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
  - 10 atoms

- Molecular Dynamics
  - KMC, TDMC Experiments
  - Long time structural
  - up to 100s of ns

- Hyperdynamics
  - up to sec., hours

Molecular Electronics with Nanotube Hetero-junctions

- Dr. Madhu Menon (U. Ky) and Dr. Antonios 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
  - AI Global (NASA Ames)

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

- Redistribution of strain
- 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 Functionalization, Thermal Conductivity, Gas Storage

- Prof. Don Brenner (UC Santa), Prof. M. Osiran (Washington State)

Molecular Electronics with Nanotube Hetero-junctions

- Dr. Madhu Menon (U. Ky) and Dr. Antonios 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

- AI Global (NASA Ames)
- 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

- Transition State Theory Derived Formula

- Experimental feasible conditions: length ~ 1µm; 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 (polyvinyl alcohol) ribbon contained CNT fibers & knotted CNT fibers

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

Work hardening of composite with stretching
TEM images of alignment of CNTs in a polymer matrix by stretching

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

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 Herrera's group at Rice University)

C. Wei, D. Srivastava, and K. Cho (submitted 2001)
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<tr>
<th>V1</th>
<th>V2</th>
<th>V3</th>
<th>OR</th>
<th>XOR</th>
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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

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

Carbon Nanotube: Dendritic Tree
- Electronic, acoustic, thermal, and chemical signal transmission and information processing
- Information processing can be based on (a) branching, (b) switching, and (c) 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

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

Nanotechnology for Solid-State Quantum Computers Using Fullerenes

- Kane Model: Solid state quantum bits: Nuclear spin of \(^7^P\) dopant atoms in bulk Si, controlled by external electronic gates using hyperfine interactions, serve as solid-state qubits [1]
- Problem: Uniform arrays of individual \(^7^P\) dopant atoms in bulk Si are experimentally difficult to fabricate

Solution: Use Encapsulated Atoms as Qubits

Electronic Control Gates

Example: H encapsulated in C

Electronic charge density shows a weak meta-stable state of H at the center of C

Suitable Solid-state Qubits Identified:
- H encapsulated in a C_60 fullerene
- 31P encapsulated in a diamond nanocrystallite

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

Example 1: \(^1\text{H}\) Encapsulated in C_60

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

<table>
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<th>Formation Energy (eV)</th>
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<tr>
<td>Center: -0.46</td>
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<tr>
<td>Carbon A: -1.28</td>
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<tr>
<td>Carbon B: -1.54</td>
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<tr>
<td>Carbon C: -1.40</td>
</tr>
</tbody>
</table>

Mechanism:
- H on Carbon B

Charge Density of \(^1\text{H}\) Encapsulated in C_60

- The valence electron charge density of \(^1\text{H}\) leaks out of C_60 cage molecule. This is good and needed for neighboring qubit interactions.


Reactivity Control to Encapsulate \(^1\text{H}\): C_30D_20

\(^1\text{H}\) prefers to make a bond with C atom within fullerene.
- Reduce the chemical reactivity of the interior surface.
- sp\(^3\) 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_30D_20.

Model 2: \(^{31}\text{P}\) 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.

\(^{31}\text{P}\) in Diamond

\(^{31}\text{P}\) in Silicon


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)