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Computational Nanotechnology of Materials, Devices and Machines: Carbon Nanotubes

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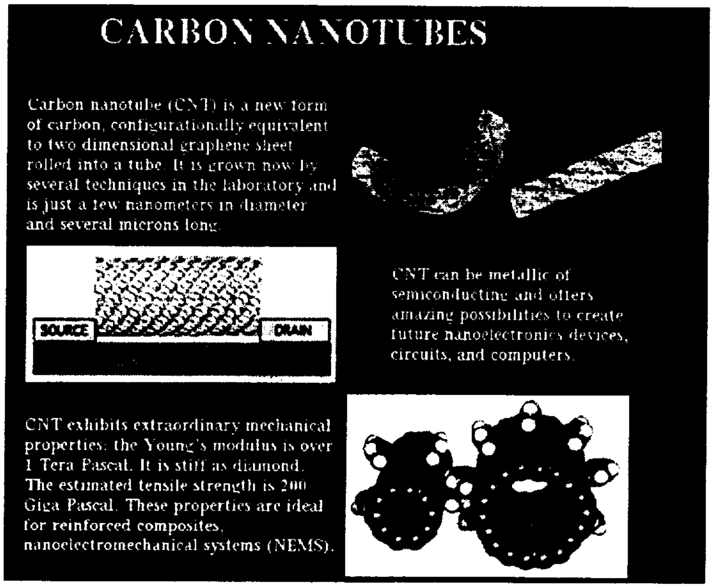
NASA Mission Needs

- Onboard computing systems for future autonomous intelligent vehicles
  - powerful, compact, low power consumption, radiation hard

- High performance computing (Tera- and Peta-flops)
  - processing satellite data
  - integrated space vehicle engineering
  - climate modeling
- Revolutionary computing technologies
- Smart, compact sensors, ultrasmall probes
- Advanced miniaturization of all systems
- Microspacecraft
- 'Thinking' spacecraft
- Micro-, nano-rovers for planetary exploration



CARBON NANOTUBES

Carbon nanotube (CNT) is a new form of carbon, configurationally equivalent to two dimensional graphene sheet rolled into a tube. It is grown now by several techniques in the laboratory and is just a few nanometers in diameter and several microns long.

CNT can be metallic of semiconducting and offers amazing possibilities to create future nanoelectronics devices, circuits, and computers.

CNT exhibits extraordinary mechanical properties: the Young's modulus is over 1 Tera Pascal. It is stiff as diamond. The estimated tensile strength is 200 Giga Pascal. These properties are ideal for reinforced composites, nanoelectromechanical systems (NEMS).

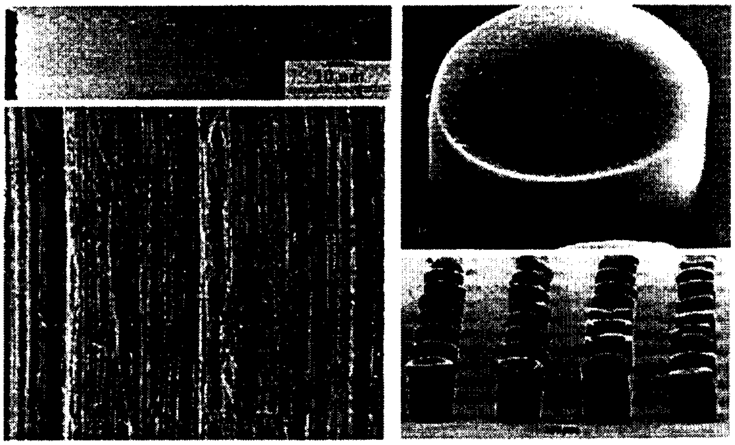
http://www.ipt.arc.nasa.gov at Ames Research Center

Simulation Techniques

- **Large-scale Classical Molecular Dynamics Simulations on a Shared Memory Architecture Computer**
  - **Tersoff-Brenner reactive many-body potential for hydrocarbons with long range LJ(6-12) Van der Walls interactions**
  - **Parallel implementation on a shared memory Origin2000**
- **Quantum Molecular Dynamics Simulations**
  - **Tight-binding MD in a non-orthogonal atomic basis.**
  - **Previous parametrization: silicon and carbon (M. Menon and K. R Subbaswami, Phys. Rev. B 1993-94).**
  - **Extended to heteroatomic systems including C, B, N, H**

Experimental Nanotechnology at Ames Research Center

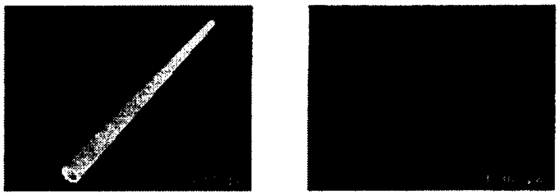
CVD Carbon Nanotube SEM Images



http://www.ipt.arc.nasa.gov at Ames Research Center

Nanomechanics of Nanomaterials: Characterization

- Nanotubes are extremely strong, highly elastic nanofibers.
  - ~ **High value of Young's modulus (1.2 -1.3 T Pa for SWNTs)**
  - ~ **Elastic limit up to 10-15% strain**
- Dynamic response under axial compression, bending and torsion.



- *Redistribution of strain*
- *Sharp buckling leading to bond rupture*
- *SWNT is stiffer than MWNT*

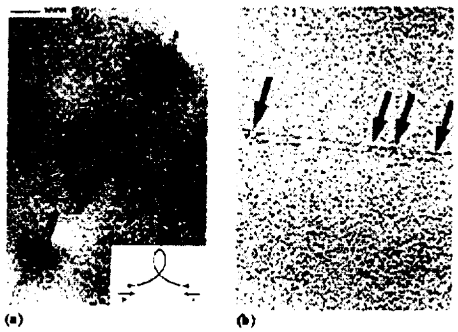
Application: Nanotubes in Composites

- Experiment: Buckling and collapse of nanotubes embedded in polymer composites.

- **Experiment : Buckling and Collapse of Embedded Carbon Nanotubes**

O. Lourie et. al. Phys. Rev. Lett. Vol. 81, 1638 (1998).

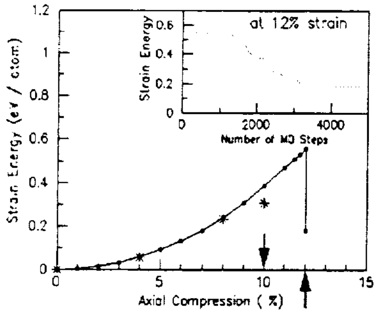
Buckle, bend and loops of thick tubes.



Local collapse or fracture of thin tubes.

Stiffness and Plasticity of Compressed C Nanotubes

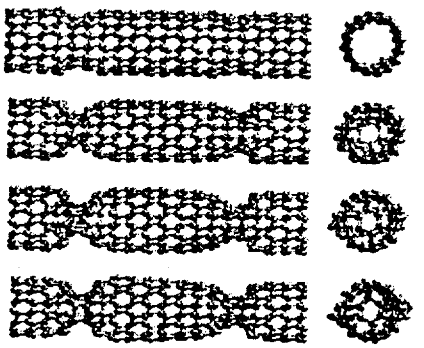
- **Energetics of collapse-plasticity of (8,0) CNT at 12% compression strain.**



Quantum GTBMD Method
classical atomistic (with Tersoff-Brenner potential)

- **Linear response regime (Y = 1.3 TPa) followed by pinching/buckling (classical MD) or collapse/plasticity (quantum MD).**

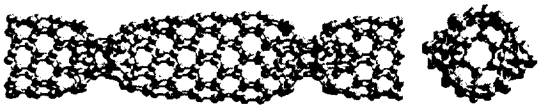
- **Spontaneous collapse-plasticity of (8.0) CNT through graphitic (sp2) to diamond like (sp3) type transition.**



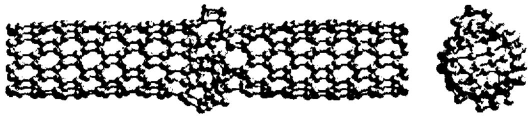
(a) side view (b) top view

Shows the same collapse as observed in experiment.

Plastic Collapse by Design



- With a single B point defect

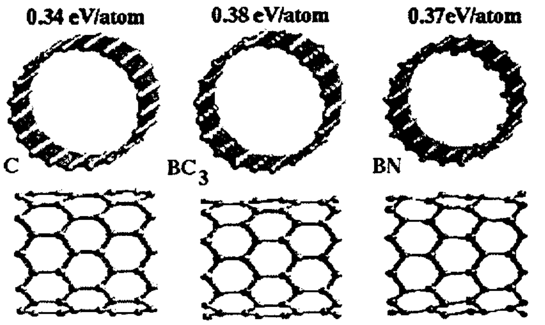


- Tube plastically collapses at the location of the defect.
- New types of hetero-junctions can be created.
- Quantum dot effect in one-dimensional system.
- Application: Molecular electronics.

Heteroatomic CxByNz Nanotubes

- **Band gap engineering over a larger range is possible**

• BN	~ 5 eV
• BC2N	~ 2 eV
• C	~ 0 - 1 eV
• BC3	~ 0.5 eV

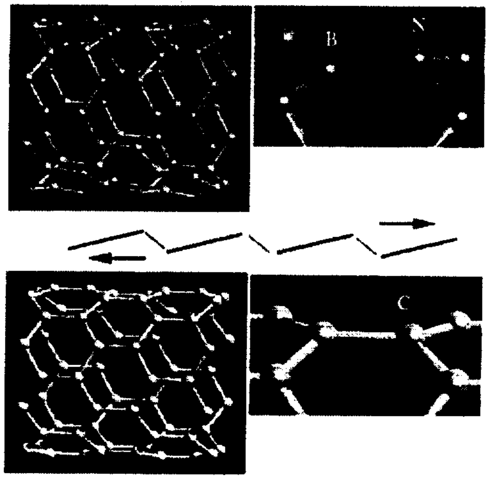


reconstruction due to
polar BN bond

BN Nanotubes - Structural Characteristics

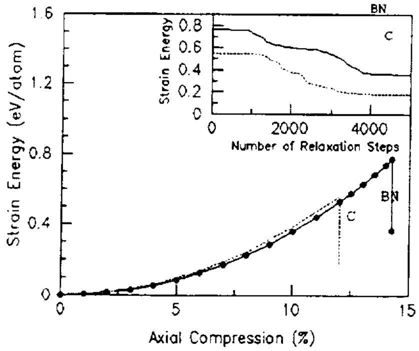
- BN bond buckling effect to minimize the energy

- BN bond buckling effect



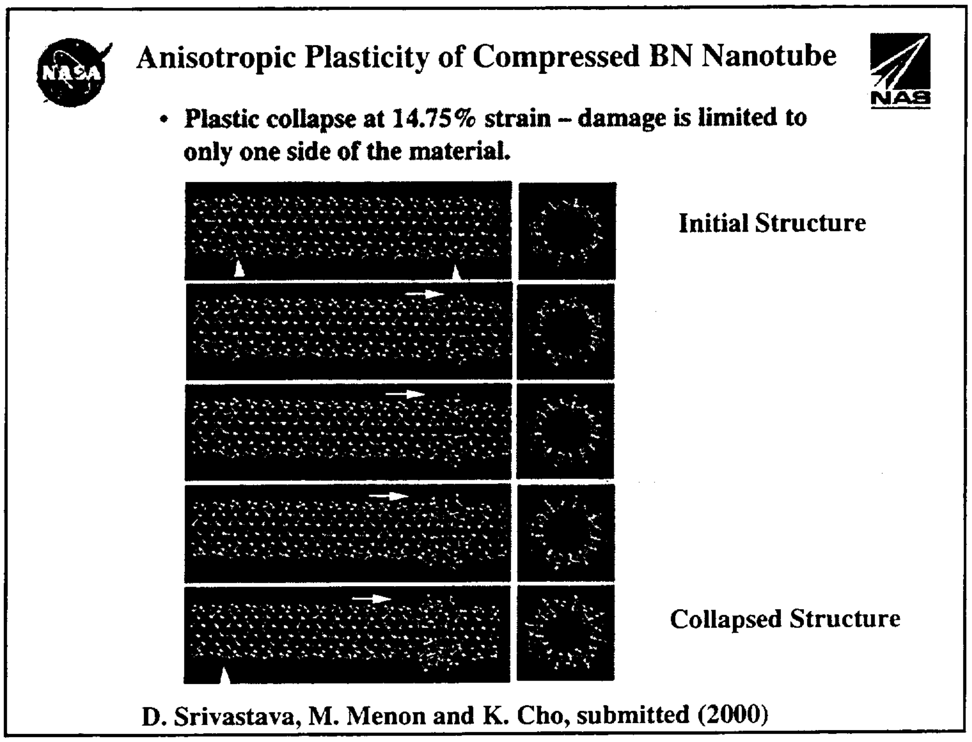
BN Nanotubes: Nanomechanics and Plasticity

- Comparison of Young's modulus and elastic limit with carbon nanotubes



- Y (BN) = 1.2 TPa ~ BN is 92% as strong as CNT !
  Y (C) = 1.3 TPa
- BN nanotube plastically collapses at even higher strain than C nanotube.

D. Srivastava, M. Menon and K. Cho, submitted (2000)



Anisotropic Plasticity of Compressed BN Nanotube

- **Plastic collapse at 14.75% strain – damage is limited to only one side of the material.**

Initial Structure

Collapsed Structure

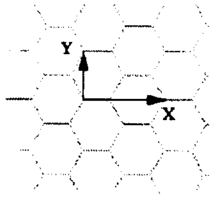
D. Srivastava, M. Menon and K. Cho, submitted (2000)

Nanotube Electronics: Scheme

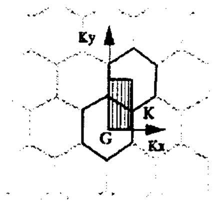
Carbon-based Electronics

- molecular wires
- topological defect mediated hetero-junctions ~ switching
  transisting
  tunneling devices
- C nanotubes doped with B and N
  BN nanotubes (insulator ~ 5eV gap)
  heterojunctions
  superlattices
- Combination of the above two ~ to tailor the probable device characteristics
- interconnects - Carbon/metal junctions

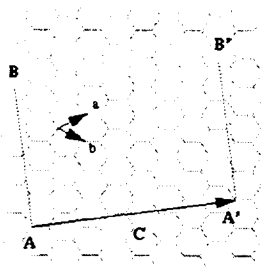
Nanotube Electronics (Characterization)



Hexagonal Lattice of a Graphene Sheet – (2xunit cell)



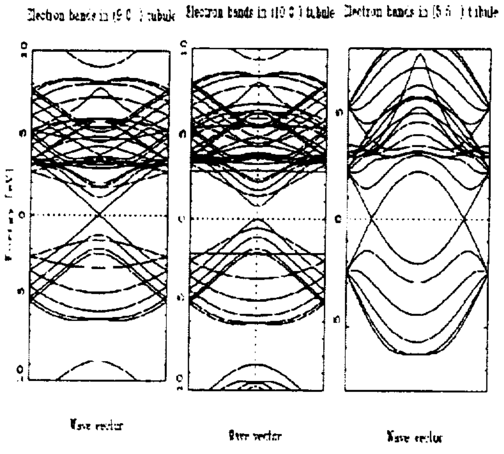
First Brillouin zone for an arm-chair tube.



Ch = n a + m b (chiral vector)

Boundry condition decide if nanotube is metalic or semiconducting

Band Structure of Different Nanotubes



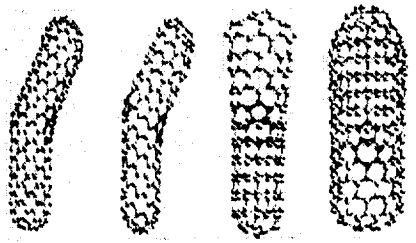
(9,0) tube **(10,0) tube** **(5,5) tube**

Arm chair tubes (n,n) ~ metal like

Otherwise m−n = 3l (l~ integer) metal like

Nanotube Heterojunctions: 2-point

2- point Nanotube Heterojunctions
Molecular Electronic Switches

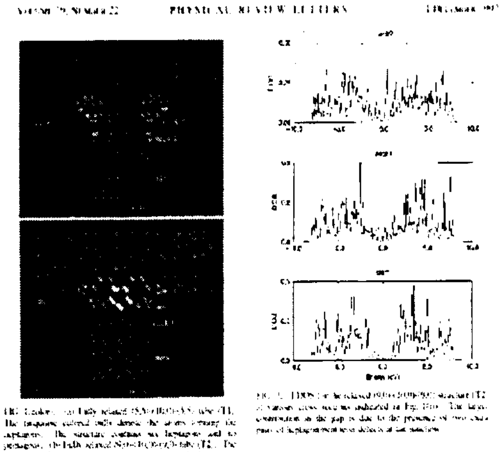


Chico et. al. Phys. Rev. Lett., 96
Charlier et. al. Phys. Rev. B, 96
Lambine et. al. Chem. Phys. Lett., 96
Saito et. al. Phys. Rev. B, 96

Semiconductor-Metal
Semimetal-Metal

We studied the effect of capping the tubes and relaxing the junctions with a quantum GTBMD method.

Nanotube Heterojunctions: 3-point

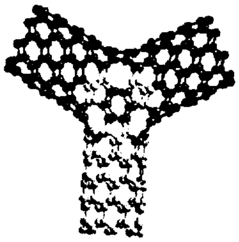


LDOS of (10,0)–(9,0) "T-junction"

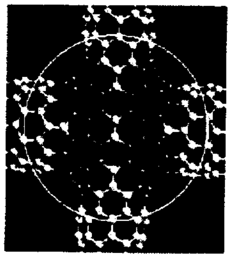
3-terminal "T-tunnel" Junctions of Nanotubes

Molecular Networks with Nanotubes

Pathways to Two Dimensional Molecular "Networks"



Metal–Semiconductor–Metal
"Y" Tunnel Junction



A four–terminal nanotube heterojunction

"It turns out that all of our proposed junctions satisfy – Generalized Euler's Rule about the global topology of connected networks"

Nanotube Electronics with Doping

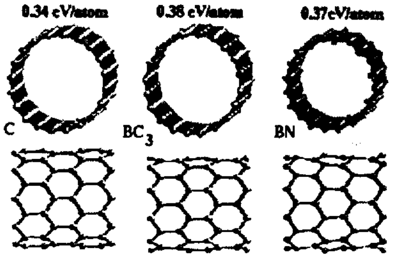
- Band gap engineering over a larger range should be possible:

BN	~5.5 eV
BC_2N	~2.0 eV
C	~0 – 1 eV
BC_3	~0.5 eV

~ a variety of junctions, quantum dots and superlattices should be possible

~ should be more robust

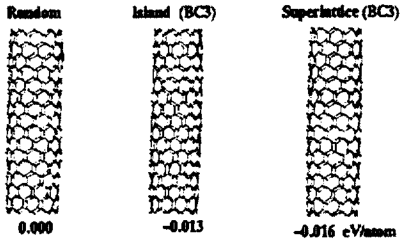
- Example: Composite (10,0) nanotube



reconstruction due to polar BN bond

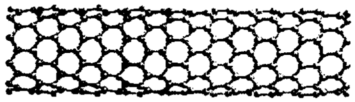
Nanotube Electronics with Doping

- B doping of Carbon Nanotube



phase separation of doped and undoped regions is thermodynamically stable !

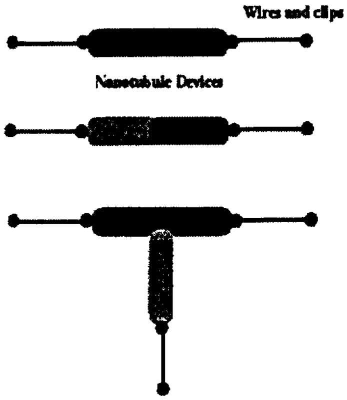
- BN/C Junctions



Interface Energy = 2*BN/C – BN – C
Interface Energy = 0.33eV/CB bond

Stable interfaces should be possible !

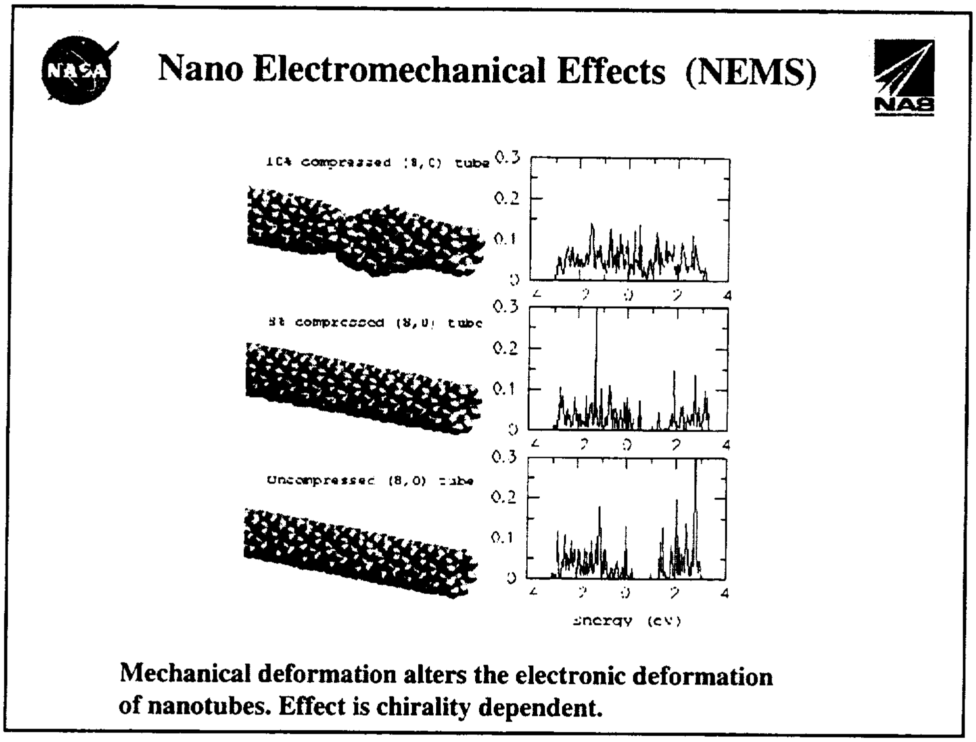
Nanotube/Molecules Hybrid Electronics



Negative
"World-image
is also
possible

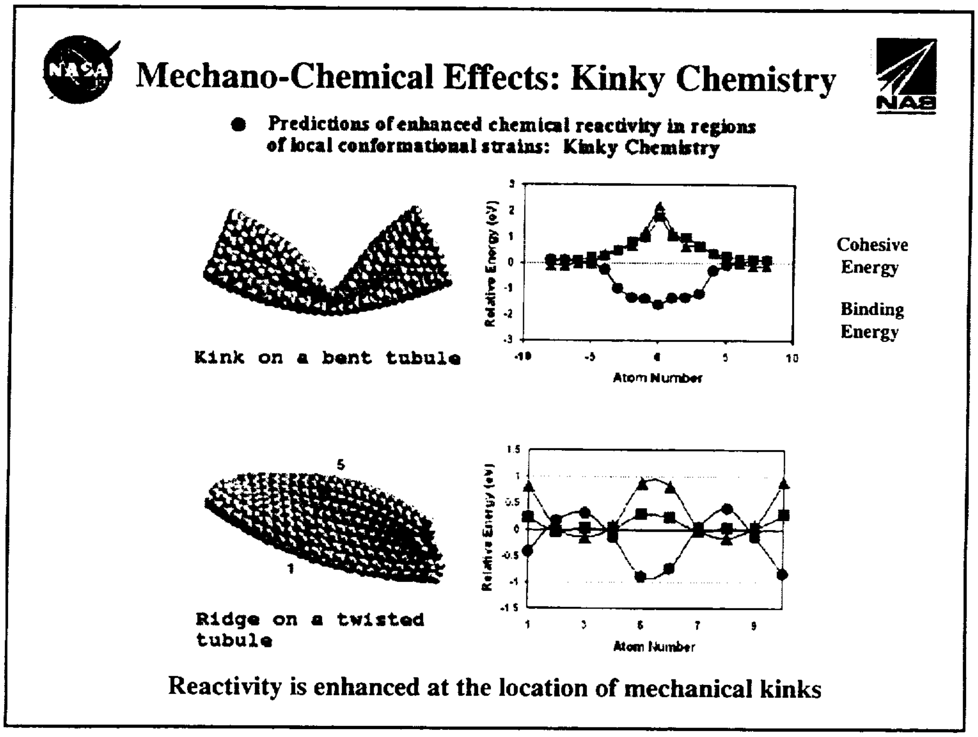
- Amenable to self-assembly through shape and color interactions

- Provision for molecular interconnects to the outside metallic contacts



Nano Electromechanical Effects (NEMS)

Mechanical deformation alters the electronic deformation of nanotubes. Effect is chirality dependent.



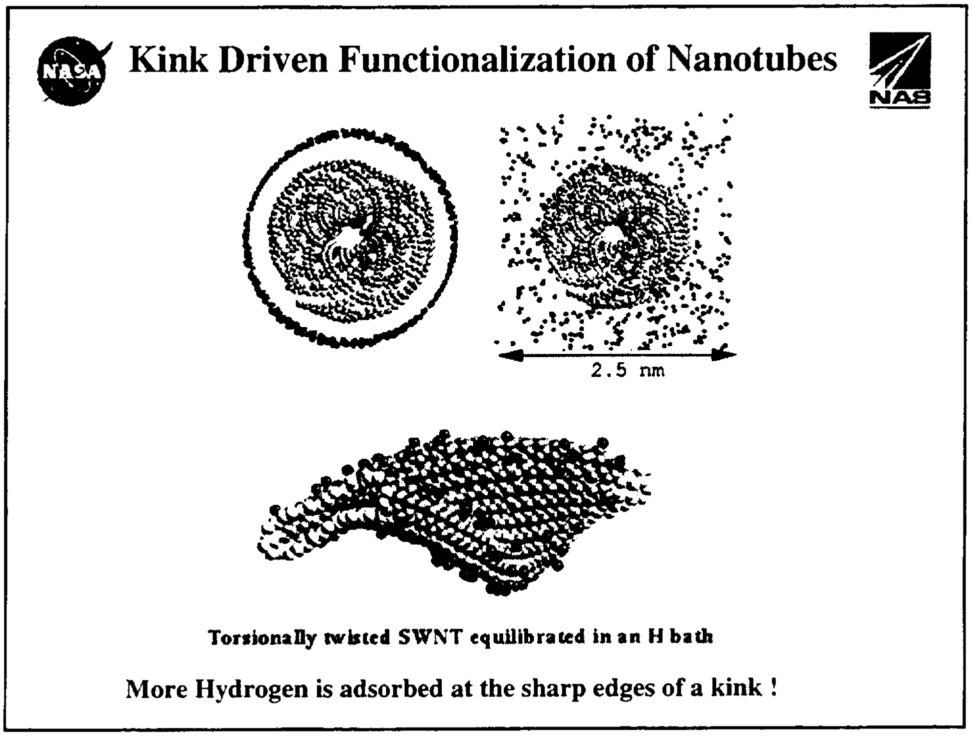
Mechano-Chemical Effects: Kinky Chemistry

- **Predictions of enhanced chemical reactivity in regions of local conformational strains: Kinky Chemistry**

Kink on a bent tubule

Ridge on a twisted tubule

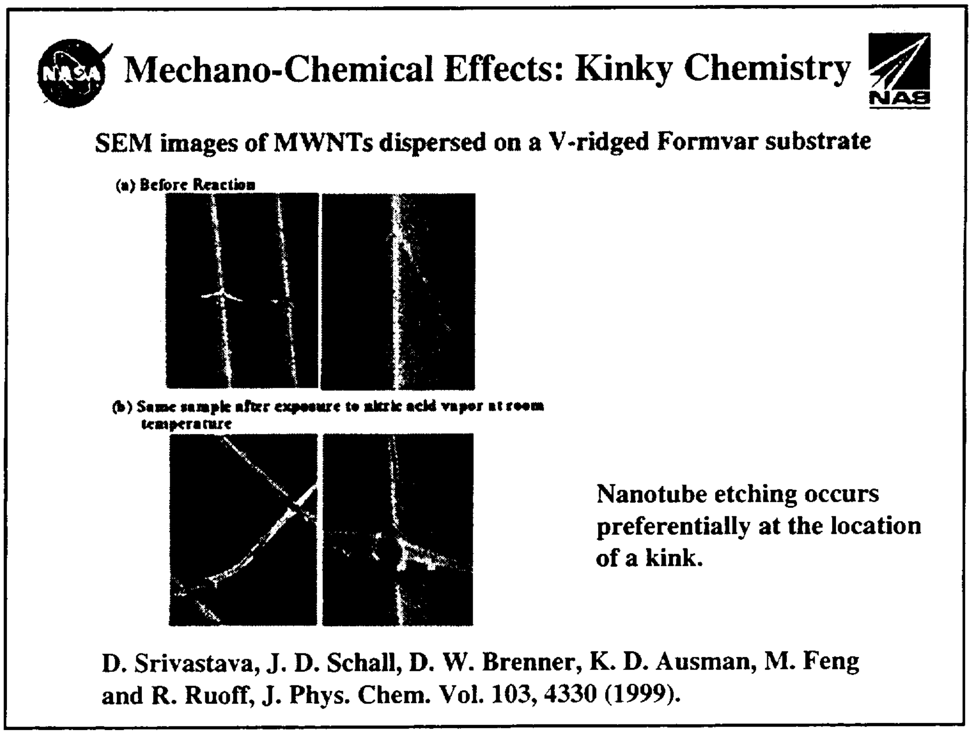
Reactivity is enhanced at the location of mechanical kinks



Kink Driven Functionalization of Nanotubes

Torsionally twisted SWNT equilibrated in an H bath

More Hydrogen is adsorbed at the sharp edges of a kink !



Mechano-Chemical Effects: Kinky Chemistry

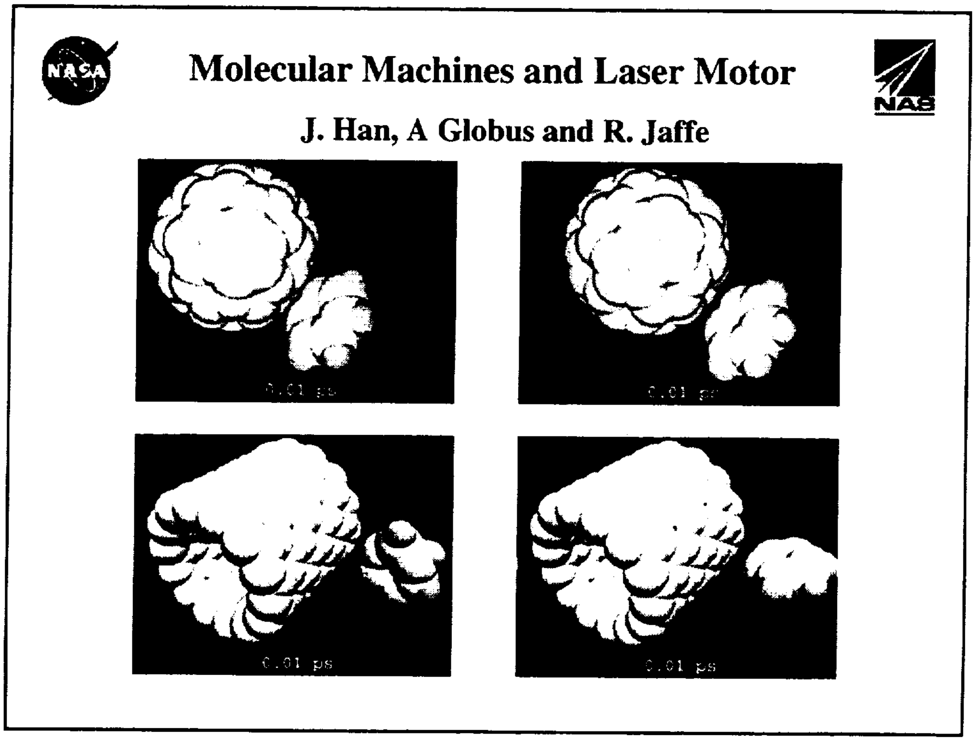
SEM images of MWNTs dispersed on a V-ridged Formvar substrate

(a) Before Reaction

(b) Same sample after exposure to nitric acid vapor at room temperature

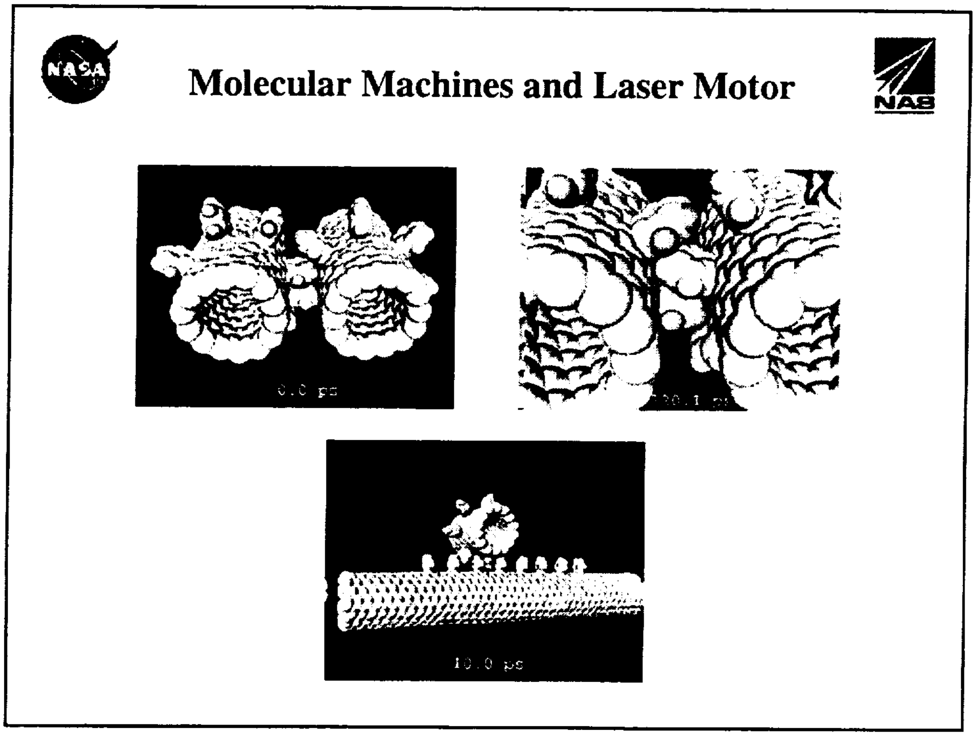
Nanotube etching occurs preferentially at the location of a kink.

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



Molecular Machines and Laser Motor

J. Han, A Globus and R. Jaffe

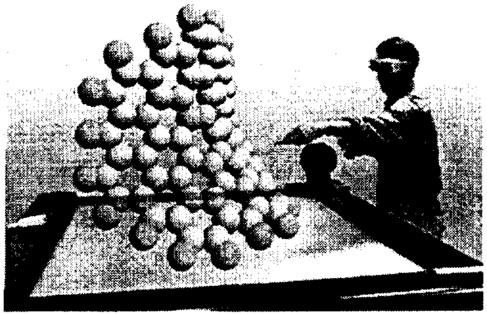


Molecular Machines and Laser Motor

Computational Nanotechnology: Future: PSE

Nanomanipulation in Virtual World

Simulations



Experiments

Next Generation of Technology and Products