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**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**

- High value of Young's Modulus (1.2-1.3 T Pa for SWNTs)
- Elastic limit up to 10-15% strain
- Redistribution of stress
- Sharp buckling leading to bond rupture
- SWNT is stiffer than MWNT

**Nanomechanics of Nanotubes and Nanotube+Polymer Composites**

- Dr. Chengyu Wei (Princeton), Prof. K. Cho (Stanford University)
- Chemical Functionalisation, Thermal Conductivity, Gas Storage
  - Prof. Don Brenner (NC State), Prof. M. Osman (Washington State)
- Molecular Electronics with Nanotube Hetero-junctions
  - Dr. Madhu Menon (U. Ky) and Dr. Ameen Andriotis (U. Crete)
- Quantum Computing with Doped Bucky Onions and Fullerenes
  - Seongjun Park (Student), Prof. K. Cho (Stanford)
- Genetic Algorithm based Searches for New Molecular Force Field
  - Al Globus (NASA Ames)

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

- Local collapse or fracture of thin tubes.

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

**Local collapse or fracture of thin tubes.**

- Structural and thermal properties
- Load transfer and mechanical properties

**SEM images of epoxy-CNT composite**

**SEM images of polymer (polyvinyl alcohol) ribbon containing CNT fibers & knotted CNT fibers**

- Transition State Theory Derived Formula

- Experimental feasible conditions: length ~ 10nm, strain rate ~ 1000s^-1, T ~ 300K

**Transition State Theory Derived Formula**

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

• Thermal conductivity of single-wall nanotubes
• Nanotube/polymer composites as high thermal expansion coefficient materials
• Thermal conductivity of nanotube/polymer composite

* C. Wei, D. Sirevaag, and K. Cho (submitted 2001)

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**Diffusion coefficient of polymer with CNTs embedded**

* Experimental data on diffusivity in ABS/CNT & RTV/CNT show larger increase (Rick Perrera's group at Rice University)

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**Elastic modulus of CNT composites**

- Young's modulus of CNT composites 30% higher than polymer matrix
- Stretched treatments enhance Y by 50%
  (L/D-2, Np=10)

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

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 Model**: Solid-state quantum bits. Nuclear spin of $^{79}$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 $^{79}$P dopant atoms in bulk Si are experimentally difficult to fabricate.


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

Carbon Nanotube: Dendritic Tree

- 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)

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

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Solution: Use Encapsulated Atoms as Qubits

Example: \(^1H\) encapsulated in \(C_{20}\)

Electronic Caged Gate

Electronic charge density shows a weak meta-stable state of \(^1H\) at the center of \(C_{20}\).

Suitable Solid-state Qubits Identified:
- \(^1H\) encapsulated in \(C_{20}\) fullerene
- \(^31P\) encapsulated in a diamond nanocrystallite

Example 1: \(^1H\) Encapsulated in \(C_{20}\)

- Center is a meta-stable site.
- \(^1H\) strongly prefers to make a bond with a carbon atom, then it is not suitable as a qubit.

Formation Energy (eV)

<table>
<thead>
<tr>
<th></th>
<th>Center</th>
<th>Carbon A</th>
<th>Carbon B</th>
<th>Carbon C</th>
<th>Center</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>-1.26</td>
<td>-1.54</td>
<td>-1.40</td>
<td>-0.46</td>
</tr>
</tbody>
</table>

Reactivity Control to Encapsulate \(^1H\): \(C_{20}D_{20}\)

- \(^1H\) prefers to make a bond with C atom within fullerene.
  - Reduce the chemical reactivity of the interior surface.
- \(^1p\) hybrid on C atom will reduce the electron density at the interior surface.
  - Hydrogenation on exterior.
- Hexagon has lower escape barrier than a pentagon.
  - Non-hexagon smaller fullerene structure is preferred.
  - As a conclusion, we examined \(C_{20}D_{20}\).

Charge Density of \(^1H\) Encapsulated in \(C_{20}D_{20}\)

- The valance electron charge density of \(^1H\) leaks out of \(C_{20}D_{20}\) cage molecule. This is good and needed for neighboring qubit interactions.

Model 2: \(^31P\) 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.

\(^31P\) in Diamond, \(^31P\) in Si


J. Han, A Globus and R. Jaffe

Nanomanipulation in Virtual World

- 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)