60! 7?6

Computational Nanotechnology of Molecular Materials, Electronics and Machines

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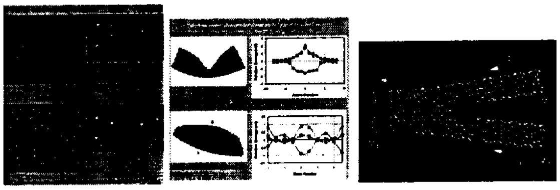
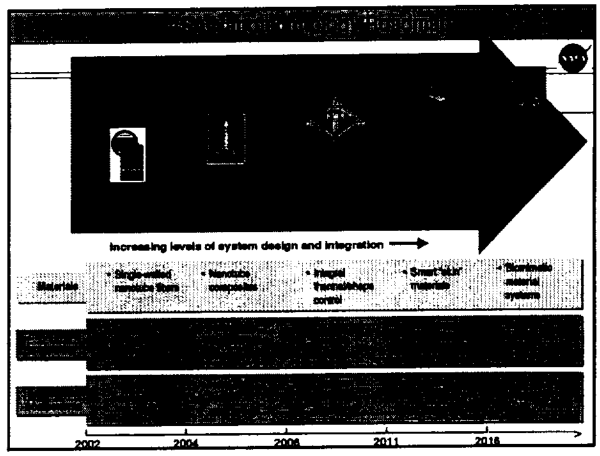
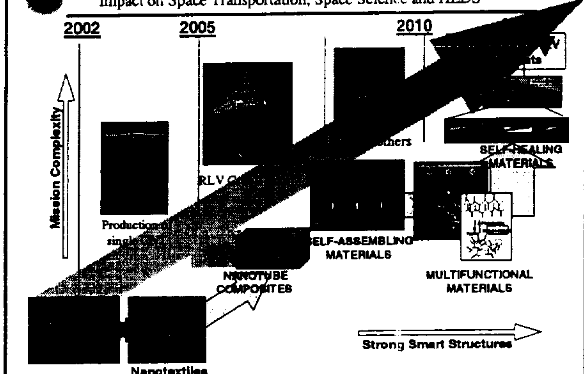




Nano-Materials Roadmap

Impact on Space Transportation, Space Science and HEDS

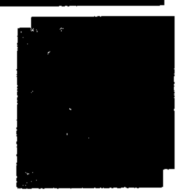


CNT = Carbon Nanotube

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.



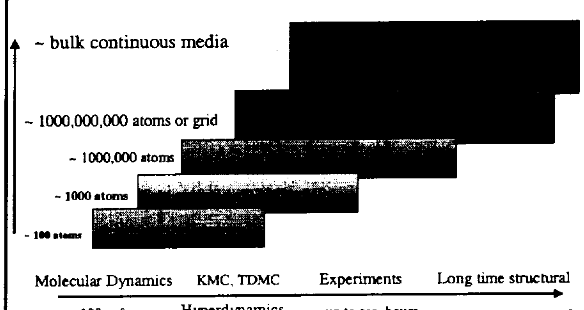
CNT exhibits extraordinary mechanical properties: Young's modulus over 1 Tera Pascal, as stiff as diamond, and tensile strength ~ 200 GPa.

CNT can be metallic or semiconducting, depending on chirality.

Computational Nanotechnology Projects – Collaborators (Acknowledgement)

- **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. 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**
  → Al Globus (NASA Ames)

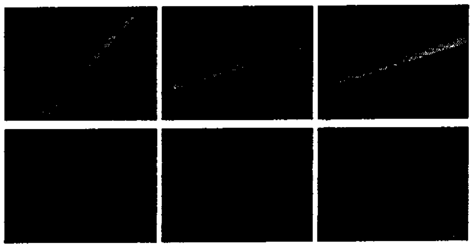
Spatio-Temporal Resolution



Nanomechanics Examples: Nanotubes

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

[redacted]



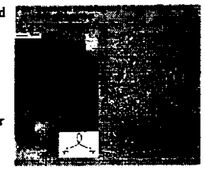
Computer Simulations: Characterization of New Materials!

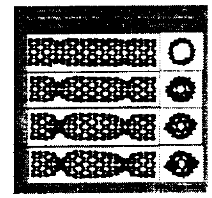
Experimental validation: Nanotubes in Composites

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

Buckle, bend and loops of thick tubes..

Local collapse or fracture of thin tubes.





New Prediction: Anisotropic Plastic Collapse

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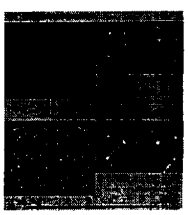
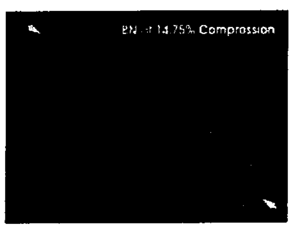




Nanostructured skin effect !

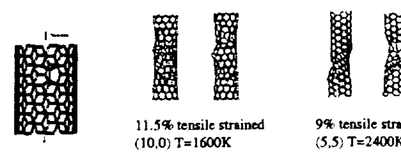
Computer Simulations Generating new IP !

Bridging the Spatio-Temporal Scales

Example: Yielding of Nanotube under Tension

Simulation: 30% yielding strain from fast strain rate (1/ps) molecular dynamics simulations (B. Yakobson et. al. 1997)

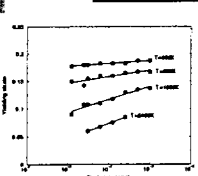
Experiments: 6% maximum strain in SWCNT ropes; 12% maximum strain in MWCNTs ?



11.5% tensile strained (10,0) T=1600K

9% tensile strained (5,5) T=2400K

Spatio-temporal dependence



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

Transition State Theory Derived Formula

·Experimental feasible conditions: length ~ 1μm; strain rate ~ /hour; T ~ 300K

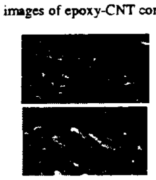
⟹ **Yield strain: 9 ± 1 %,** Experiments: 6-12% strain for SWNT ropes

C. Wei, K. Cho and D. Srivastava, submitted Phys. Rev. Lett.

Polymer CNT composite

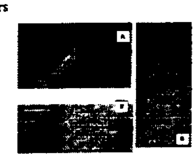
- Structural and thermal properties
- Load transfer and mechanical properties

SEM images of epoxy-CNT composite



(L.S.Schadler et.al., Appl. Phys. Lett. V73 P3842. 1998)

SEM images of polymer (polyvinylacohol) ribbon contained CNT fibers & knotted CNT fibers

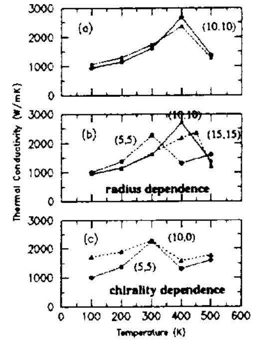


(B. Vigolo et.al., Science. V290 P1331. 2000)

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

Temperature Dependence of Thermal Conductivity [illegible] of Carbon Nanotube [illegible]

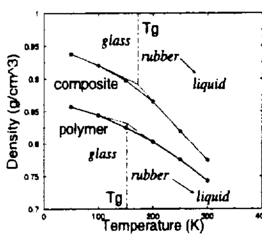


- **Thermal peak position has a strong dependence on the radius of the tube and weak dependence on chirality**
- **Typical peak thermal conductivity is about 2000-3000 W/mK**
- **High thermal conductivity material with highly directional heat-flow and weak dependence on chirality**

M. Osman and D. Srivastava, Nanotechnology, Vol. 12, 21 (2001)

High Thermal Expansion Coefficient Composite

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



Results:

-Glass transition temperature Tg increased from 150K to 1?5K

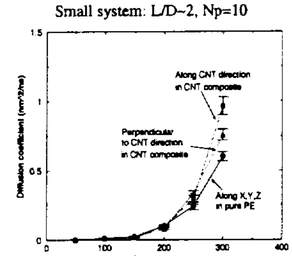
-Thermal expansion coefficients: (K^{-1})

	PE	PE-CNT	
$T<Tg$	3.8×10^{-4}	4.5×10^{-4}	↑18%
$T>Tg$	8.6×10^{-4}	12.0×10^{-4}	↑40%

(Experimental value: $1.0\times10^{-4}K^{-1}$; T <Tg)

Thermal Diffusion coefficients

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



Diffusion coefficients of polymer with CNTs embedded

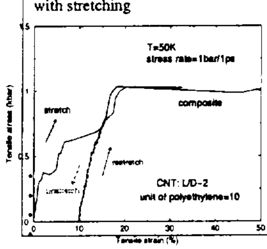
Diffusion coefficient increased, especially along CNT axis direction, indicating enhancement of thermal conductivity

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

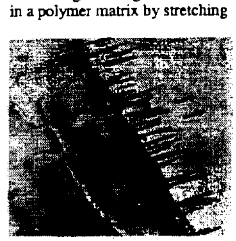
* C. Wei, D. Srivastava, and K. Cho (submitted 2001)

Stretching Sequence

Work hardening of composite with stretching



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



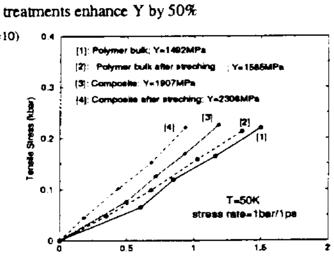
(L. Jin et al., Appl.Phys. Lett., V73 P1197, 1998)

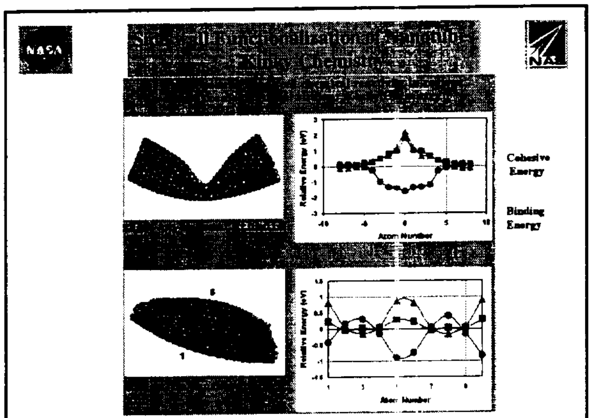
Young's Modulus

-Young's modulus of CNT composites 30% higher than polymer matrix

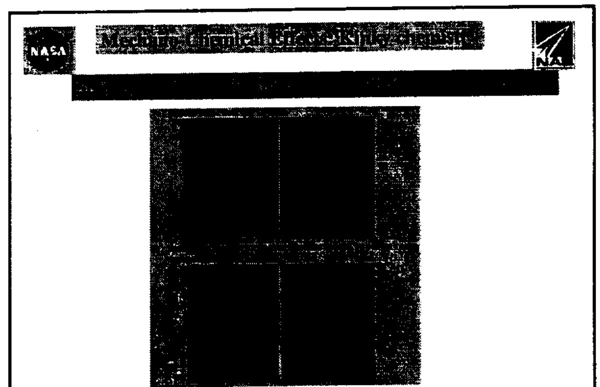
-Stretching treatments enhance Y by 50%

(L/D~2, Np=10)

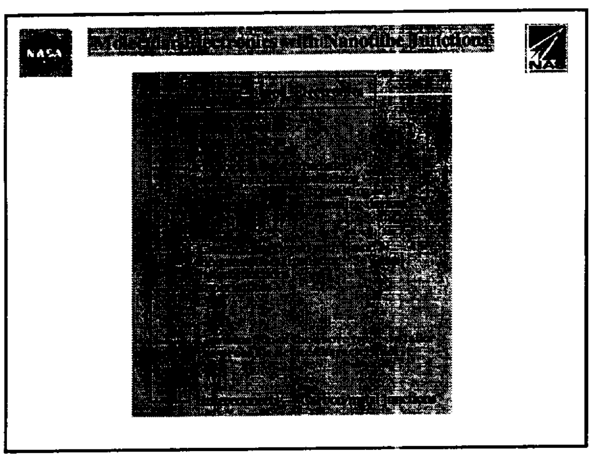


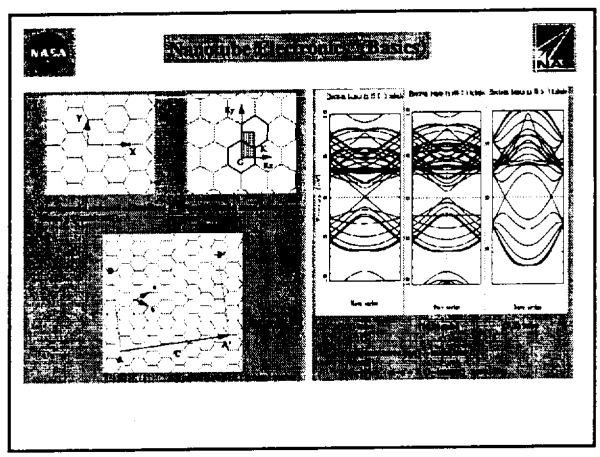


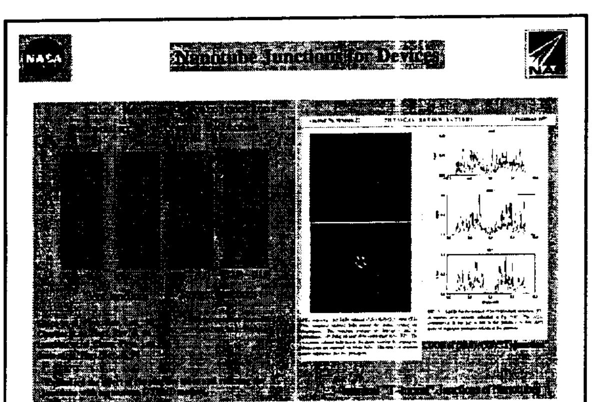
D. Srivastava, J. D. Schall, D. W. Brenner, K. D. Ausman, M. Feng And R. Ruoff, . Phys. Chem. Vol. 103, 4330 (1999).



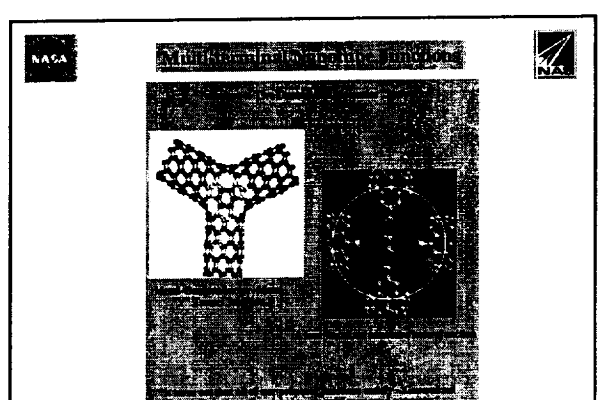
D. Srivastava, J. D. Schall, D. W. Brenner, K. D. Ausman, M. Feng And R. Ruoff, J. Phys. Chem. Vol. 103, 4330 (1999).



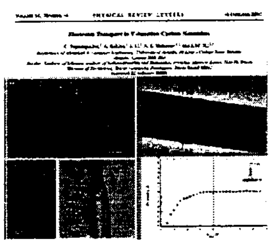


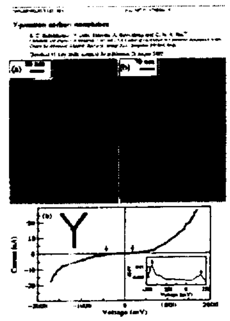


M. Menon and D. Srivastava, Phys. Rev. Lett. Vol. 74, 4453 (1997)

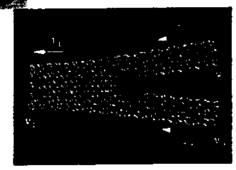


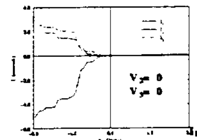
M. Menon and D. Srivastava, J. Mat. Res. Vol. 13, 2357 (1998)
D. Srivastava, S. Saini and M. Menon, *Molecular Electronics*, Ed. Aviram and Ratner, 178 (1998)



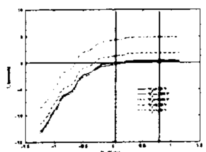


Rectification and Analog Logic Devices



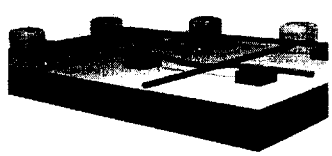


V2	V3	OR	XOR
0	0	0	0
0	1	1	1
1	0	1	1
1	1	1	0



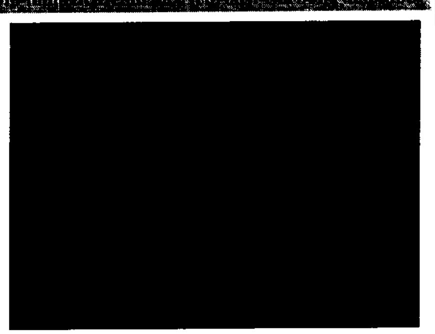
Andriotis, Menon, Srivastava, Chernozatonskii, Phys. Rev. Lett. (2001)

- 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)

Ceral Sensory System (inter-neuron) of a cricket



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

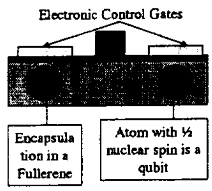
D. Srivastava et al., Comp. in Science and Engineering, IEEE, APS (2001)

Bio-mimetic Dendritic Neurons: Carbon Nanotubes

Biological Dendritic Neural Tree	Carbon Nanotube: Dendritic 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	• 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

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

Solution: Use Encapsulated Atoms as Qubits !



Proposal: Arrays of "encapsulated" atoms (with ½ nuclear spin – qubits) will be easy to fabricate as compared to the arrays of the similar bare atoms.

Example: ^{1}H encapsulated in C_{34}

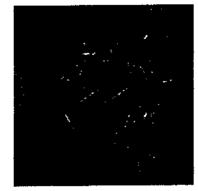
Electronic charge density shows a weak meta-stable state of ^{1}H at the center of C_{34}

Suitable Solid-state Qubits Identified:

- ^{1}H encapsulated in a $C_{20}D_{20}$ fullerene
- ^{31}P encapsulated in a diamond nanocrystallite

Charge Density of ^{1}H Encapsulated in $C_{20}D_{20}$

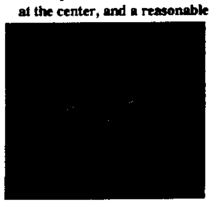
- **The valance electron charge density of ^{1}H leakes out of $C_{20}D_{20}$ cage molecule. This is good and needed for neighboring qubit interactions.**



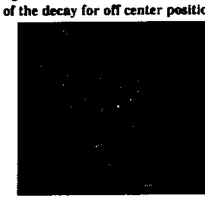
S. Park, D. Srivastava and K. Cho, J. NanoSc. NanoTech. (2001)

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

S. Park, D. Srivastava and K. Cho, J. NanoSc. and NanoTech. (2001)

NASA

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J. Han, A Globus and R. Jaffe

NASA

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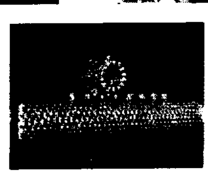

NASA

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Nanomanipulation in Virtual World

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