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**Nano-Materials Roadmap**
Impact on Space Transportation, Space Science and HEDS

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

**Spatio-Temporal Resolution**
- bulk continuous media
- 1,000,000,000 atoms or grid
- 1,000,000 atoms
- 100,000 atoms
- 500 atoms

Molecular Dynamics
KMC, TDMC
Experiments
Long time structural

- up to 100s of ns
- Hyperdynamics
- up to sec. hours
- High value of Young's Modulus (1.2 - 1.3 TPa for SWNTs)
- Elastic limit up to 10-15% strain

Computer Simulations: Characterization of New Materials

Nanostructured skin effect!

Computer Simulations Generating new IP!

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

Transition State Theory Derived Formula

- Experimental feasible conditions: length = 1 mm; strain rate = 1/min; 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/epoxy/CNT/ribbon contained CNT fibers & knotted CNT fibers

Thermal Characterization of Nanotubes and Polymer-Nanotube Composites

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

High Thermal Expansion Coefficient Composite

- Glass transition temperature \( T_g \) increased from 150K to 170K
- Thermal expansion coefficients \( (K^{-1}) \)
  - PE: \( 3.3 \times 10^{-4} \) \( \quad \) 18%
  - PE-CNT: \( 10 \times 10^{-4} \) \( \quad \) 40%

Diffusion coefficients of polymer with CNTs embedded

- Diffusion coefficient increased, especially along CNT axis direction, indicating enhancement of thermal conductivity
- Experiments on diffusivity in ABS/CNT & RTV/CNT show larger increase (Rick Berrera's group at Rice University)

Loading sequence

- Young's modulus of CNT composites 30% higher than polymer matrix
- Stretching treatments enhance Y by 50%
There is not much out there, except emulation of Si based paradigms for some sort of hybrid technology.

Nanotube-Crossbar based memory and computing

C. Lieber (Harvard)
S. Williams (HP), J. Heath (UCLA)

Revolutionary Computing: Architecture

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- Nanotube-Crossbar based memory and computing

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Our Proposed Model: Neural Signal Processing/Seizing in Biological Systems

Cerebral Sensory System (inner-ear) of a cricket

Bio-mimetic Dendritic Neurons: Carbon Nanotube

A 4-level dendritic neural tree: 14 branched carbon nanotube junctions

Bio-mimetic Dendritic Neurons: Carbon Nanotube

- Electronic, acoustic, thermal, and chemical signal transduction and information processing

- Information processing can be based on
  - (a) branching - switching at the branch junctions
  - (b) time series sequencing of signal spikes
  - (c) structural details of the branching and junctions
  - (d) chemical environment
  - (e) physical contacts at the ends

- Short and long term memory can be part of structure by default and chemical adhesion placements design for specific purpose/functionality

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Solution: Use Encapsulated Atoms as Qubits!

<table>
<thead>
<tr>
<th>Encapsulated Atom</th>
<th>Example: 'H encapsulated in C₆₀</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electronic Charge</td>
<td>Electronic charge density shows a</td>
</tr>
<tr>
<td>Gate</td>
<td>weak meta-stable state of 'H at</td>
</tr>
<tr>
<td></td>
<td>the center of C₆₀.</td>
</tr>
</tbody>
</table>

Proposal: Arrays of "encapsulated" atoms (with ⅓ nuclear spin - qubits) will be easy to fabricate as compared to the arrays of similar bare atoms.

<table>
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<tr>
<th>Suitable Solid-state Qubits Identified:</th>
</tr>
</thead>
<tbody>
<tr>
<td>- 'H encapsulated in a C₆₀ fullerene</td>
</tr>
<tr>
<td>- ³¹P encapsulated in a diamond</td>
</tr>
</tbody>
</table>

Charge Density of 'H Encapsulated in C₂₀D₂₀

- The valance electron charge density of 'H leaks out of C₂₀D₂₀ cage molecule. This is good and needed for neighboring qubit interactions.

Model 2: ³¹P doped in Diamond or Silicon

- Weakly bound donor electrons have 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