Nanotechnology with Carbon Nanotubes: Mechanics, Chemistry, and Electronics

Deepak Gokhale
Computational Nanotechnology
NASA Ames Research Center, CA
Ph: (650) 604-3486, email: deepak@nasa.gov
http://people.nasa.gov/~deepak/panel.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

Mechanics dynamics for nano-architected systems
- Atomic MD, many-body force fields
- Semi-empirical tight-binding MD
- Classical finite elements

Source of Acquisition
NASA Ames Research Center
Manomechanics 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. Creto)

Experiment: buckling and collapse of nanotubes embedded in polymer composites.


Yielding of Single-Wall Nanotubes

- Yielding strongly dependent on the strain rate and temperature
- Linear dependence of Yielding on Transition State Theory based Formula

Experimental feasible conditions: length ~ 1μm; strain rate ~ 1%/hour; T ~ 300K

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


Computational Nanotechnology Project: Collaborators (Acknowledgements)

Nanomechanics Examples: Nanotubes

- High value of Young's Modulus (1.2 -1.3 T Pa for SWNTs)
- Elastic limit up to 10-15% strain

Computer Simulations: Characterization of New Materials!
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 composites
Ribbons contain CNT fibers & blended CNT fibers

(L. J. Schuller et al., Appl. Phys. Lett. 73, 2382, 1998)

Solid system: L/D-2, Np=10
Results:
- Glass transition temperature $T_g$ increased from 150K to 175K
- Thermal expansion coefficients ($K/T$)
  - PE: $T>T_g$, $3.3 \times 10^{-4}$; $T<T_g$, $6.7 \times 10^{-4}$
  - PE-CNT: $T>T_g$, $4.5 \times 10^{-4}$; $T<T_g$, $1.4 \times 10^{-3}$


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 ABGNT & RTV/CNT show larger increase (Rick Bereera’s group at Rice University)


Young’s modulus

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

(L/D-2, Np=10)

TEM images of alignment of CNTs in a polymer matrix by stretching

Model of a 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)

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) chemical environment
- Short and long term memory is part of the structure: evolutionary in nature
<table>
<thead>
<tr>
<th>Acknowledgements</th>
</tr>
</thead>
<tbody>
<tr>
<td>* Prof. K. Cho (Stanford University)</td>
</tr>
<tr>
<td>* Dr. Madhu Manoh (University of Kentucky)</td>
</tr>
<tr>
<td>* Prof. Antonios Andriotis (University of Crete, Greece)</td>
</tr>
<tr>
<td>* Prof. Don Brenner (North Carolina State University)</td>
</tr>
<tr>
<td>* Prof. Mohamed Osman (Washington State University)</td>
</tr>
<tr>
<td>* Dr. Chenyu Wei (Stanford University/NASA Ames)</td>
</tr>
<tr>
<td>* Dr. Petr Dezhigilenko (ex NASA Ames)</td>
</tr>
<tr>
<td>* Soong Jun Park (Stanford University)</td>
</tr>
<tr>
<td>* Eva Gonzales (University of Kentucky/Spain)</td>
</tr>
<tr>
<td>* Christine Anderson (University of Minnesota, MN)</td>
</tr>
<tr>
<td>* Vadim Smelyanskiy (IC/NASA Ames)</td>
</tr>
<tr>
<td>* Al Globus (CSC/NASA Ames)</td>
</tr>
<tr>
<td>* Chris Hennes (AMT/NASA Ames)</td>
</tr>
<tr>
<td>* Steve Barnard (MRJ/NASA Ames)</td>
</tr>
<tr>
<td>* Glen Deardorff (AMTI/NASA Ames)</td>
</tr>
</tbody>
</table>