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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

- Bulk continuous media
- 100,000,000 atoms or grid
  - 1000,000 atoms
  - 1000 atoms
  - 100 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
- Redistribution of stress
- Sharp buckling leading to bond rupture
- SWNT is stiffer than MWNT

Nanomechanics of Nanotubes and Nanotube+Polymer Composites
- Dr. ChenguWei (Princeton), 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. Antonis 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.

- Transition State Theory Derived Formula

- Yielding: strongly dependent on strain rate and temperature.

- 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

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 Brenner's group at Rice University)

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

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

(Received Applied Phys. Lett. 2011, 1869)

*B. Srivastava, J. Cho (submitted 2001)
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

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

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 after sequences 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

Nanotechnology for Solid-State Quantum Computers Using Fullerenes
- Kane Model: Solid-state quantum bits: Nuclear spin of the P dopant atom in bulk Si, controlled by external electronic gates using hyperfine interactions, serve as solid-state qubits [1]
- Problem: Uniform arrays of individual P dopant atoms in bulk Si are experimentally difficult to fabricate!

Solution: Use Encapsulated Atoms as Qubits!

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

Example: 1H encapsulated in C36

Suitable Solid-state Qubits Identified:
- 1H encapsulated in a C36 fullerene
- 31P encapsulated in a diamond nanocrystallite

Reactivity Control to Encapsulate 1H: C36D20

- 1H prefers to make a bond with C atom within fullerene.
  - Reduce the chemical reactivity of the interior surface.
- sp3 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 C36D20.

Charge Density of 1H Encapsulated in C36D20

- The valance electron charge density of 1H leaks out of C36D20 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.

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)