

21st century space elevator would revolutionize the delivery into space of payloads and people. CREDIT: NASA artwork by Pat Rawlings/SAIC

Twenty tons of cable and reel would be kicked up to geosynchronous altitude by spacecraft to get the project started.



http://science.nasa.gov/headlines/y2000/ast07sep_1.htm

http://www.space.com/business/technology/space_elevator_021120.html



Carbon Nanotube based Nanotechnology: Molecular Materials and Electronics



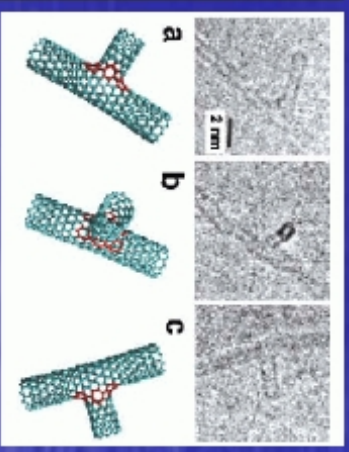
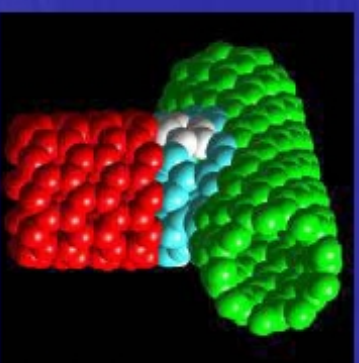
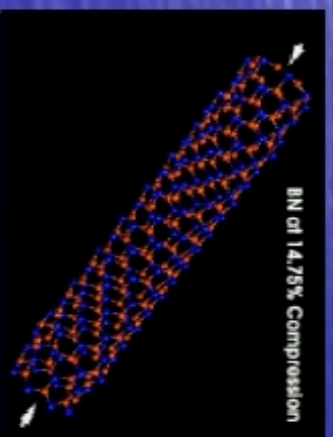
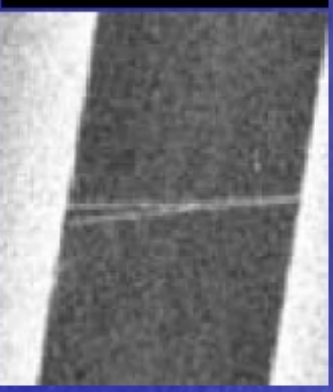
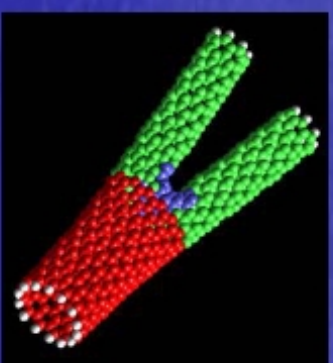
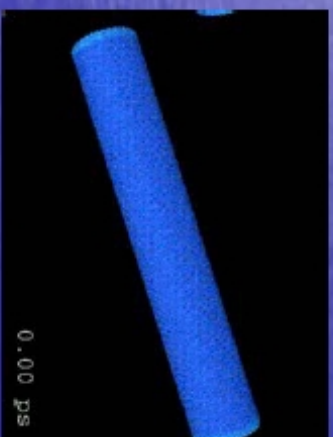
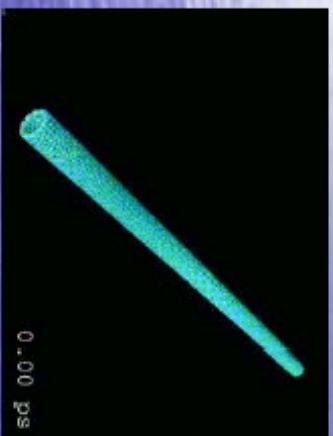
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NASA Nanotechnology Roadmap

C A P A B I L I T Y



Multi-Functional Materials



High Strength Materials
(>10 GPa)



Reusable Launch Vehicle (20% less mass, 20% less noise)



Revolutionary Aircraft Concepts
(30% less mass, 20% less emission, 25% increased range)



Autonomous Spacecraft
(40% less mass)



Adaptive Self-Repairing Space Missions

Bio-Inspired Materials and Processes

Increasing levels of system design and integration →

Materials

- Single-walled nanotube fibers
- Nanotube composites
- Integral thermal/shape control
- Smart "skin" materials
- Biomimetic material systems

Electronics/ computing

- Low-Power CNT electronic components
- Molecular computing/data storage
- Fault/radiation tolerant electronics
- Nano electronic "brain" for space Exploration
- Biological computing

Sensors, s/c components

- In-space nanoprobes
- Nano flight system components
- Quantum navigation sensors
- Integrated nanosensor systems
- NEMS flight systems @ 1 μ W

2002

2004

2006

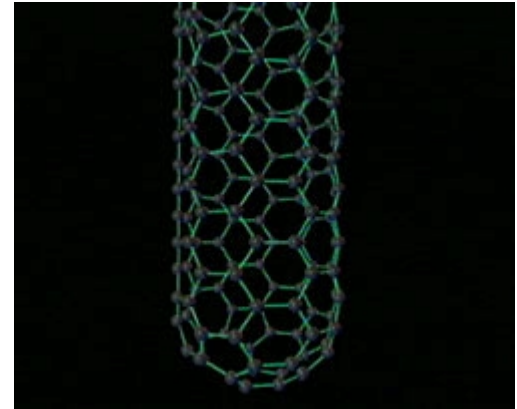
2011

2016



What Are They?

- SP² Hybridized carbon atoms
- Each atom is bonded to three other atoms
- Essentially, a sheet of graphite rolled into a tube
- Can be single or multi-walled
- Can be found in many different shapes and sizes



S. Iijima, *Nature*, **354** 56 (1991)

Introduction

Carbon nanotubes, long, thin cylinders of carbon, were discovered in 1991 by S. Iijima. These are large macromolecules that are unique for their size, shape, and remarkable physical properties. They can be thought of as a sheet of graphite (a hexagonal lattice of carbon) rolled into a cylinder. These intriguing structures have sparked much excitement in the recent years and a large amount of research has been dedicated to their understanding. Currently, the physical properties are still being discovered and disputed. What makes it so difficult is that nanotubes have a very broad range of electronic, thermal, and structural properties that change depending on the different kinds of nanotube (defined by its diameter, length, and chirality, or twist). To make things more interesting, besides having a single cylindrical wall (SWNTs), nanotubes can have multiple walls (MWNTs)--cylinders inside the other cylinders.

Why Are They Interesting?

- **Extremely Strong**
 - Tensile Strength of 45 billion pascals
- **High Current Capacity**
 - 1 billion amps/cm²
- **Good Temperature Stability**
 - Stable up to 2,800 degrees in a vacuum, 750 in air
- **Conducting or Semi-Conducting Characteristics**
 - Depending on its diameter, a nanotube can have either set of properties
- **Very Small**
 - Diameters from .6 to 1.8 nanometers

Quick Facts

Average Diameter of SWNT's

Distance from opposite Carbon Atoms (Line 1)

Analogous Carbon Atom Separation (Line 2)

Parallel Carbon Bond Separation (Line 3)

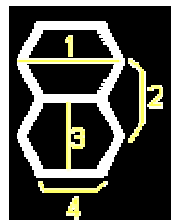
Carbon Bond Length (Line 4)

Density:

(10, 10) Armchair

(17, 0) Zigzag

(12, 6) Chiral



1.2-1.4 nm

2.83 Å [\[1\]](#)

2.456 Å [\[1\]](#)

2.45 Å [\[1\]](#)

1.42 Å [\[1,23\]](#)

1.33 g/cm³ [\[3\]](#)

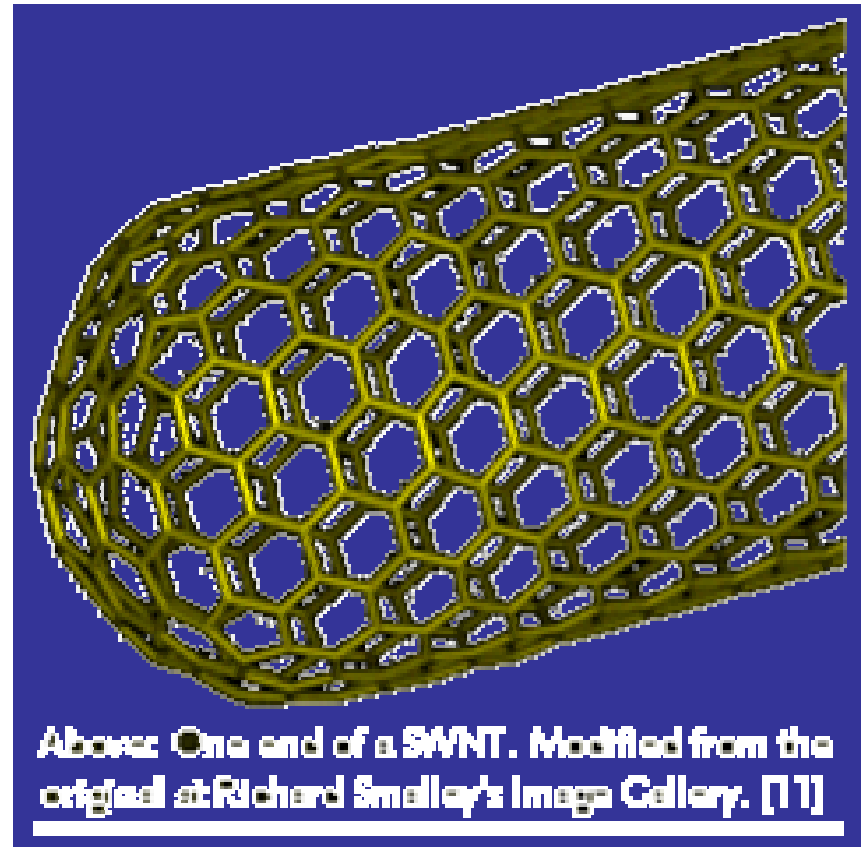
1.34 g/cm³ [\[3\]](#)

1.40 g/cm³ [\[3\]](#)

Interlayer Spacing:				
	(n, n) Armchair		3.38 Å	
	(n, 0) Zigzag		3.41 Å	
	(2n, n) Chiral		3.39 Å	
<u>Electrical Transport</u>				
Resistivity		10^{-4} Ω-cm		
Maximum Current Density		10^{13} A/m ²		
<u>Thermal Transport</u>				
Thermal Conductivity		~ 2000 W/m/K		
Phonon Mean Free Path		~ 100 nm		
Relaxation Time		~ 10^{-11} s		
<u>Elastic Behavior</u>				
Young's Modulus (SWNT)		~ 1 TPa		
Young's Modulus (MWNT)		1.28 TPa		
Maximum Tensile Strength		~30 GPa		

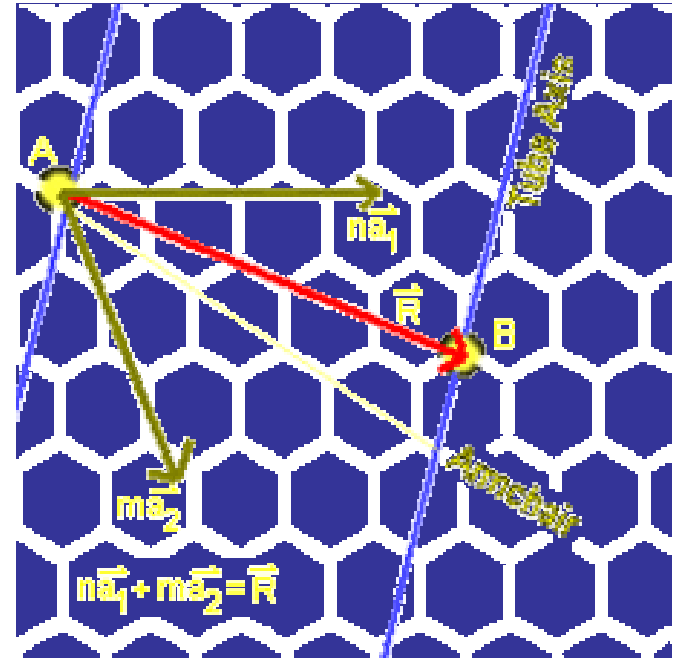
Basic Structure:

Simply put, carbon nanotubes exist as a macro-molecule of carbon, analagous to a sheet of graphite (the pure, brittle form of cabon in your pencil lead) rolled into a cylinder. Graphite looks like a sheet of chicken wire, a tessellation of hexagonal rings of carbon. Sheets of graphite in your pencil lay stacked on top on one another, but they slide past each other and can be separated easily, which is how it is used for writing. However, when coiled, the carbon arrangement becomes very strong. In fact, nanotubes have been known to be up to one hundred times as strong as steel and almost two millimeters long! These nanotubes have a hemispherical "cap" at each end of the cylinder. They are light, flexible, thermally stabile, and are chemically inert. They have the ability to be either metallic or semi-conducting depending on the "twist" of the tube.



Types of SWNT

Nanotubes form different types, which can be described by the chiral vector (n, m) , where n and m are integers of the vector equation $\vec{R} = n\vec{a}_1 + m\vec{a}_2$. The chiral vector is determined by the diagram at the right. Imagine that the nanotube is unraveled into a planar sheet. Draw two lines (the blue lines) along the tube axis where the separation takes place. In other words, if you cut along the two blue lines and then match their ends together in a cylinder, you get the nanotube that you started with. Now, find any point on one of the blue lines that intersects one of the carbon atoms (point A). Next, draw the Armchair line (the thin yellow line), which travels across each hexagon, separating them into two equal halves. Now that you have the armchair line drawn, find a point along the other tube axis that intersects a carbon atom nearest to the Armchair line (point B). Now connect A and B with our chiral vector, \vec{R} (red arrow). The wrapping angle ϕ ; (not shown) is formed between \vec{R} and the Armchair line. If \vec{R} lies along the Armchair line ($\phi=0^\circ$), then it is called an "Armchair" nanotube. If $\phi=30^\circ$, then the tube is of the "zigzag" type. Otherwise, if $0^\circ < \phi < 30^\circ$ then it is a "chiral" tube. The vector \vec{a}_1 lies along the "zigzag" line. The other vector \vec{a}_2 has a different magnitude than \vec{a}_1 , but its direction is a reflection of \vec{a}_1 over the Armchair line. When added together, they equal the chiral vector \vec{R} . [\[Adapted from 23\]](#)



The values of n and m determine the chirality, or "twist" of the nanotube. The chirality in turn affects the conductance of the nanotube, its density, its lattice structure, and other properties. A SWNT is considered metallic if the value $n - m$ is divisible by three. Otherwise, the nanotube is semiconducting. Consequently, when tubes are formed with random values of n and m , we would expect that two-thirds of nanotubes would be semi-conducting, while the other third would be metallic, which happens to be the case. [\[23\]](#)

Given the chiral vector (n,m) , the diameter of a carbon nanotube can be determined using the relationship

$$d = (n^2 + m^2 + nm)^{1/2} 0.0783 \text{ nm}$$

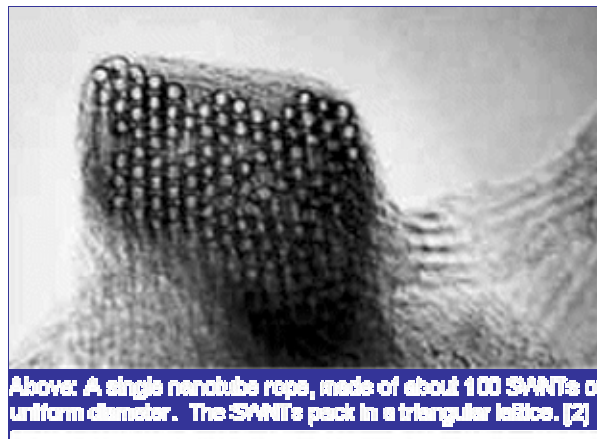
Detailed structure

- The average diameter of a SWNT is 1.2 nm. [1] However, nanotubes can vary in size, and they aren't always perfectly cylindrical. The larger nanotubes, such as a (20, 20) tube, tend to bend under their own weight. [12] The diagram at right shows the average bond length and carbon separation values for the hexagonal lattice. The carbon bond length of 1.42 Å was measured by Spires and Brown in 1996 [1] and later confirmed by Wilder *et al.* in 1998. [23] The C-C tight bonding overlap energy is in the order of 2.5 eV. Wilder *et al.* estimated it to be between 2.6 eV - 2.8 eV [23] while at the same time, Odom *et al.* estimated it to be 2.45 eV [24]

Ropes of Carbon Nanotubes

In 1996, Thess *et al.* measured the properties of "ropes" of carbon nanotubes. [2] As shown in the diagram at right, ropes are bundles of tubes packed together in an orderly manner. They found that the individual SWNTs packed into a close-packed triangular lattice with a lattice constant of about 17 Å. This was later confirmed by Gao, Cagin, and Goddard in 1997. [3] In addition, they concluded that the density, lattice parameter, and interlayer spacing of the ropes was dependent on the chirality of the tubes in the mat. (10, 10) Armchair tubes had a lattice parameter of 16.78 Å and had a density of 1.33 g/cm³. Zigzag tubes of the chirality (17, 0) had a lattice parameter of 16.52 Å and a density of 1.34 g/cm³. Mats made of (12, 6) chiral SWNT's had a lattice parameter of 16.52 Å and a density of 1.40 g/cm³. The space between the tubes was also dependent on chirality. Armchair tubes had a spacing of 3.38 Å, zigzag tubes had a spacing of 3.41 Å, and (2n, n) chiral tubes had an interlayer spacing value of 3.39 Å. Compare these values to the spacing between the layers of graphite sheets, and the spacing between the variant walls of a MWNT, both about 3.4 Å. [13]

As a good estimate, the lattice parameter in CNT ropes (bundled nanotubes) is $d + 0.34$ nm, where d is the tube diameter given above.



Above: A single nanotube rope, made of about 100 SWNTs of uniform diameter. The SWNTs pack in a triangular lattice. [2]

Optical Properties.

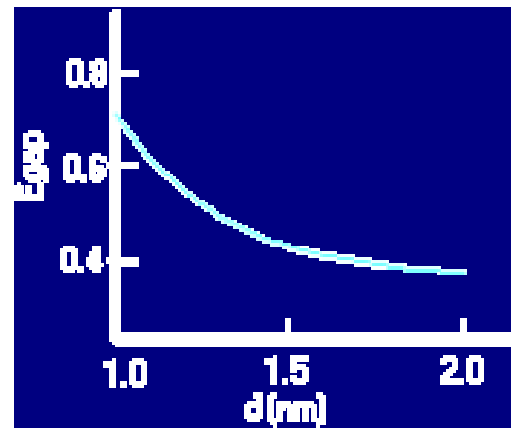
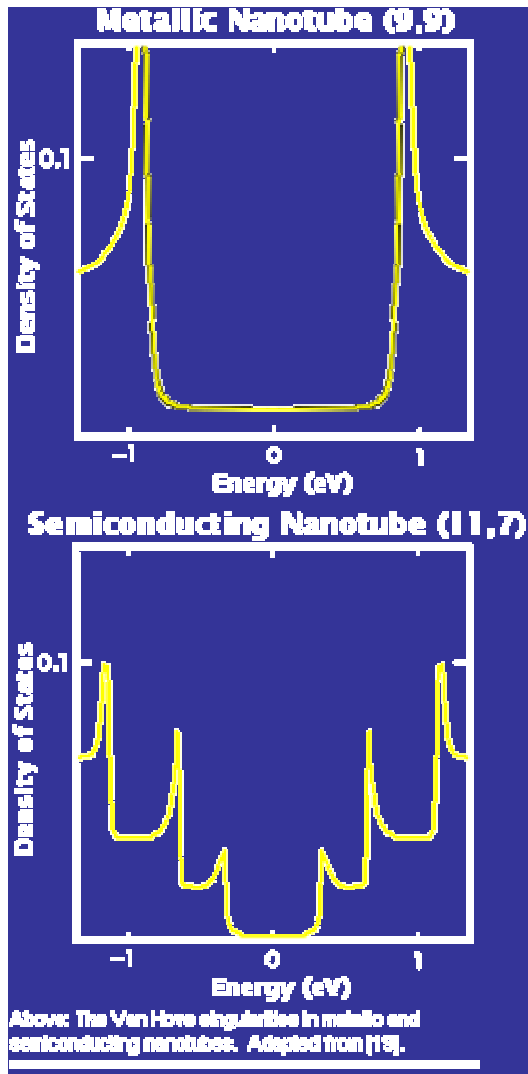
In 1998, Wilder *et al.* [23] conducted research into the fundamental gap of carbon nanotubes.

The Fundamental Gap

The study by Wilder *et al.* showed that nanotubes of type $n-m=3l$, where l is zero or any positive integer, were metallic and therefore conducting. The fundamental gap (HOMO-LUMO) would therefore be 0.0 eV. All other nanotubes, they showed, behaved as a semi-conductor. The fundamental gap, they showed, was a function of diameter, where the gap was in the order of about 0.5 eV. Their data showed that the energy gap reflected the graph at right (adapted from [23]. This graph can be modelled by the function:

$$E_{\text{gap}} = 2 y_0 a_{\text{cc}} / d$$

Where y_0 is the C-c tight bonding overlap energy, a_{cc} is the nearest neighbor C-C distance (0.142 nm) and d is the diameter.



Electrical Transport

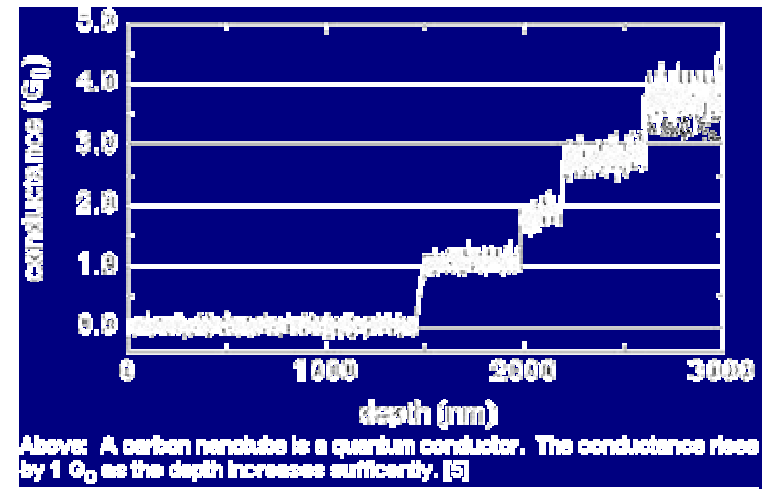
The electrical transport properties of SWNTs has been recently studied has raised some controversy. The conductance of a tube is quantized, and a nanotube acts as a ballistic conductor. Nanotubes also have a constant resistivity, and a tolerance for very high current density.

Ballistic Conductance

In 1998, Stephan Frank *et al.* experimented on the conductance of nanotubes. [5] Using a SPM, he carefully contacted nanotube fibers with a mercury surface. His results revealed that the nanotube behaved as a ballistic conductor with quantum behavior. The MWNT conductance jumped by increments of $1 G_0$ as additional nanotubes were touched to the mercury surface. The value of G_0 was found to be $1/12.9 \text{ k-1}$, where $G_0 = 2e^2/h$. The coefficient of the conductance quantum was found to have some surprising integer and non-integer values, such as $0.5 G_0$. Later, in 1999, Sanvito, Kwon, Tománek, and Lambert, [4] used a scattering technique to calculate the ballistic quantum conductance of MWNTs. They found that their results explained these unexpected conductance values found by Frank in 1998. Sanvito *et al.* stated that some of the quantum conductance channels were blocked by interwall reactions. Also, the interwall reactions of MWNTs were found to redistribute the current over individual tubes across the structure nonuniformly.

Resistivity and Maximum

Current Density Relatively early in the research of nanotubes, Thess *et al.* calculated the resistivity of ropes of metallic SWNTs to be in the order of 10^{-4} -cm at 300 K. [2] They did this by measuring the resistivity directly with a four-point technique. One of their values they measured was 0.34×10^{-4} , which they noted would indicate that the ropes were the most highly conductive carbon fibers known, even factoring in their error in measurement. In the same study his measurements of the conductivity, Frank *et al.* [5] was able to have reach a current density in the tube greater than 10^7 A/cm^2 . Later, Phaedon Avouris [12] suggested that stable current densities of nanotubes could be pushed as high as 10^{13} A/cm^2 .



Thermal Conductivity.

The thermal conductivity of carbon nanotubes is dependent on the temperature and the large phonon mean free paths. On the graph of thermal conductivity vs temperature, the slope of the line at low temperatures can be modelled using the heat capacity, sound velocity, and relaxation time of the tube.

Thermal Conductivity

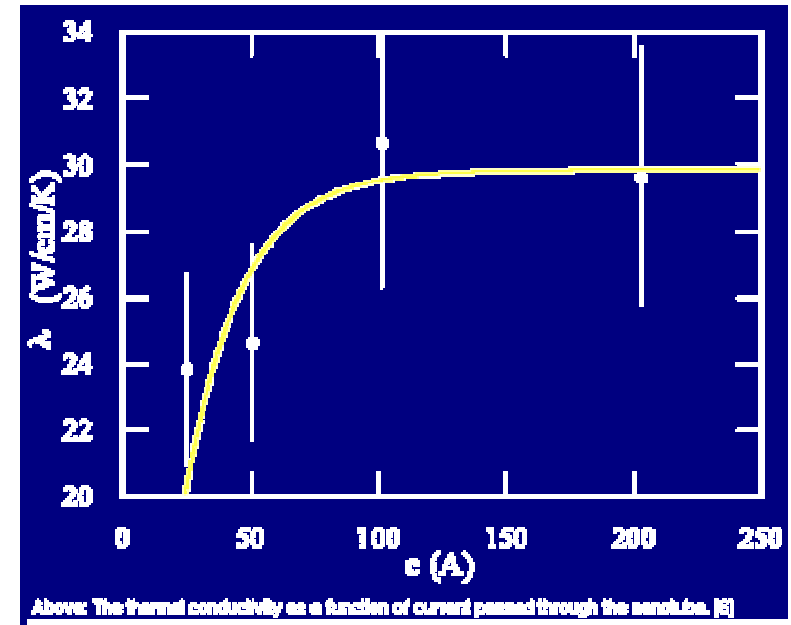
There seems to be some disagreement into the exact nature of the thermal conductivity of carbon nanotubes, although most agree that thermal conductivity seems to change depending on temperature, and possible also on current and vacancy concentration. In 1999, J. Hone, M. Whitney, and A. Zettle [\[15\]](#) found that the thermal conductivity was temperature dependent, and was almost a linear relationship. They suggested that the conductivity was linear in temperature from 7 K to 25 K. From 25 K to 40 K, the line increases in slope, and it arises monotonically with temperature to above room temperature. They proposed a model to explain the low temperature behavior, which is:

$$k_{zz} = C v^2 \tau$$

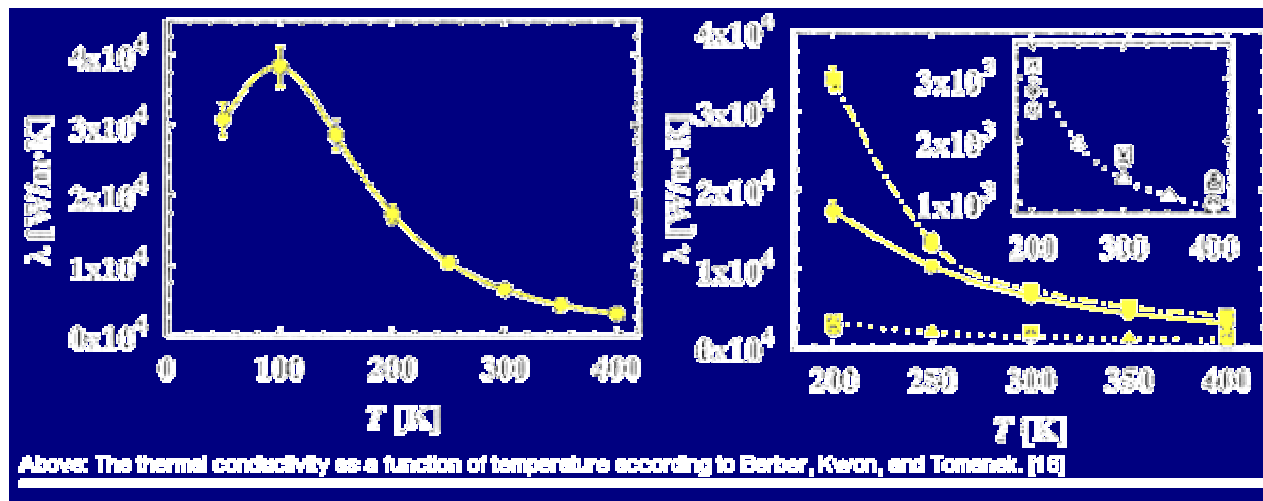
Where k_{zz} is the slope of the line on the graph, C is the heat capacity,

v is the sound velocity (Hone *et al.* used 1, 2, and 0.8×10^6 cm/s), and

τ is the relaxation time, which is approximately 10^{-11} s. They also found that the thermal conductivity for a single rope at room temperature could vary between 1800 - 6000 W/m-K.



Also that year, Che, Cagin, and Goddard [6] numerically calculated the thermal conductivity of a (10, 10) nanotube to approach 2980 W/m-K as the current applied to it is increased (see figure at right.) In 2000, Berber, Kwon, and Tomànek [16] determined the thermal conductivity of carbon nanotubes and its dependence on temperature. They confirmed the suggestion of Hone *et al.* in 1999 by suggesting an unusually high value of 6,600 W/m-k for the thermal conductivity at room temperature. They theorized that these high values would be due to the large phonon mean free paths, which would concur with Hone's model suggested above. Both groups stated that these values for thermal conductivity are comparable to diamond or a layer of graphite. However, Berber *et al.* suggested that the graphs of the temperature dependence of thermal conductivity looked much less linear than previously proposed by Hone *et al.* Instead of a near-linear graph with a positive slope, their graph showed a positive slope from low temperatures up to 100K, where it peaks around 37,000 W/m-K. Then, the thermal conductivity drops dramatically down to around 3000 W/m-k when the temperature approaches 400 K.





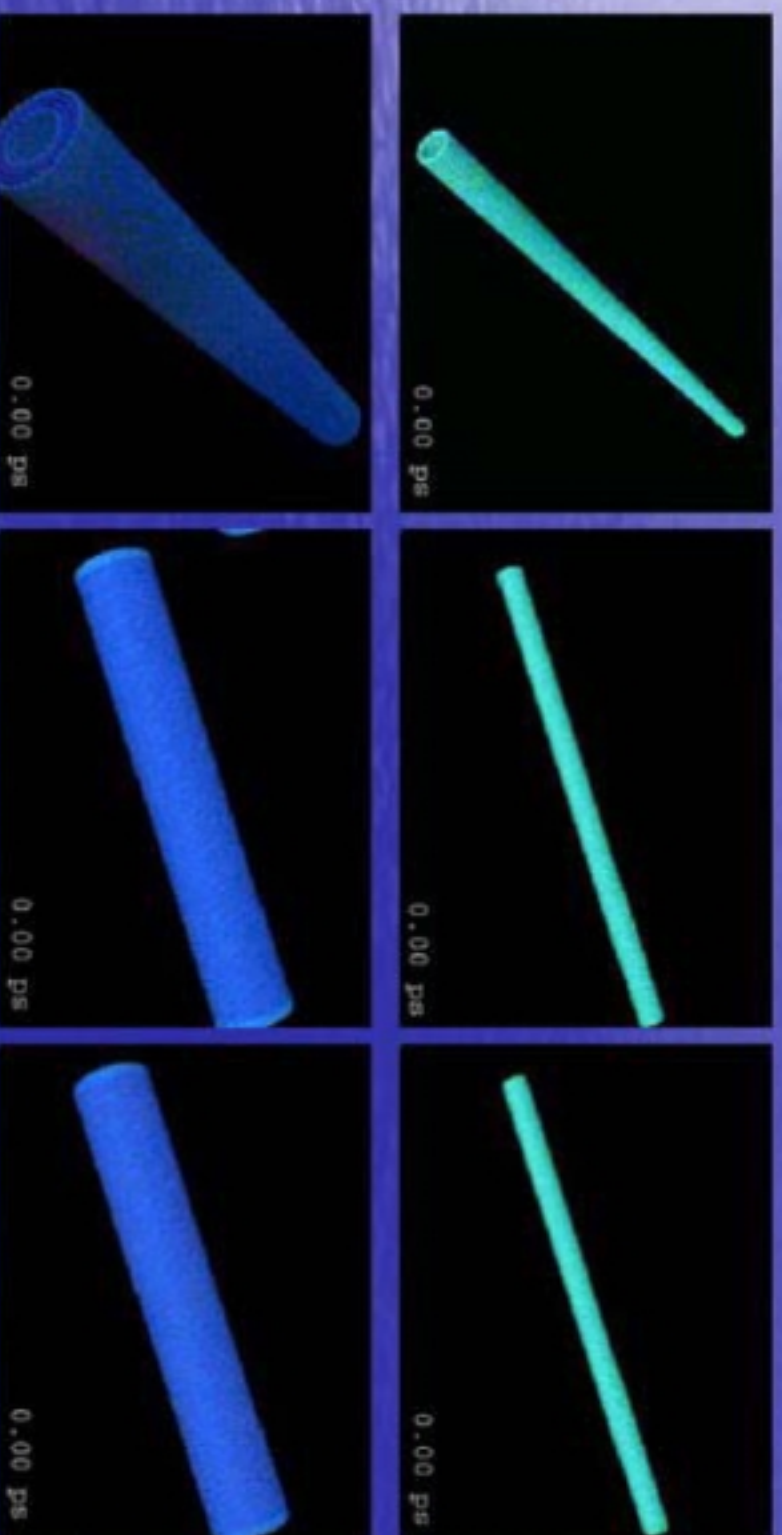
Nanomechanics Examples: Nanotubes



~ High value of Young's Modulus (1.2 - 1.3 TPa for SWNTs)

~ Elastic limit up to 10-15% strain

- Dynamic response under axial compression, bending torsion



Computer Simulations: Characterization of New Materials!

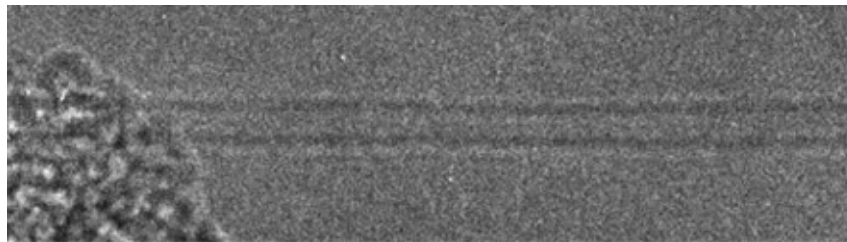
Determining the Elastic Properties of SWNTs has been one of the most hotly disputed areas of nanotube study in recent years. On the whole, SWNTs have are stiffer than steel and are resistant to damage from physical forces. Pressing on the tip of the nanotube will cause it to bend without damage to the tip or the whole CNT. When the force is removed, the tip of the nanotube will recover to its original state. [19] Quantizing these effects, however, is rather difficult and an exact numerical value cannot be agreed upon.

Elastic Behavior

The Young's modulus (elastic modulus) of SWNTs lies close to 1 TPa. The maximum tensile strength is close to 30 GPa.

Reference: *M.-F. Yu et al., Phys. Rev. Lett.* **84**, 5552 (2000).

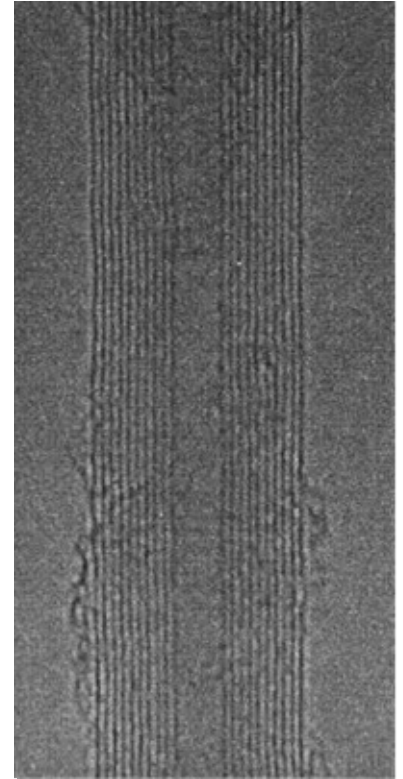
The results of various studies over the years has shown a large variation in the value reported. In 1996, researchers at NEC in Princeton and the University of Illinois measured the average modulus to be 1.8 TPa. [9] This was measured by first allowing a tube to stand freely and then taking a microscopic image of its tip. The modulus is calculated from the amount of blur seen in the photograph at different temperatures. In 1997, G. Gao, T. Cagin, and W. Goddard III [3] presented a talk at the Fifth Foresight Conference on Molecular Nanotechnology where they reported three variations on the Young's Modulus to five decimal places that were dependent on the chiral vector. They concluded that a (10,10) armchair tube had a modulus of 640.30 GPa, a (17,0) zigzag tube had a modulus of 648.43 GPa, and a (12,6) tube had a value of 673.94 GPa. These values were calculated from the second derivatives of potential. Using these two different methods, a discrepancy arises.



Further studies were conducted. In 1998, Treacy *et al.* [7] reported an elastic modulus of 1.25 TPa using the same basic method as done two years earlier. This compared well with the modulus of MWNTs (1.28 TPa), found by Wong *et al.* in 1997. Using an AFM, they pushed the unanchored end of a freestanding nanotube out of its equilibrium position and recorded the force that the nanotube exerted back onto the tip. [8] In 1999, E. Hernández and Angel Rubio showed using tight-binding calculations, the Young's Modulus was dependent on the size and chirality of the SWNT, ranging from 1.22 TPa for the (10, 0) and (6, 6) tubes to 1.26 TPa for the large (20,0) SWNT. However, using first principal calculations, they calculated a value of 1.09 TPa for a generic tube. [8]

The previous evidence would lead us to assume that the diameter and shape of the nanotube was the determining factor for its elastic modulus. However, when working with different MWNTs, Forró *et al.* noted that their modulus measurements of MWNTs in 1999 (using AFM) did not strongly depend on the diameter, as had been recently suggested. Instead, they argued that the modulus of MWNTs correlates to the amount of disorder in the nanotube walls. However, their evidence showed that the value for SWNTs does in fact depend on diameter; an individual tube had a modulus of about 1 TPa while bundles (or ropes) of 15 to 20 nm in diameter had a modulus of about 100 GPa.[20]

It has been suggested that the controversy into the value of the modulus is due to the author's interpretation of the thickness of the walls of the nanotube. If the tube is considered to be a solid cylinder, then it would have a lower Young's modulus. If the tube is considered to be hollow, the modulus is gets higher, and the thinner we treat the walls of the nanotube, the higher the modulus will become. [13]



TEM image of MWNT

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Location: <http://cnst.rice.edu/ropes.html>
3. Energetics, Structure, Mechanical and Vibrational Properties of Single Walled Carbon Nanotubes (SWNT)", by Guanghua Gao, Tahir Cagin*, and William A. Goddard III, [1997]
Location: http://www.wag.caltech.edu/foresight/foresight_2.html
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¹ School of Chemistry, Physics and Environmental Science, University of Sussex, Brighton BN1 9QJ, England UK
² Departamento de Física Teórica, Universidad de Valladolid, E-47011 Valladolid, Spain.
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Location: <http://www.msu.edu/~pfaffeli>

11. "Richard E Smalley's Homepage", Richard Smalley

Location: <http://cnst.rice.edu/reshome.html>

Image Gallery: <http://cnst.rice.edu/pics.html>

12. Lecture given at Michigan State University by Phaedon Avouris, a nanotube researcher at the IBM labs. [2000]

13. David Tomànek

Personal Web Site: <http://www.pa.msu.edu/~tomanek/tomanek.html>

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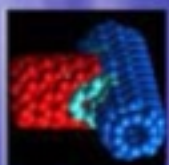
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24. Teri Wang Odom; Jin-Lin Huang; Philip Kim; Charles M. Lieber; *Nature* **391**, 6662, 62-64 (1998).

A@(n, m)	system A enclosed in an (n, m) nanotube
AFM	atomic force microscopy / atomic force microscope
CNT	carbon nanotube
DFT	density functional theory
DWNT	double-wall nanotube
EG	exfoliated graphite
ESR	electron spin resonance
FEM	field emission microscopy
GIC	graphite intercalation compounds
HREM	high-resolution electron microscopy
HRTEM	high-resolution transmission electron microscopy
ICP	inductively coupled plasma
IR	infrared spectroscopy
LDOS	local density of states
MR	magnetoresistance
MWNT	multi-wall nanotube
(n, m)	topological characterization of a nanotube by the chiral vector
SEM	scanning electron microscopy
SPM	scanning probe microscopy (includes STM, AFM, etc.)
STM	scanning tunneling microscopy
STS	scanning tunneling spectroscopy
SWNT	single wall nanotube
TGA	thermogravimetric analysis
XRD	x-ray diffraction

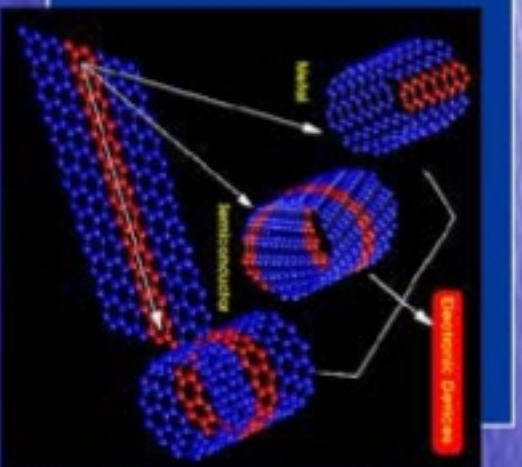


Carbon Nanotube

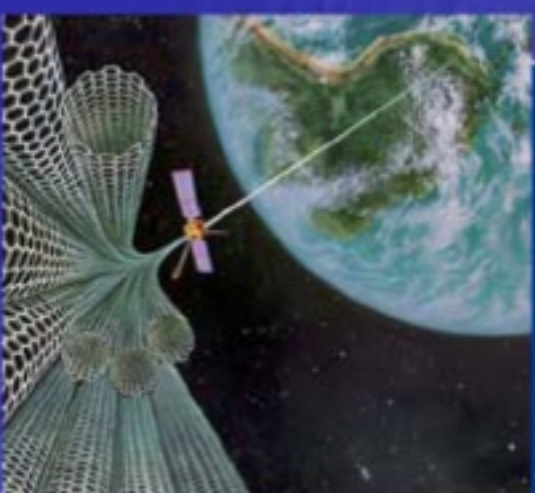
CNT is a tubular form of carbon with diameter as small as 1 nm.

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.

How Are They Made?

■ Arc Discharge

- Send a large current through graphite rods
- Carbon vaporizes and some of it reforms as nanotubes

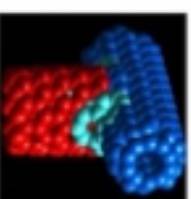
■ Chemical Vapor Deposition

- Pump carbon bearing gas into an oven with a substrate
- Carbon forms nanotubes on the substrate

■ Laser Generation

- Use a laser to superheat graphite rods and vaporize carbon
- Nanotubes form on a catalyst

NASA Ames Nanotechnology Research Focus



* Carbon Nanotubes

- Growth (CVD, PECVD)
- Characterization
- AFM tips
 - Metrology
 - Imaging of Mars Analog
 - Imaging Bio samples
- Electrode development
- Biosensor (cancer diagnostics)
- Chemical sensor
- Logic Circuits
- Chemical functionalization
- Gas Absorption
- Device Fabrication

* Molecular Electronics

- Synthesis of organic molecules
- Characterization
- Device fabrication

* Inorganic Nanowires

* Protein Nanotubes

- Synthesis
- Purification
- Application Development

* Genomics

- Nanopores in gene sequencing
- Genechips development

* Computational Nanotechnology

- CNT - Mechanical, thermal properties
- CNT - Electronic properties
- CNT based devices: physics, design
- CNT based composites, BN nanotubes
- CNT based sensors
- DNA transport
- Transport in nanopores
- Nanowires: transport, thermoelectric effect
- Transport: molecular electronics
- Protein nanotube chemistry

* Quantum Computing

* Computational Quantum Electronics

- Noneq. Green's Function based Device Simulator

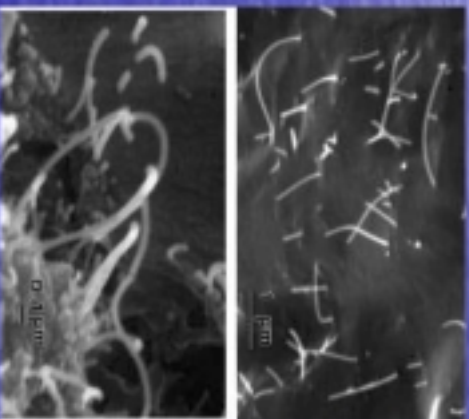
* Computational Optoelectronics

* Computational Process Modeling

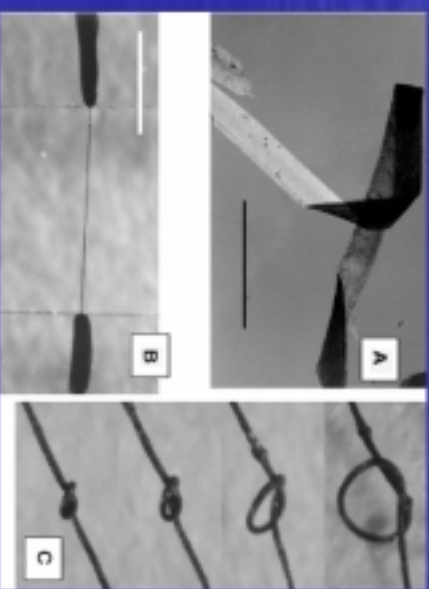
Polymer-CNT composite

- 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



High Thermal Expansion Coefficient Composite

Small system: $L/D \sim 2$, $N_p = 10$

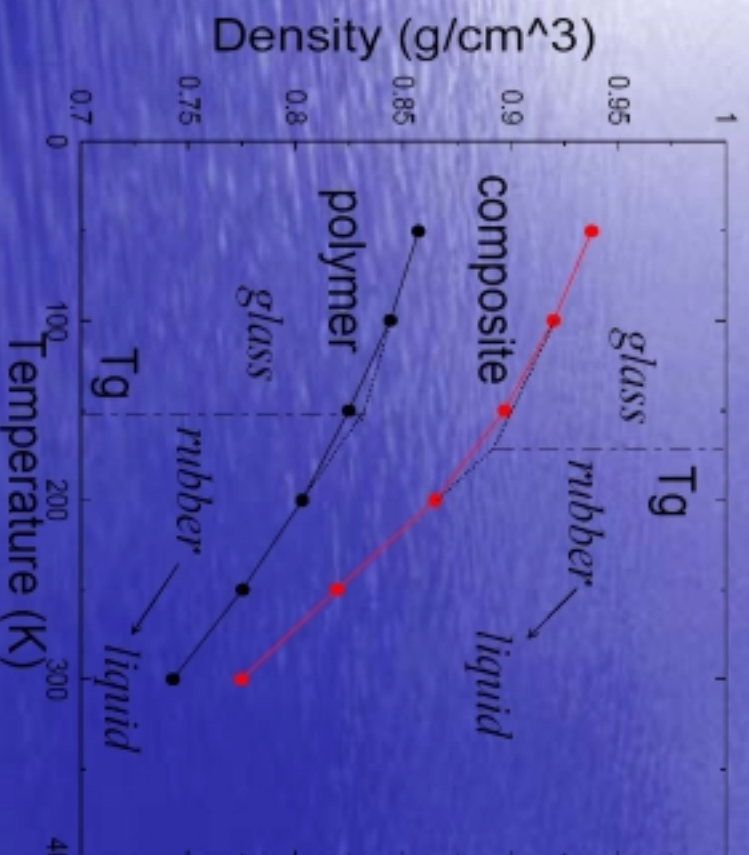
Results:

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

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

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

(Experimental value: $1.0 \times 10^{-4} K^{-1}$; $T < T_g$)



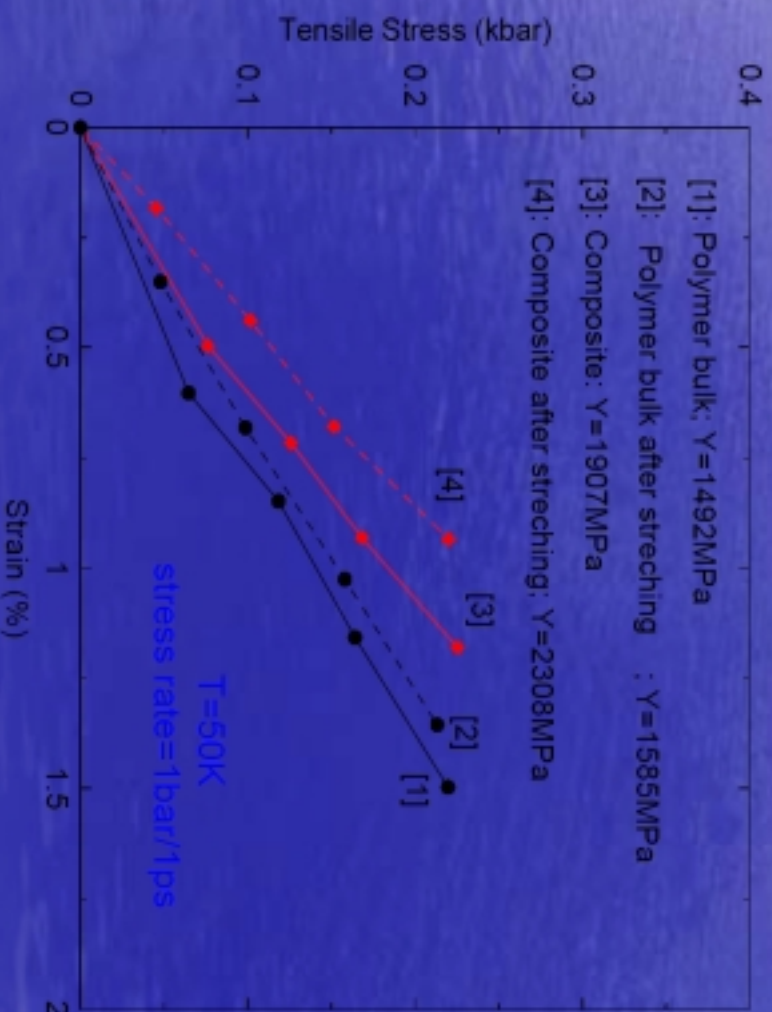


Young's Modulus



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

($L/D \sim 2$, $N_p = 10$)



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

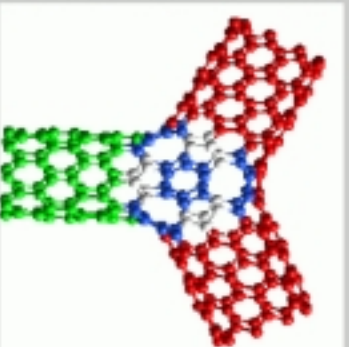
interconnects – Carbon/metal junctions



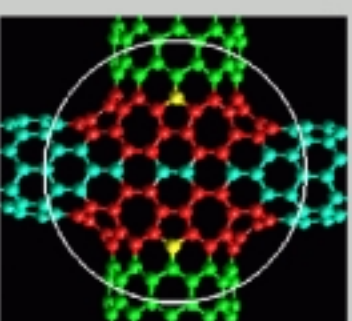
Nanotube Junctions for Devices



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"

VOLUME 75, NUMBER 22 PHYSICAL REVIEW LETTERS FEBRUARY 1995

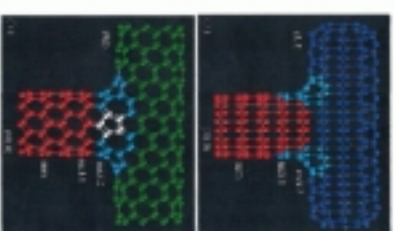


FIG. 1. STM images of a single carbon nanotube (left) and a Y-junction (right). The images were taken at a bias voltage of 1 V. The scale bar is 1 nm. The images were taken at a bias voltage of 1 V. The scale bar is 1 nm. The images were taken at a bias voltage of 1 V. The scale bar is 1 nm.

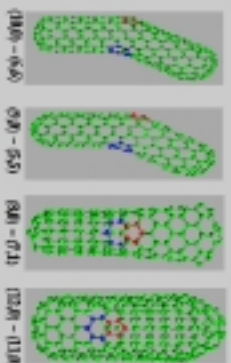


FIG. 2. LDOS of a Y-junction. The figure shows four panels (a, b, c, d) of the local density of states (LDOS) for different parts of the Y-junction. Panel (a) shows the LDOS for the central region, panel (b) for the top arm, panel (c) for the bottom arm, and panel (d) for the side arm. The x-axis is energy in eV, and the y-axis is LDOS in units of 1/eV.

LDOS of (10,0)-(9,0) "T-junction"

3-terminal "T-tunnel" Junctions of Nanotubes

2-point Nanotube Heterojunctions Molecular Electronic Switches



Bent Junctions

Straight Junctions

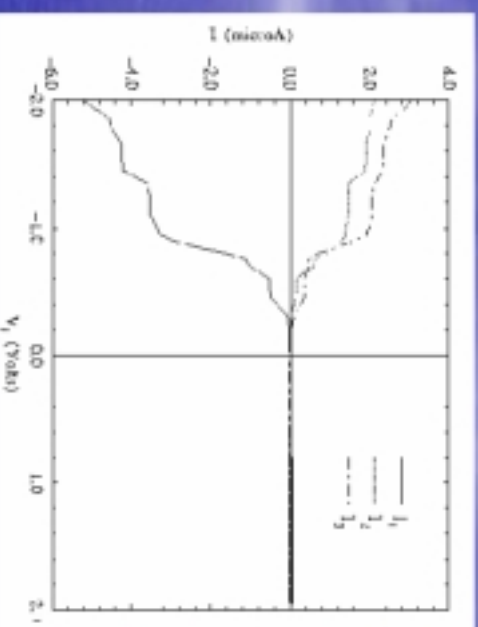
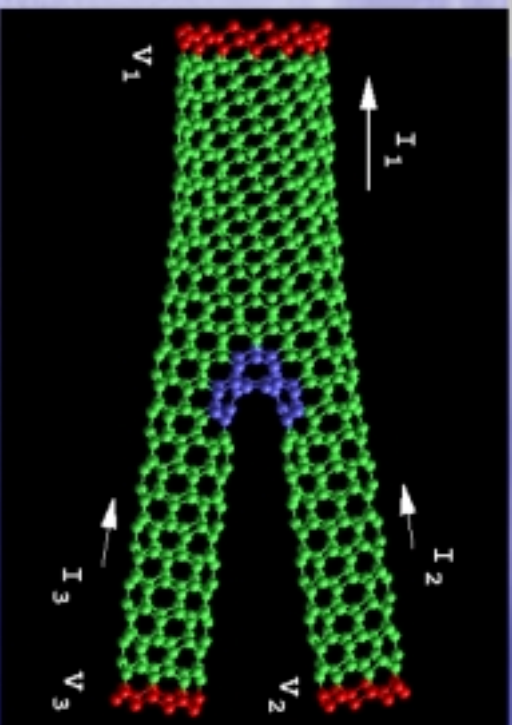
Chen et al. Phys. Rev. Lett. 76, 156
Chen et al. Phys. Rev. Lett. 76, 156
Lambert et al. Chem. Phys. Lett. 255
Suh et al. Phys. Rev. B, 96

We modeled the effect of coupling the tubes and reducing the junction with a quantum GTEM method.

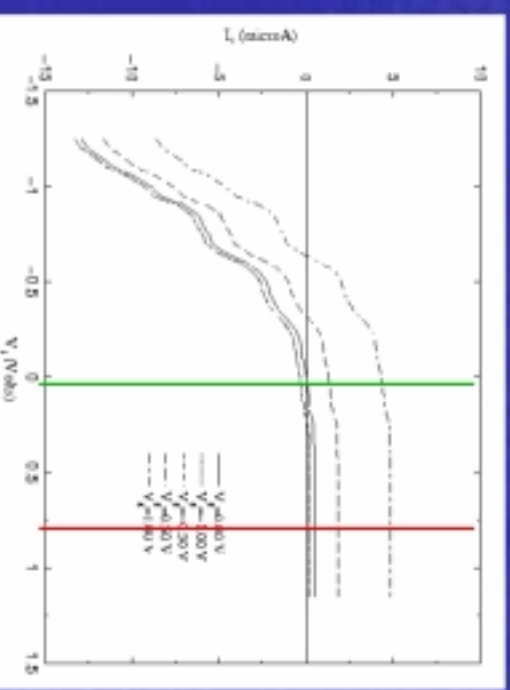
M. Menon and D. Srivastava, Phys. Rev. Lett. Vol. 74, 4453 (1997)

M. Menon and D. Srivastava, J. Mat. Res. Vol 13, 2357 (1998)

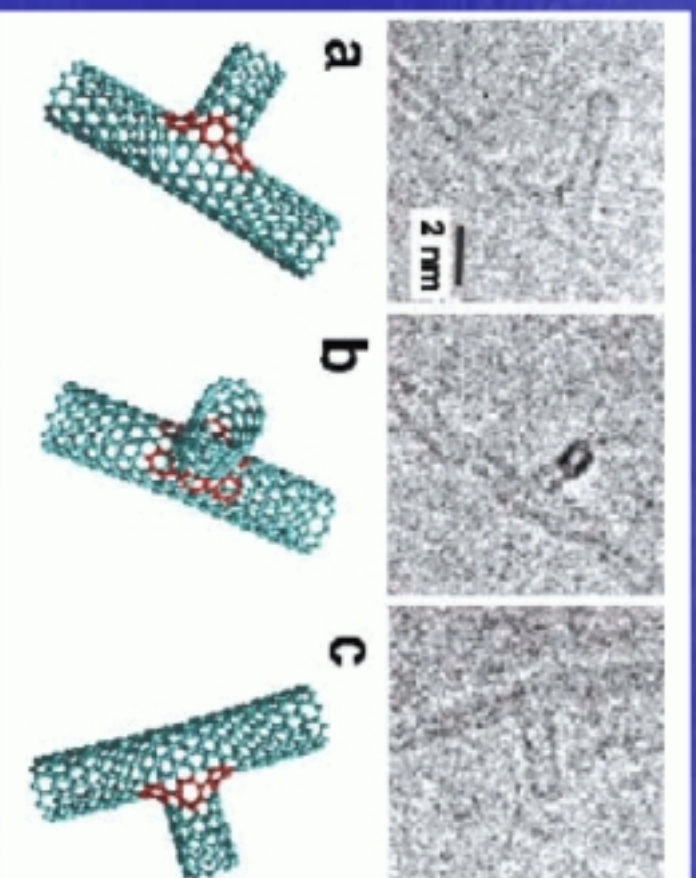
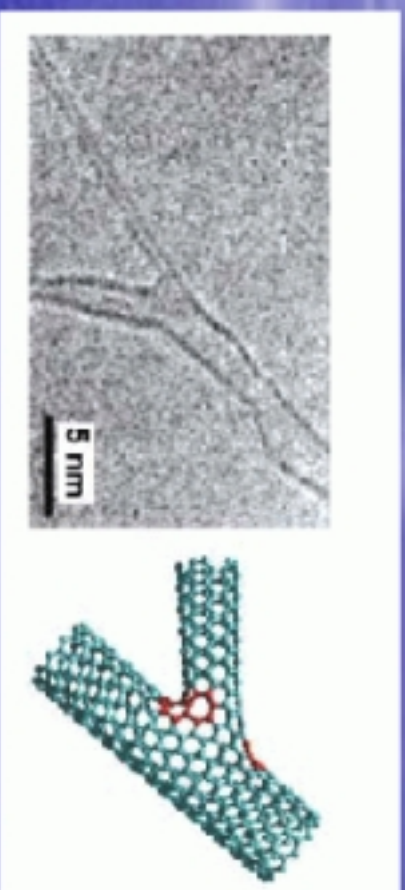
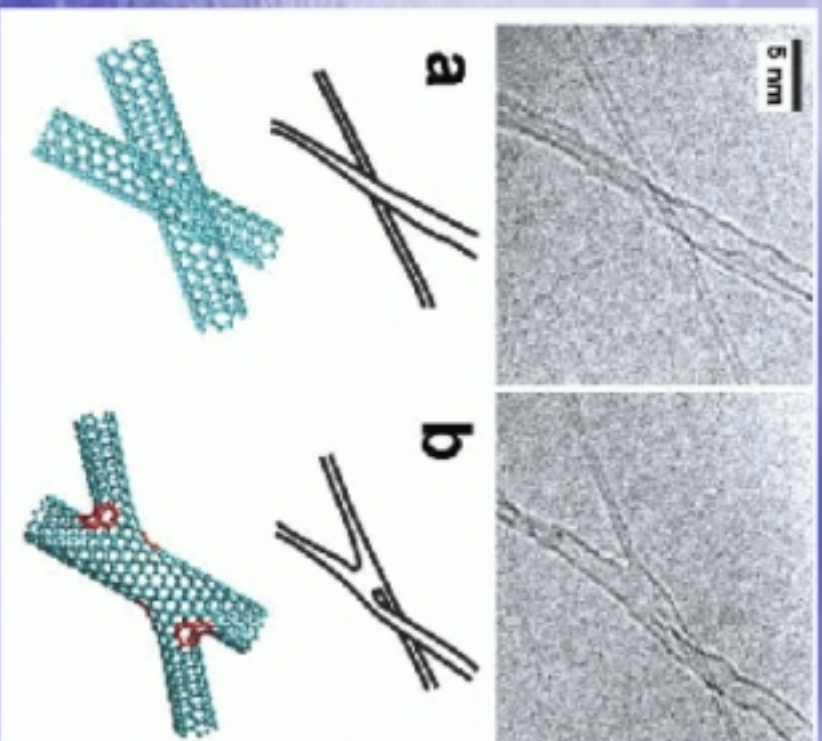
Rectification and Analog Logic Devices



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



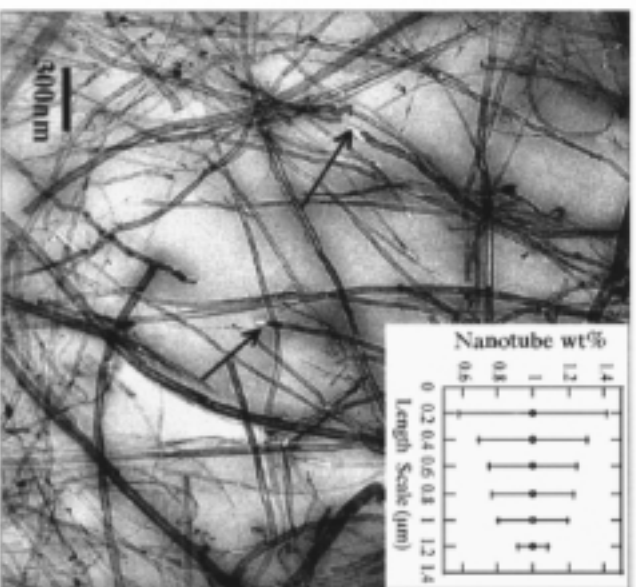
Single-wall Carbon Nanotube Junctions: Welding



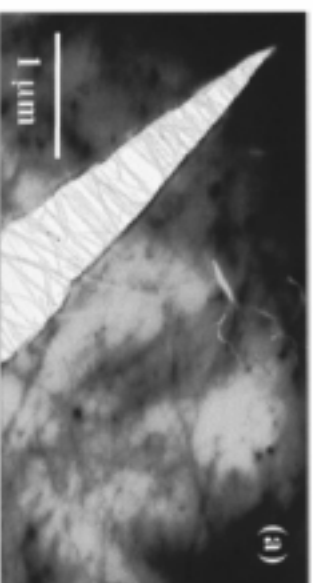
Terrones et. al., Phys. Rev. Lett.
12 August (2002)

Deformation in CNT-Polystyrene Composite

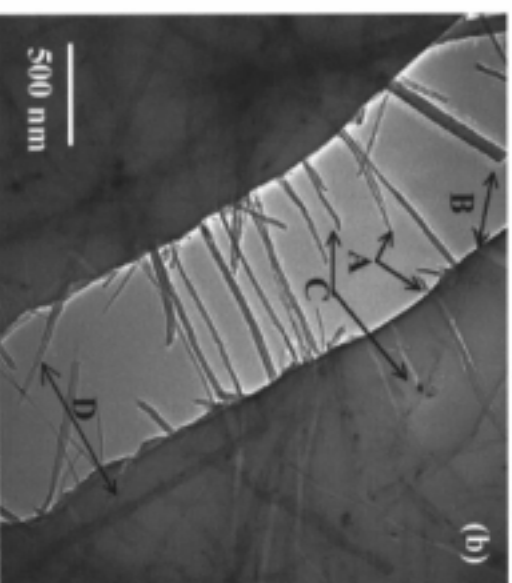
MWNT-PS composite sample
prepared by simple solution evaporation
assisted by sonication



- 1 wt% addition of NT
- 36-42% increase in elastic modulus
- ~25 increase in break stress



Crack nucleation
at low NT density
areas
Propagation
weak NT-PS
interface or
relatively low NT
density region



Bridging of crack
faces in the wake
Providing closure
stresses across
the crack faces.

What About Electronics?

- **Better Interconnects on Chips**
 - The high conducting capacity, temperature tolerance, and small size of nanotubes make them ideal for on chip wiring
- **Field Emission Properties**
 - Allows the creation of efficient flat panel displays
- **Field Effect Transistors (FETs)**
 - Transistors made with nanotubes appear to have properties comparable to current silicon devices
 - Miniaturization introduces the possibility of switching using much less power, allowing clock speeds of up to one terahertz

How are these FETs Made?

■ NTFET Geometry

- Initially the FETs were back gated, but this was inefficient
- Now they use a top gated design that is very similar to silicon MOSFETs

■ N or P type devices can be created

- CNFETs in air are p-type
- Doping with potassium, or exposure to vacuum can change the CNFET to n-type

■ Making Logic Gates

- NTFETs can be used to construct gates in the standard way
- Also, because of their ability to be p or n-type, multiple FETs, and therefore entire gates, can be made on one nanotube

So, what's the Problem?

■ Creating Nanotubes

- Extremely expensive processes
- Low yield
- Highly Heterogeneous product
- One gram of carbon nanotubes costs \$1,500

■ Creating FETs

- All the CNFETs created so far have been made "by hand"
- Manufacture is complex, involving both traditional lithography and high resolution tools
- For CNFETs to be viable new, more efficient manufacturing processes will be needed

1991 Discovery of multi-wall carbon nanotubes ["Helical microtubules of graphitic carbon", S. Iijima, Nature **354**, 56 (1991)]

1992 Conductivity of carbon nanotubes ["Are fullerene tubules metallic?", J. W. Mintmire, B. I. Dunlap and C. T. White, Phys. Rev. Lett. **68**, 631 (1992)]

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"Electronic structure of graphene tubules based on C₆₀", R. Saito, M. Fujita, G. Dresselhaus and M. S. Dresselhaus, Phys. Rev. B **46**, 1804 (1992)]

1993 Structural rigidity of carbon nanotubes ["Structural Rigidity and Low Frequency Vibrational Modes of Long Carbon Tubules", G. Overney, W. Zhong, and D. Tománek, Z. Phys. D **27**, 93 (1993)]

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"Cobalt-catalysed growth of carbon nanotubes with single-atomic-layer walls", D S Bethune, C H Kiang, M S DeVries, G Gorman, R Savoy and R Beyers, Nature, **363**, 605 (1993)]

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1997 Quantum conductance of carbon nanotubes ["Individual single-wall carbon nanotubes as quantum wires", SJ Tans, M H Devoret, H Dai, A Thess, R E Smalley, L J Geerligs and C Dekker, Nature, **386**, 474 (1997).]

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1998 Chemical Vapor Deposition synthesis of aligned nanotube films ["Synthesis of large arrays of well-aligned carbon nanotubes on glass", Z F Ren et al., Science, **282**, 1105 (1998).]

1998 Synthesis of nanotube peapods ["Encapsulated C60 in carbon nanotubes", B.W. Smith, M. Monthieux, and D.E. Luzzi, Nature **396**, 323 (1998).]

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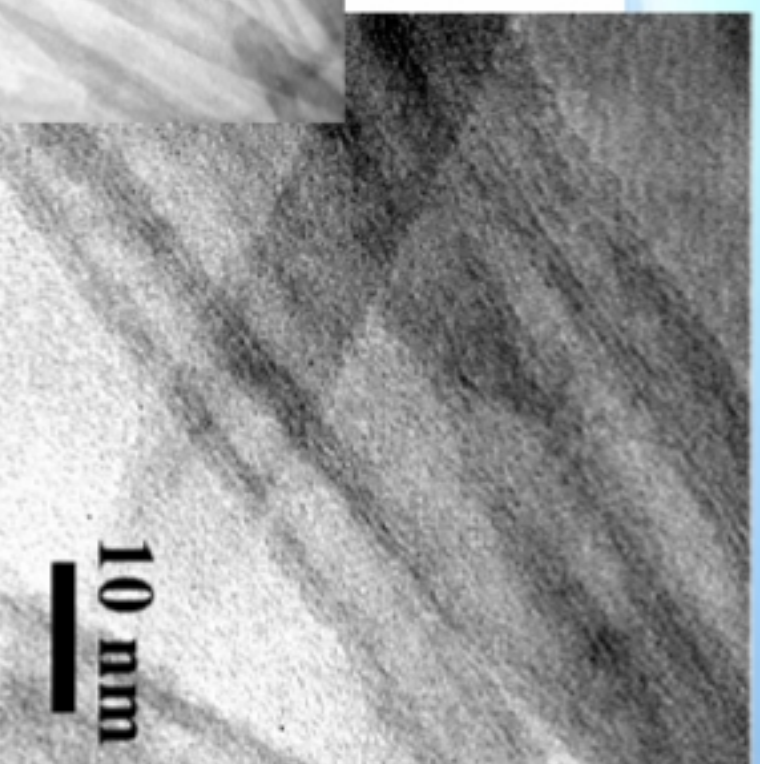
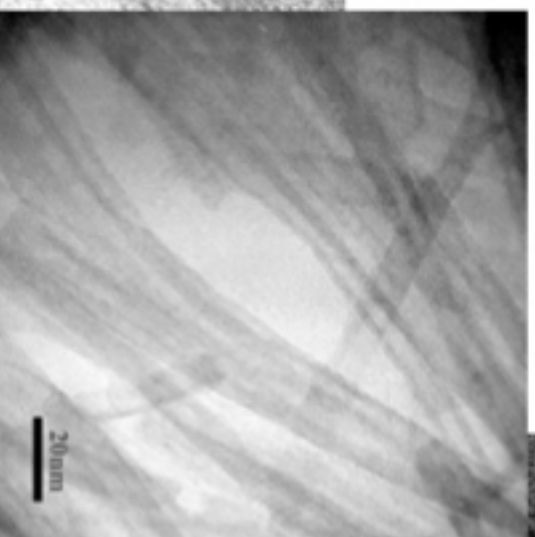
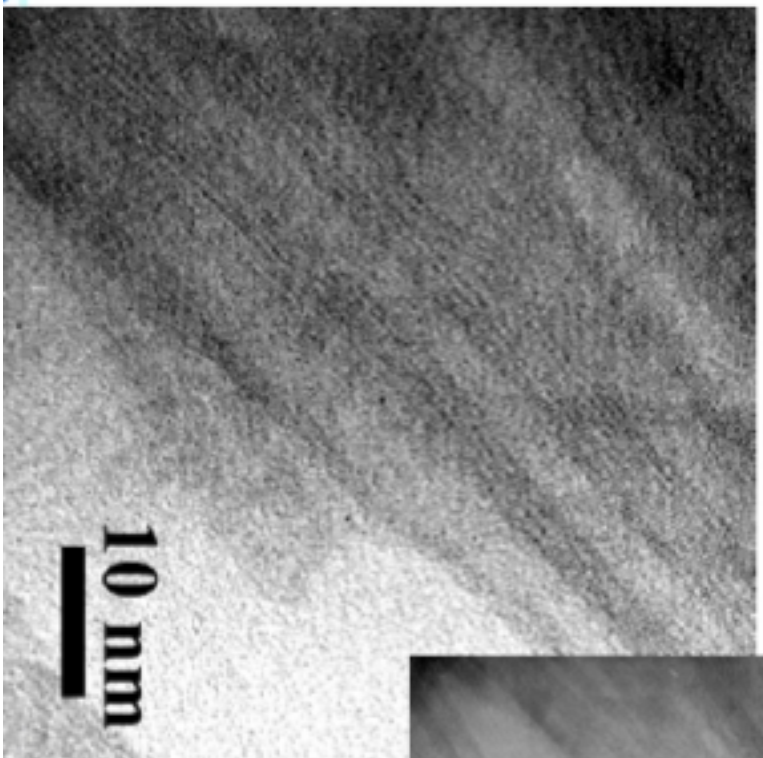
2000 Macroscopically aligned nanotubes ["Macroscopic Fibers and Ribbons of Oriented Carbon Nanotubes" , Brigitte Vigolo, Alain Pénicaud, Claude Coulon, Cédric Sauder, René Pailier, Catherine Journet, Patrick Bernier, and Philippe Poulin, Science **290**, 1331 (2000).]

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TiO_x nanotubes

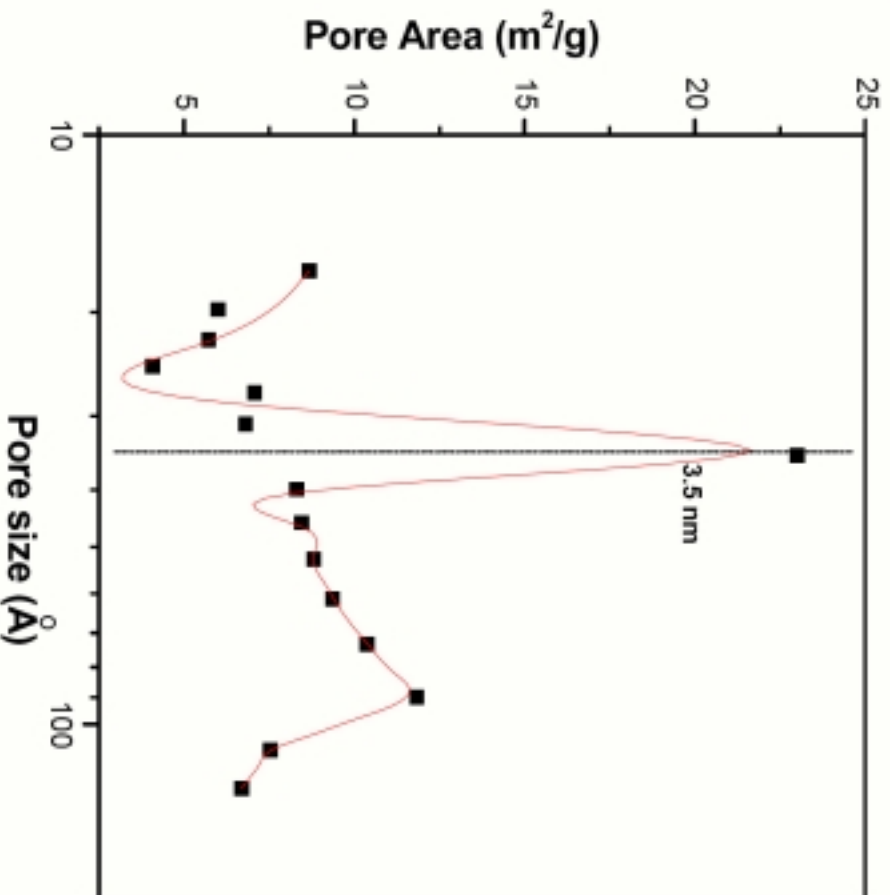
- Hydrothermal Synthesis
 - TiO₂ : 10 g/L
 - NaOH : 10M
 - 130°C, 24 hours



- Tube length : ~ 200 nm
- Outer Diameter : ~10 nm
- Inner Diameter : ~3 nm
- Surface area : 149 m²/g

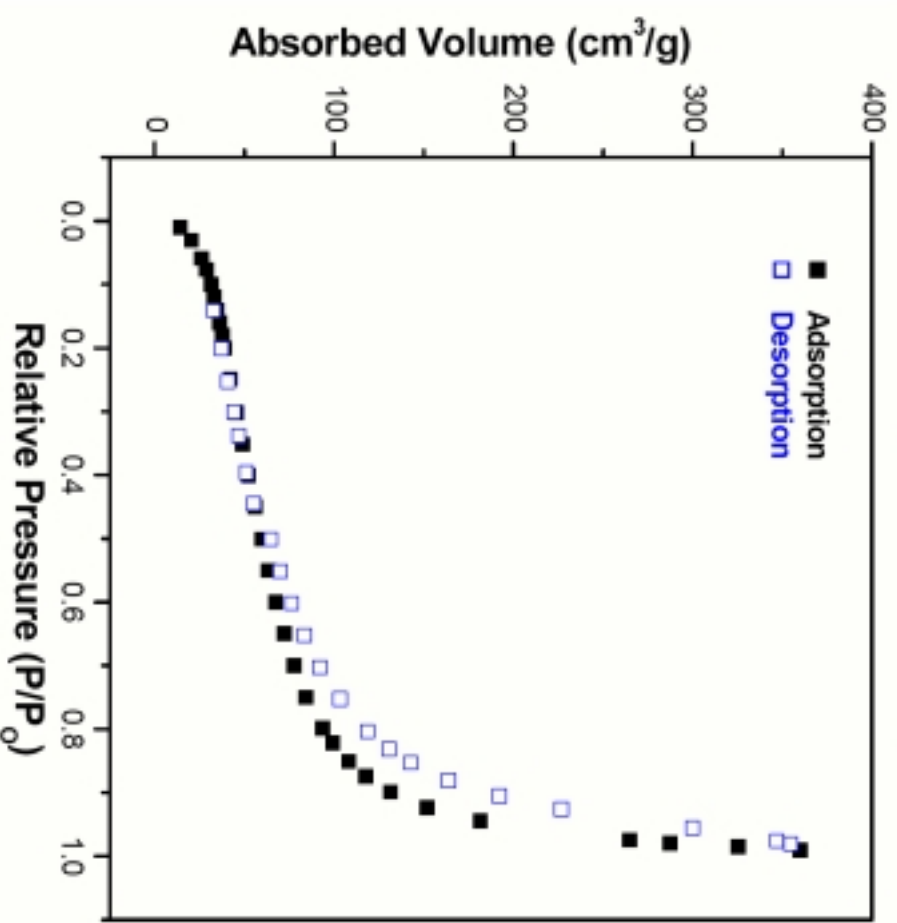
TiOx Nanotubes

• Pore size distribution



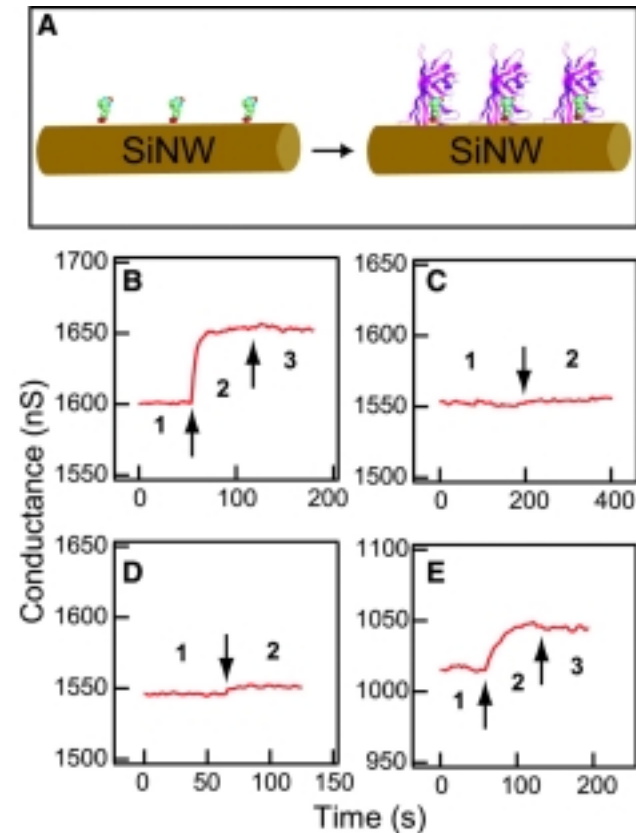
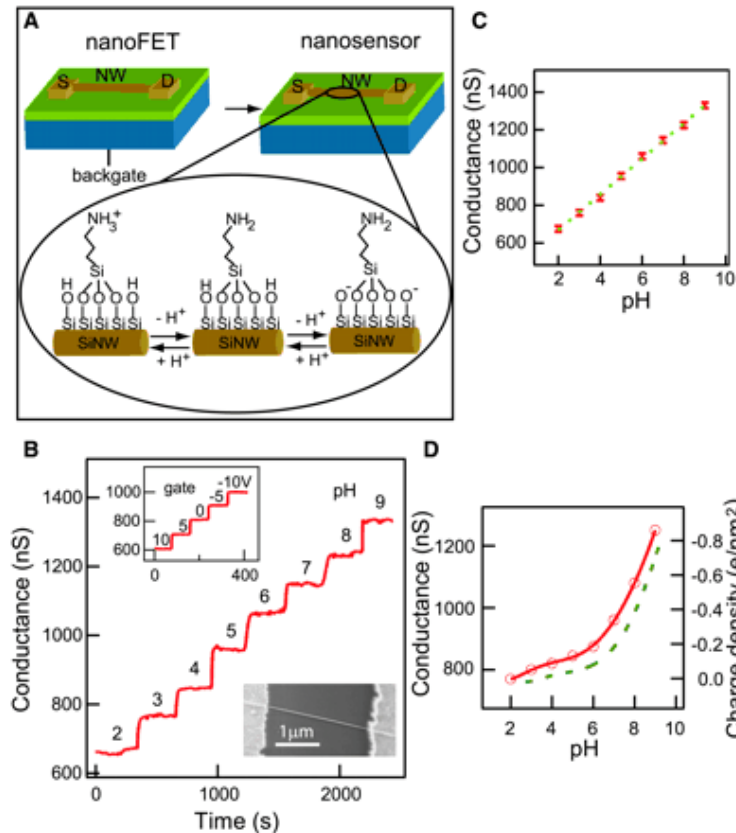
- BJH desorption method
- Maximum proportion: $\approx 3.5\text{nm}$
- Well matched with TEM micrograph

• Isotherm hysteresis loop

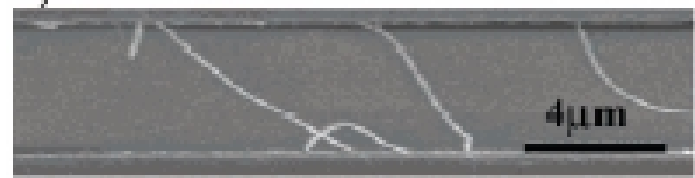
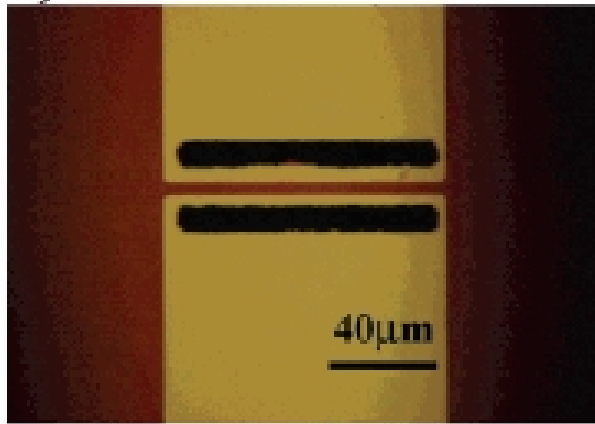


- Type IV : pore structure

Nanotube-based Chemical/Biological Sensors?



Cui, Lieber, etc. Science 2001



<http://msnbc-cnet.com.com/2100-1001-957709.html>

Nanowire or nanotube? Intel looks ahead

A good website for nanomaterials

www.mrs.org/gateway/matl_news_ext_2004a.html