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
- 1000,000 atoms
- 100 atoms
- 10 atoms

Molecular Dynamics, KMC, TDMC, Experiments, Long time structural

- up to 100s of ns
- Hyperdynamics - up to sec, hours

• Nanomechanics of Nanotubes and Nanotube-Polymer Composites
  - Dr. Chengyu Wei (Postdoc), Prof. K. Cho (Stanford University)
• Chemical Functionalization, 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. 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
Experiments: buckling and collapse of nanotubes embedded in polymer composites.

- Local collapse or fracture of thin tubes.

Transition State Theory Derived Formula

\[ \text{Yield strain: } 9 \pm 1\% \]

Experimental feasible conditions: length - 1µm; strain rate - 1/hour; T = 300K

- 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

\[ (1.5 \text{ Schaller et al., Appl. Phys. Lett. } 71, \text{1580, 1997}) \]  
\[ (B. Veprek et al., Science } 290, \text{7551, 2000}) \]
- Thermal conductivity of single-wall nanotubes
- Nanotube/polymer composites as high thermal expansion coefficient materials
- Thermal conductivity of nanotube/polymer composite

Small system: L/D-2, Np=10

* Experiments on diffusivity in ABS/CNT & RTV/CNT show larger increase (Rick Herrera’s group at Rice University)

- Work hardening of composite with stretching
- Young's modulus of CNT composites 30% higher than polymer matrix
- Stretching treatments enhance Y by 50%

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

Nanotechnology for Solid-State Quantum Computers Using Fulleranes

- Kane Model: Solid state quantum bits. Nuclear spin of 3P dopant atoms in bulk Si, controlled by external electric gates using hyperfine interactions, serve as solid-state qubits.

- Problem: Uniform arrays of individual 3P 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
- $^{31}$P encapsulated in a diamond nanocrystallite

Reactivity Control to Encapsulate H: C$_{20}$D$_{20}$

- 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$_{20}$D$_{20}$.

Charge Density of H Encapsulated in C$_{20}$D$_{20}$

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

Example 1: H Encapsulated in C$_{36}$

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

Charge Density of $^{1}$H Encapsulated in C$_{20}$D$_{20}$

- The valance electron charge density of 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.

$^{31}$P in Diamond
$^{31}$P in Si

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- 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.

$^{31}$P in Diamond
$^{31}$P 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)