Nanotechnology with Carbon Nanotubes: Mechanics, Chemistry, and Electronics

Deepak R. Sarvestani
Computational Nanotechnology
NASA Ames Research Center, CA
Ph: (650) 604-3496, email: deepak@nano.nasa.gov

https://people.nasa.nasa.gov/~deepak/nanotube.html

CNT is a tubular form of carbon with diameter as small as 1 nm. Length: few nm to microns.

CNT is configurationally equivalent to a two-dimensional graphene sheet rolled into a tube.

CNT exhibits extraordinary mechanical properties: Young's modulus over 1 Tera Pascal, as stiff as diamond, and tensile strength ~ 200 GPa.

CNT can be metallic or semiconducting, depending on chirality.

Software-Simulations: Expanding Sphere

Size Scale

- ~100,000 atoms
- ~1000 atoms
- ~500 atoms

Response/Transport Properties

- Magnetic
- Chemical
- Spectral/ Optical
- Electrical
- Thermal

Time Scale

- MD (100 ns)
- Experiments

Source of Acquisition
NASA Ames Research Center
**Computational Nanotechnology Project Collaborators (Acknowledgments)**

- Nanomechanics of Nanotubes and Composites
  - Dr. Chengyu Wei (Postdoc), Prof. K. Cho (Stanford University)
- Reactivity and Chemistry of Carbon Nanotubes
  - Prof. Don Brenner (NC State) and Prof. Rod Ruoff
  - Seongjun Park and Prof. K. Cho (Stanford University)
- Molecular Electronics with Nanotube Hetero-Junctions
  - Dr. Madhu Menon (U. Ky) and Prof. Antonis Andriotis (U. Crete)

**Nanomechanics Examples: Nanotubes**

- High value of Young’s Modulus (1.2-1.3 TPa for SWNTs)
- Elastic limit up to 10-15% strain
- Dynamic response under axial compression, bending, torsion

**Computer Simulations: Characterization of New Materials**

- **Experimental validation: Nanotubes in Composites**
  - Experiment: buckling and collapse of nanotubes embedded in polymer composites.

- **New Prediction: Anisotropic Plastic Collapse**
  - Nanostructured skin effect!

**Simulation: 30% yielding strain from fast strain rate (1/ps)**
molecular dynamics simulations (B. Yakobson et al. 1997)
- Experiments: 6% maximum strain in SWCNT ropes; 12% maximum strain in MWCNTs?

**Nanostrucured skin effect!**

- Yielding strain: 9 ± 1 %, Experiments: 6-12% strain for SWNT ropes

**Yielding of Single-Wall Nanotubes**

- yield strain strongly dependent on the strain rate and temperature!
- Linear dependence = Activated Process
  
  **Transition State Theory based Formula**

- Experimental feasible conditions: length ~ 1µm; strain rate ~ 1%/hour; 
  
  \[ T \approx 300K \]

  \[ \Rightarrow \] Yield strain: 9 ± 1 %, Experiments: 6-12% strain for SWNT ropes

Double-wall nanotube with contact to outermost wall

- At the experimentally feasible strain-rate and temperature:
  - MWNT yields at higher strain than equivalent SWCNT


- Structural and thermal properties
- Load transfer and mechanical properties

SEM images of epoxy-CNT composite
ribbon-cast CNT fibers & basalt CNT fibers

(O. Vigil et al., Science, V294, 713, 2002)

Small system: L/D-2, Np=10

Results:
- Glass transition temperature Tg increased from 150K to 175K
- Thermal expansion coefficients (K-1)
  
<table>
<thead>
<tr>
<th></th>
<th>PE</th>
<th>PE-CNT</th>
</tr>
</thead>
<tbody>
<tr>
<td>T&lt;Tg</td>
<td>3.3x10^-4</td>
<td>4.5x10^-4</td>
</tr>
<tr>
<td>T&gt;Tg</td>
<td>8.6x10^-4</td>
<td>12.0x10^-4</td>
</tr>
</tbody>
</table>

  (Experimental value: 1.0x10^-10 K^-1; T < Tg)


Small system: L/D-2, Np=10

Diffusion coefficients of polymer with CNTs embedded

Diffusion coefficients increased, especially along CNT axis direction, indicating enhancement of thermal conductivity

* Experiments on diffusivity in AROCN & RTV/CNT show larger increase (Rick Barrera’s group at Rice University)


Young’s modulus:

- Young’s modulus of CNT composites 30% higher than polymer matrix
- Stretching treatments enhance Y by 50%

(L/D-2, Np=10)
A 4-level dendritic neural tree: 14 branched carbon nanotube junctions

Biological Dendritic Neural Tree
- One dimensional cable theory
- Hodgkin-Huxley model for action-potential based information flow
- Information processing is coded in (a) branching at the junctions, and (b) time-series sequencing of the signal spikes
- Input - output - control: is based on (a) structural details of the branches and junctions, and (b) via chemical environment
- Short and long term memory is part of the structure: evolutionary in nature

Bio-mineral Dendritic Neuron: Carbon Nanotube
- Electronic, acoustic, thermal, and chemical signal transmission and information processing
- Information processing can be based on (a) branching + switching at the junctions, and (b) time-series sequencing of signal spikes
- Input - output - control: can be based on (a) structural details, (b) chemical environment, and (c) physical contacts at the ends
- Short and long term memory can be part of structure by defect and chemical adsorbate placements: design for specific purpose/functionality

Model of 4-level dendritic neural tree that could be made of branched carbon nanotubes

D. Srivastava et al., Comp. in Science and Engineering, IEEE, APS (2001)
Acknowledgements

• Prof. K. Cho (Stanford University)
• Dr. Madhu Menon (University of Kentucky)
• Prof. Antonios Arampatzis (University of Crete, Greece)
• Prof. Don Brenner (North Carolina State University)
• Prof. Mohamed Osman (Washington State University)

• Dr. Chenyu Wei (Stanford University/NASA Ames)
• Dr. Fedor Dezgilenko (ex NASA Ames)
• Seong Jun Park (Stanford University)
• Eva Gonzales (University of Kentucky/ Spain)
• Christiane Anderson (University of Minnesota, MN)

• Vadim Smelyanskiy (IC/NASA Ames)
• Al Globus (CSC/NASA Ames)
• Chris Henze (AMTI/NASA Ames)
• Steve Barnard (MRJ/NASA Ames)
• Glen Deardorff (AMTI/ NASA Ames)