Source of Acquisition
NASA Ames Research Center

Nanotechnology with Carbon Nanotubes: Mechanics, Chemistry, and Electronics

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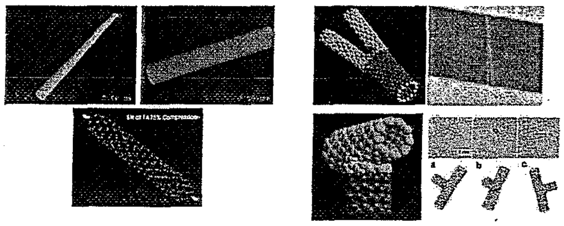
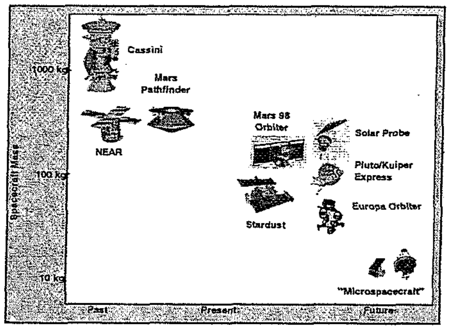
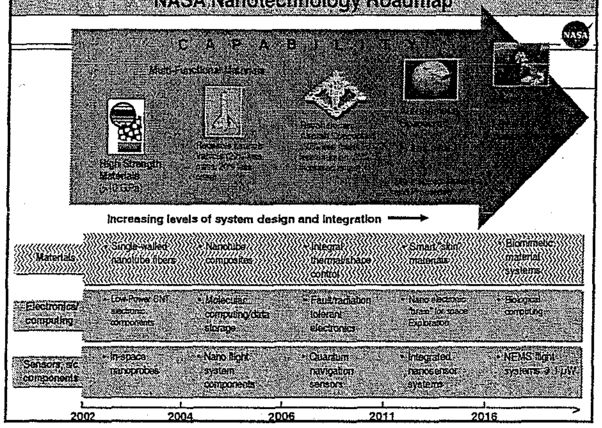


NASA's Own Moore's Law



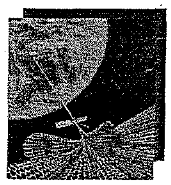
NASA Nanotechnology Roadmap

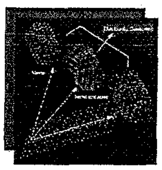


Carbon Nanotube

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.

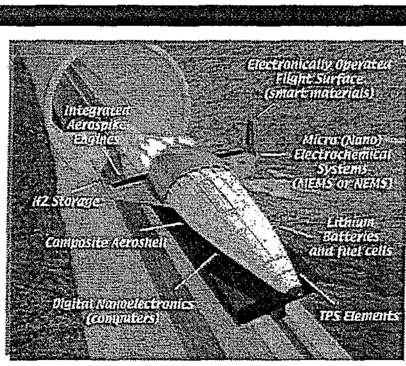




CNT exhibits extraordinary mechanical properties: Young's modulus over 1 Tera Pascal, as stiff as diamond, and tensile strength ~ 200 GPa.

CNT can be metallic or semiconducting, depending on chirality.

Just one Material, so much Potential



Software-Simulations: Expanding Sphere

Size Scale

- Mesoscopic dynamics for non-homogeneous
- ~ 1000,000 atoms — Atomistic MD, many-body force fields
- ~ 1000 atoms — Semi-emirical, tight-binding MD
- ~ 100 atoms — ab-initio, structure, energetics

MD (100 ns) — Time Scale — Experiments

Response/Transport Properties

- Magnetic
- Chemical
- Spectral/Optical
- Electrical
- Thermal

Computational Nanotechnology Projects Collaborators (Acknowledgement)

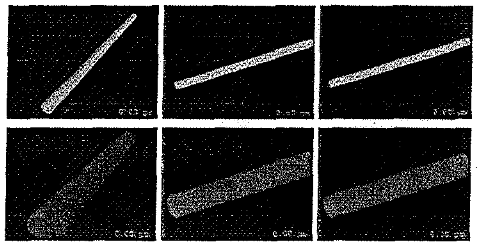
- Nanomechanics of Nanotubes and Composites
  - → Dr. Chengyu Wei (Postdoc), Prof. K. Cho (Stanford University)
- Reactivity and Chemistry of Carbon Nanotubes
  - → Prof. Don Brenner (NC State) and Prof. Rod Ruoff
  - → Seongjun Park and Prof. K. Cho (Stanford University)
- Molecular Electronics with Nanotube Hetero-junctions
  - → Dr. Madhu Menon (U. Ky) and Prof. Antonis Andriotis (U. Crete)

Nanomechanics Examples: Nanotubes

~ High value of Young's Modulus (1.2 -1.3 T Pa for SWNTs)

~ Elastic limit up to 10-15% strain

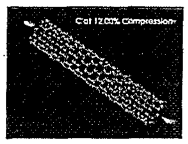
• Dynamic response under axial compression, bending torsion



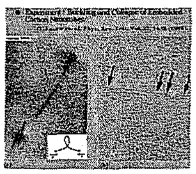
Computer Simulations: Characterization of New Materials!

Experimental validation: Nanotubes in Composites

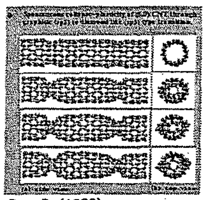
• Experiment: buckling and collapse of nanotubes embedded in polymer composites.



Buckle, bend and loops of thick tubes..



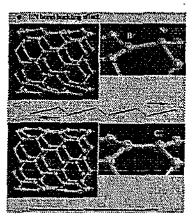
Local collapse or fracture of thin tubes.

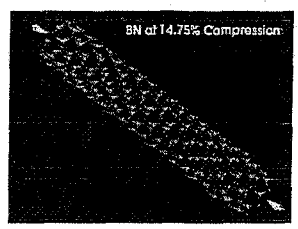


D. Srivastava, M. Menon and K. Cho, Phys. Rev. B (1999)

New Prediction: Anisotropic Plastic Collapse

•Structure and chemistry of **BN** nanotube is different





Nanostructured skin effect !

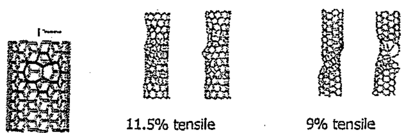
D. Srivastava, M. Menon and K. Cho, Phys. Rev. B (2001)

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)

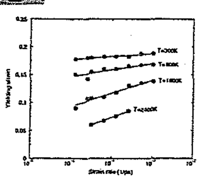
Experiments: 6% maximum strain in SWCNT ropes; 12% maximum strain in MWCNTs ?



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

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

Yielding of Single-Wall Nanotubes



- yielding: strongly dependent on the strain rate and temperature !

- Linear dependence ~ Activated Process

Transition State Theory based Formula

$$\varepsilon_Y = \frac{\bar{E}_v}{VK} + \frac{k_B T}{VK}\ln\left(\frac{N\dot{\varepsilon}}{n_{site}\dot{\varepsilon}_0}\right)$$

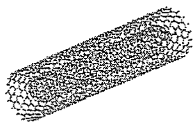
-***Experimental feasible conditions:*** length ~ 1μm; strain rate ~ 1%/hour; T ~ 300K

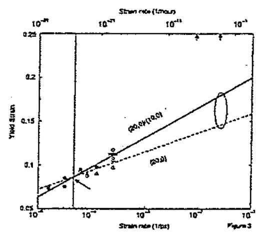
⟹ **Yield strain: 9 ± 1 %,** Experiments: 6-12% strain for SWNT ropes

C. Wei, K. Cho and D. Srivastava, to appear Phys. Rev. B (2003)

Yielding of Multi-wall Nanotubes

Double-wall nanotube with Contact to outermost wall





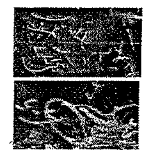
- **At the experimentally feasible strain-rate and temperature: ~ MWCNT yields at higher strain than equivalent SWCNT**

C. Wei, D. Srivastava and K. Cho, (to appear) Appl. Phys. Lett. (2003)

Polymer-CNT composite

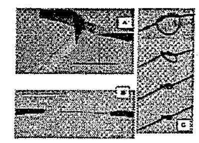
- Structural and thermal properties
- Load transfer and mechanical properties

SEM images of epoxy-CNT composite



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

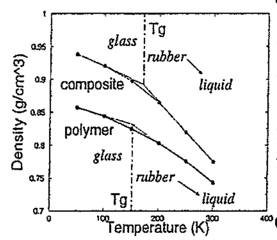
SEM images of polymer (polyvinylacohol) ribbon contained CNT fibers & knotted CNT fibers



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

High Thermal Expansion Coefficient Composite

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



Results:

-Glass transition temperature Tg increased from 150K to 175K

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

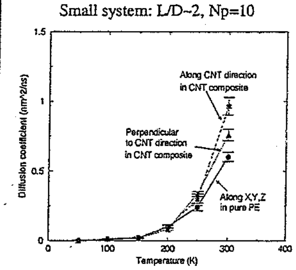
	PE	PE-CNT	
$T<Tg$	3.8×10^{-4}	4.5×10^{-4}	↑18%
$T>Tg$	8.6×10^{-4}	12.0×10^{-4}	↑40%

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

C. Wei, D. Srivastava, and K. Cho Nano Letters (2002)

Thermal Diffusion coefficients

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



Diffusion coefficients of polymer with CNTs embedded

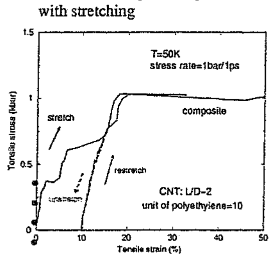
Diffusion coefficient increased, especially along CNT axis direction, indicating enhancement of thermal conductivity

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

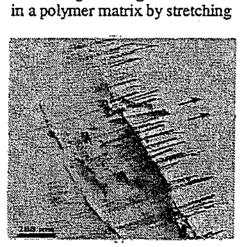
C. Wei, D. Srivastava, and K. Cho Nano Letters (2002)

Loading sequence

Work hardening of composite with stretching



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



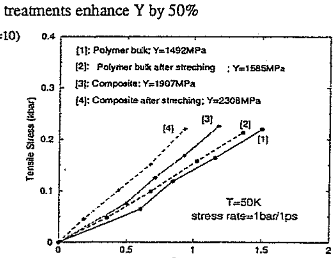
(L. Jin et.al., Appl.Phys. Lett., V73 P1197, 1998)

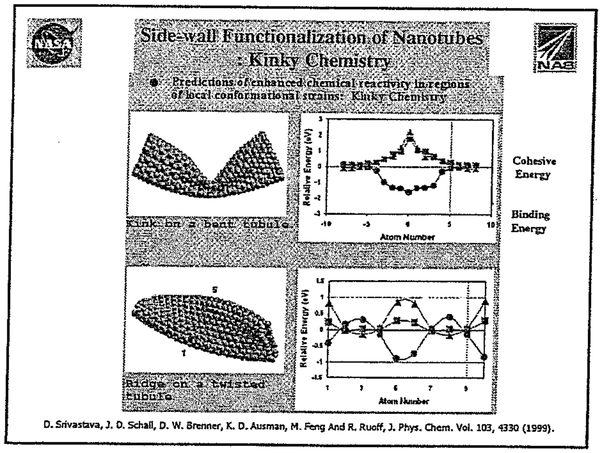
Young's Modulus

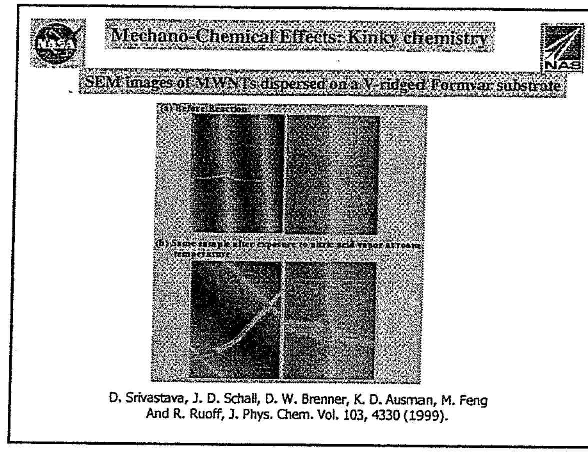
-Young's modulus of CNT composites 30% higher than polymer matrix

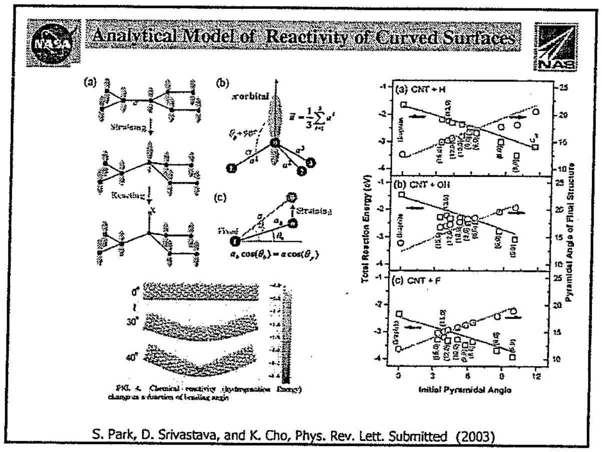
-Stretching treatments enhance Y by 50%

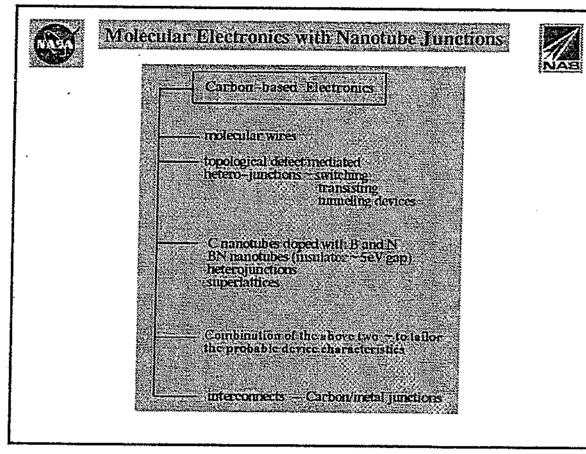
(L/D~2, Np=10)

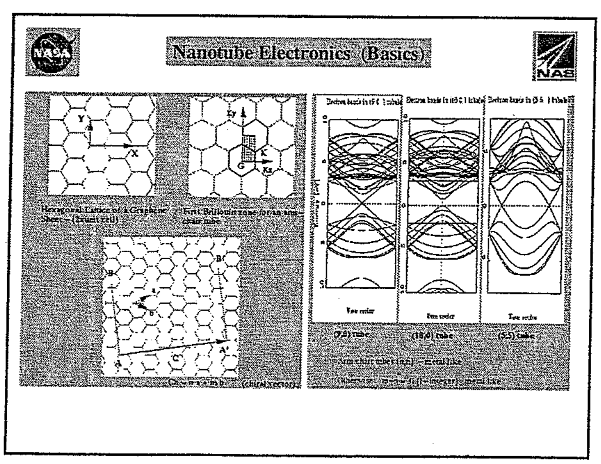


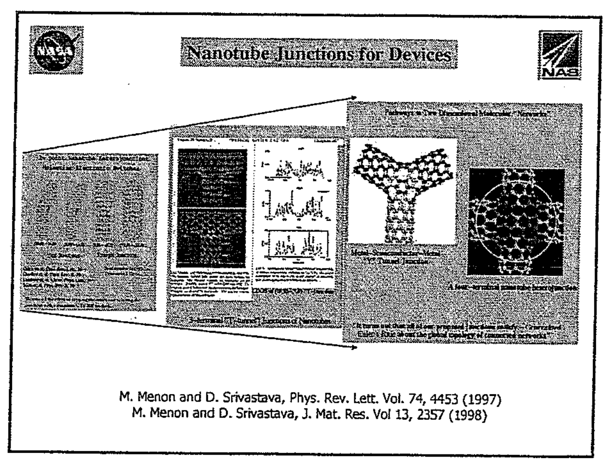

Side-wall Functionalization of Nanotubes : Kinky Chemistry
Predictions of enhanced chemical reactivity in regions of local conformational strains: Kinky Chemistry
Kink on a bent tubule
Relative Energy (eV)
Atom Number
Cohesive Energy
Binding Energy
Ridge on a twisted tubule
D. Srivastava, J. D. Schall, D. W. Brenner, K. D. Ausman, M. Feng And R. Ruoff, J. Phys. Chem. Vol. 103, 4330 (1999).


Mechano-Chemical Effects: Kinky chemistry
SEM images of MWNTs dispersed on a V-ridged Formvar substrate
(a) Before Reaction
D. Srivastava, J. D. Schall, D. W. Brenner, K. D. Ausman, M. Feng
And R. Ruoff, J. Phys. Chem. Vol. 103, 4330 (1999).


Analytical Model of Reactivity of Curved Surfaces
(a)
(b)
(c)
π orbital
Straining
Reacting
Final
(a) CNT + H
(b) CNT + OH
(c) CNT + F
Total Reaction Energy (eV)
Pyramidal Angle of Final Structure
Initial Pyramidal Angle
S. Park, D. Srivastava, and K. Cho, Phys. Rev. Lett. Submitted (2003)

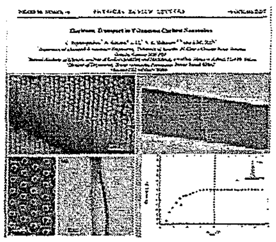

Molecular Electronics with Nanotube Junctions
Carbon-based Electronics
molecular wires
topological defect mediated
hetero-junctions – switching
transisting
tunneling devices
C nanotubes doped with B and N
BN nanotubes (insulator ~5eV gap)
heterojunctions
superlattices
Combination of the above two – to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

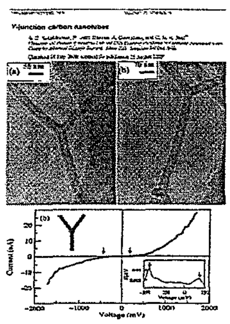

Nanotube Electronics (Basics)
(7,0) tube
(8,4) tube
(5,5) tube


Nanotube Junctions for Devices
M. Menon and D. Srivastava, Phys. Rev. Lett. Vol. 74, 4453 (1997)
M. Menon and D. Srivastava, J. Mat. Res. Vol 13, 2357 (1998)

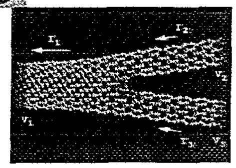
Multi-wall Y-junction Carbon Nanotubes

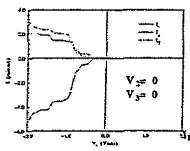
Experimental Synthesis of Multi-wall Carbon Nanotube Y-Junctions (2000)

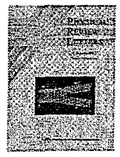




Rectification and Analog Logic Devices

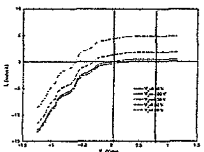






V2	V3	OR	XOR
0	0	0	0
0	1	1	1
1	0	1	1
1	1	1	0

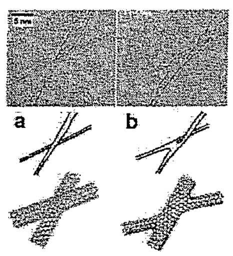
OR XOR

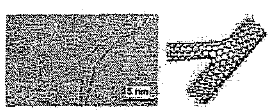


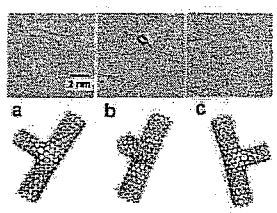
V_1

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

Single-wall Carbon Nanotube Junctions: Welding

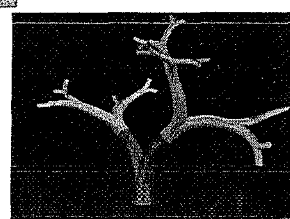


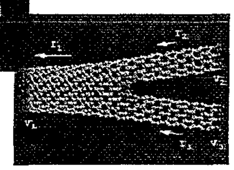




Terrones et. al., Phys. Rev. Lett. 12 August (2002)

Bio-mimetic Dendritic Neurons: Carbon Nanotube

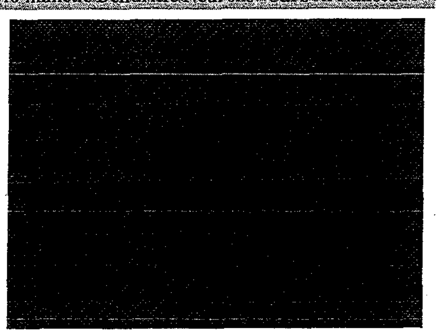




Model of 4-level dentritic neural tree that could be made of branched carbon nanotubes

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

Bio-mimetic Dendritic Neurons: Carbon Nanotube



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 Nanotube

Biological Dendritic Neural Tree	Carbon Nanotube: Dendritic Tree
• One dimensional cable theory + Hodgkin-Huxley model for action-potential based information flow	• Electronic, acoustic, thermal, and chemical signal transmission and information processing
• Information processing is coded in (a) branching at the junctions, and (b) time-series sequencing of the signal spikes	• Information processing can be based on (a) branching + switching at the junctions, and (b) time series sequencing of signal-spikes
• Input – output – control: is based on (a) structural details of the branches and junctions, and (b) via chemical environment	• 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 is part of the structure: evolutionary in nature	• 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)

Acknowledgements

- Prof. K. Cho (Stanford University)
- Dr. Madhu Menon (University of Kentucky)
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- Dr. Fedor Dezigilenko (ex NASA Ames)
- Seong Jun Park (Stanford University)
- Eva Gonzales (University of Kentucky/ Spain)
- Christiane Anderson (University of Minnesota, MN)

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- Al Globus (CSC/NASA Ames)
- Chris Henze (AMTI/NASA Ames)
- Steve Barnard (MRJ/NASA Ames)
- Glen Deardorff (AMTI/ NASA Ames)