Deepak Srivastava
Computational Nanotechnology at CSC/NAS
NASA Ames Research Center
Moffett Field, CA 95014

Carbon Nanotube

- 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.

Spatio-Temporal Resolution

- Bulk continuous media
- 1000,000,000 atoms or grid
- 1000 atoms
- 1000 atoms
- 100 atoms

Molecular Dynamics, KMC, TDMC Experiments Long time structural
- up to 100s of sec
- Hyperdynamics - up to sec, hours

Nanomechanics of Nanotubes and Nanotube-Polymer Composites
- Chemical Functionalization, Thermal Conductivity, Gas Storage
- Molecular Electronics with Nanotube Hetero-junctions
- Quantum Computing with Doped Bucky Onions and Fullerenes
- Genetic Algorithm based Searches for New Molecular Force Field
- High value of Young's Modulus (1.2-1.3 T Pa for SWNTs)
- Elastice limit up to 10-15% strain
- Redistribution of strain
- Sharp buckling leading to bond rupture
- SWNT is stiffer than MWNT

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

Buckle, bend and loops of thick tubes...

Local collapse or fracture of thin tubes.


Simulation: 30% yielding strain from fast strain rate (1ps) molecular dynamics simulations

- Experiments: 6% maximum strain in SWCNT ropes; 12% maximum strain in MWCNTs

\[
\begin{align*}
\text{11.5% tensile strained (10.0) } & \text{ T=1600K} \\
\text{9% tensile strained (5.5) } & \text{ T=2400K}
\end{align*}
\]

Transition State Theory Derived Formula

- Yielding: strongly dependent on the strain rate and temperature!
- Linear dependence on the temperature of the of the yielding strain vs strain rate – activated process

- Experimental feasible conditions: length ~ 1mm; strain rate ~ 1hour; T ~ 300K

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


- Structural and thermal properties
- Load transfer and mechanical properties

SEM images of epoxy-CNT composite

- SEM images of polymer (polyvinylalcohol) ribbon contained CNT fibers & knotted CNT fibers

(2 Nogue et al. Science 309, 1531, 2005)
• Thermal conductivity of single-wall nanotubes
• Nanotube/polymer composites as high thermal expansion coefficient materials
• Thermal conductivity of nanotube/polymer composite
A 4-level dendritic neural tree 14 branched carbon nanotube junctions

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

Nanotechnology for Solid-State Quantum Computers Using Fullerenes

- **Kane's Model**: Solid-state quantum bits. Nuclear spins of \(^{31}P\) dopant atoms in bulk Si, controlled by external electronic gates using hyperfine interactions, serve as solid-state qubits. [1]
- **Problem**: Uniform arrays of individual \(^{31}P\) dopant atoms in bulk Si are experimentally difficult to fabricate.

Solution: Use Encapsulated Atoms as Qubits!

Electronic Control Gates

Example: $^1$H encapsulated in C$_{20}$D$_{20}$
- Electronic charge density shows a weak meta-stable state of $^1$H at the center of C$_{20}$D$_{20}$
- Suitable Solid-state Qubits Identified:
  - $^1$H encapsulated in C$_{20}$D$_{20}$ fullerene
  - $^{31}$P encapsulated in a diamond nanocrystallite

Proposition: Arrays of "encapsulated" atoms (with nuclear spins - qubits) will be easy to fabricate as compared to the arrays of the similar bare atoms.

Example 1: $^1$H Encapsulated in C$_{36}$
- Center is a meta-stable site.
- $^1$H strongly prefers to make a bend with a carbon atom, then it is not suitable as a qubit.

<table>
<thead>
<tr>
<th>Formation Energy (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon A: -1.28</td>
</tr>
<tr>
<td>Carbon B: -1.54</td>
</tr>
<tr>
<td>Carbon C: -1.40</td>
</tr>
<tr>
<td>Center: -0.46</td>
</tr>
</tbody>
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Reactivity Control to Encapsulate $^1$H: C$_{20}$D$_{20}$
- $^1$H prefers to make a bond with C atom within fullerene.
- $^{31}$P hybrid on C atom will reduce the chemical reactivity of the interior surface.
- Hexagon has lower escape barrier than a pentagon.
- As a conclusion, we examined C$_{20}$D$_{20}$.

Charge Density of $^1$H Encapsulated in C$_{20}$D$_{20}$
- The valance electron charge density of $^1$H leaks out of C$_{20}$D$_{20}$ cage molecule. This is good and needed for neighboring qubit interactions.

Model 2: $^{31}$P doped in Diamond or Silicon
- Weakly bound donor electron has strong $S$-like electronic charge density at the center, and a reasonable spread of the decay for off center positions.

Charge Density of $^{31}$P in Diamond

$^{31}$P in Diamond

$^{31}$P in Si

• Nanomechanics of Individual Nanotubes and Comparison with Experiments: (Nanotube + Polymer Composite)

• Kinky Chemistry and Functionalization of Nanotubes: (Generalized to a universal theory of reaction)

• Temperature Dependence of Thermal Conductivity (Generalized to Multi-wall nanotubes and nanotube junctions)

• Rectification and Switches with Nanotube Y-Junctions (Generalized a variety of logic gates and devices)

• Solid State Quantum Bits: (Initiate Experimental Efforts)

D. Srivastava, M. Menon and K. Cho, invited review article, Computing in Engineering and Sciences, submitted (2001)