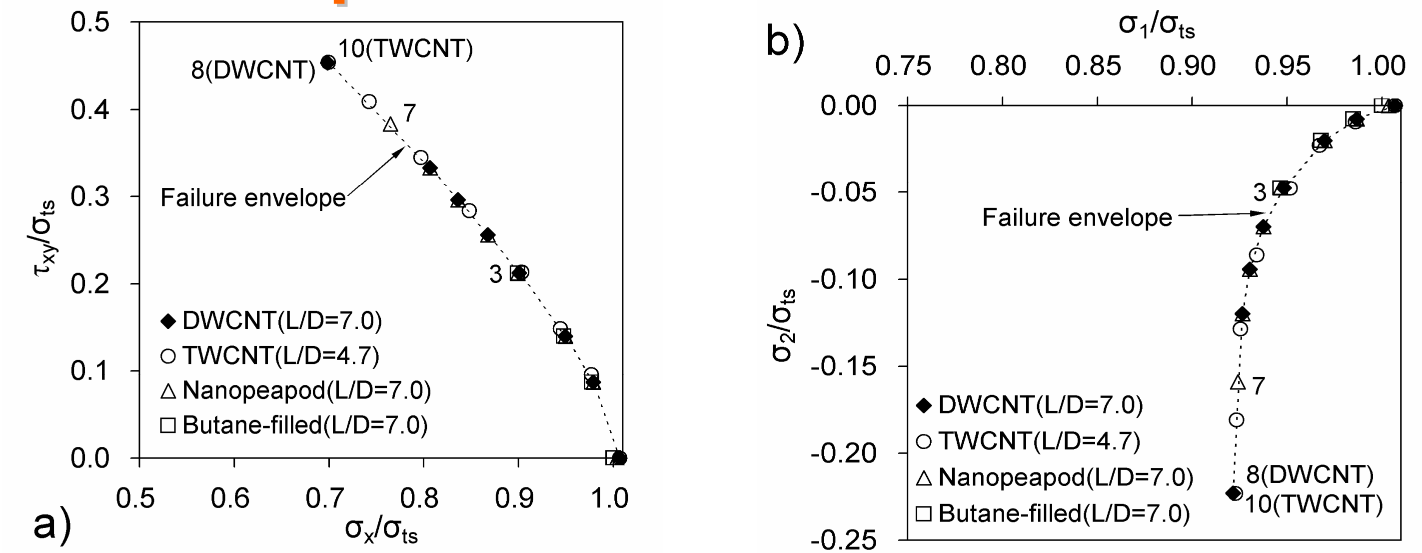
- The critical buckling moment can be modified by adjusting the system temperature and through chemical functionalization of the carbon nanotube walls.

Failure criteria under biaxial tension-torsion: Failure envelope of SWCNTs



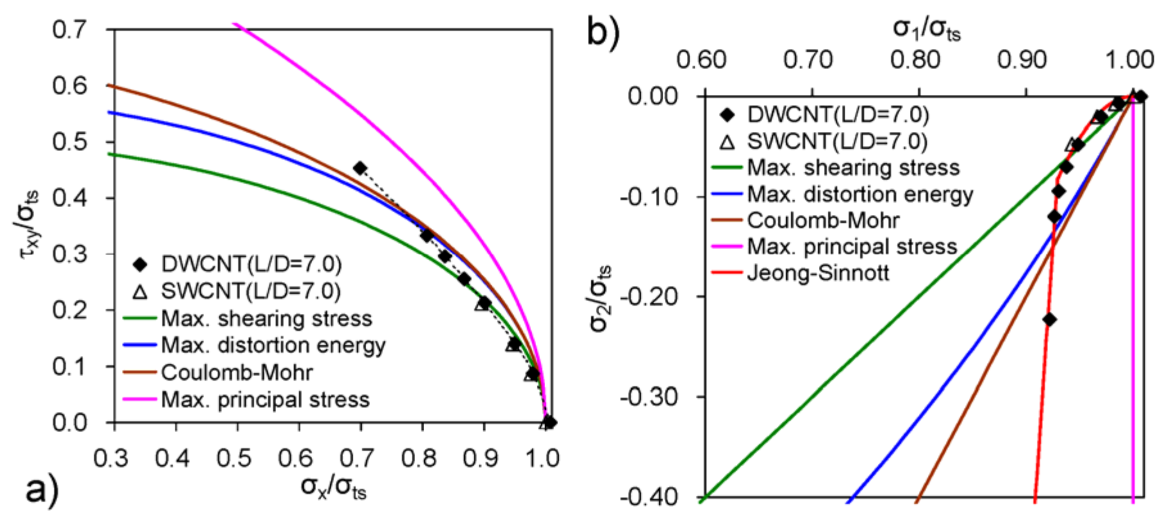
- The failure points show significant differences depending on the applied load ratio or the applied stress ratio.
- The failure envelope is unchanged by the different slenderness ratio (*L/D*) and thus a generalized failure envelope can be obtained.

Failure criteria under biaxial tension-torsion: Failure envelope of MWCNTs and filled CNTs



- The failure points show significant differences depending on the applied load ratio or the applied stress ratio.
- The failure envelope is unchanged by the different slenderness ratio (*L/D*), the types of MWCNTs, and the types of filled materials. Thus, generalized failure envelope can be obtained.

Failure criteria under biaxial tension-torsion



- Failure criteria for CNTs

$$-\left(\frac{\sigma_1}{\sigma_{ts}}\right)^2 + 2\left(\frac{\sigma_1}{\sigma_{ts}}\right) + \frac{1}{C_1}\left(\frac{\sigma_2}{\sigma_{ts}}\right) = 1 \quad \text{for} \quad \left(\frac{\sigma_1}{\sigma_{ts}}\right) \geq 0.93$$

where, C_1 = -16.5

$$C_2\left(\frac{\sigma_1}{\sigma_{ts}}\right) - \left(\frac{\sigma_2}{\sigma_{ts}}\right) = 14.3 \quad \text{for} \quad \left(\frac{\sigma_1}{\sigma_{ts}}\right) < 0.93$$

where, C_2 = 15.3

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Conclusions

- CNT filling has an effect on torsional buckling moments but not on the tensile failure loads.
- Tensile strength decreases under applied torsion.
- Chemical functionalization and higher temperatures decrease the tensile failure loads.
- The critical buckling moment of a single carbon nanotube in a bundle is higher than that of the individual carbon nanotube by itself.
- The tensile failure load and critical buckling moment can be modified by adjusting the system temperature and through chemical functionalization of the carbon nanotube walls.
- The failure envelope is unchanged by the different slenderness ratio (*L/D*), the types of MWCNTs, or the types of filling materials. Thus, generalized failure envelopes can be determined.