The orientational order/disorder transition in buckminsterfullerene (C_{60}): an experiment using the NCNR Disk Chopper Spectrometer

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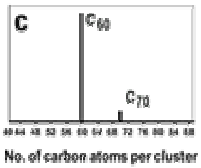
and Yiming Qiu

NIST Summer School 2005

Outline

- Carbon: don't we know everything?
  - Properties
  - Pretty Pictures
  - Applications and Interests
- How TOF works
  - Aims of the experiment
  - What other types of science is it useful for?

Finding C_{60}



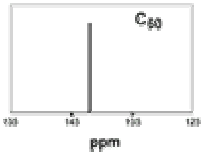
…whilst determining how carbon nucleates in the atmosphere of a cool carbon-rich red giant star

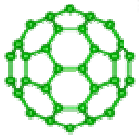

Robert F. Curl


Harold W. Kroto


Richard E. Smalley

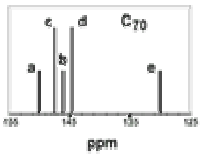
NMR Taylor, 1990

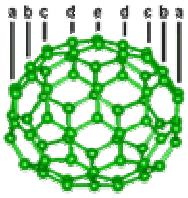




THE 1996 CHEMISTRY NOBEL PRIZE


© The Nobel Foundation.

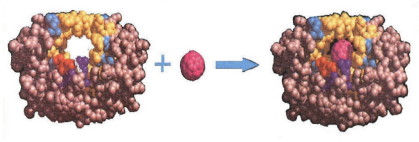




Interest and Uses

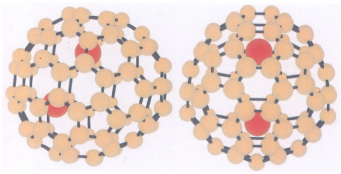
Kratschmer & Huffman 1990

HIV Protease Inhibitor



Friedman, UC San Francisco

$Sc_2@C_{84}$



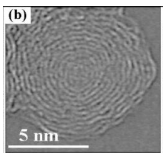
Shinohara

Superconductivity

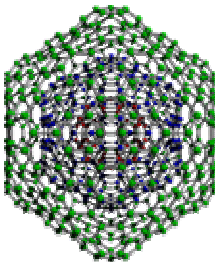
Magnetism

Lubricants

Onions



Thune, PRB, 68, 5434

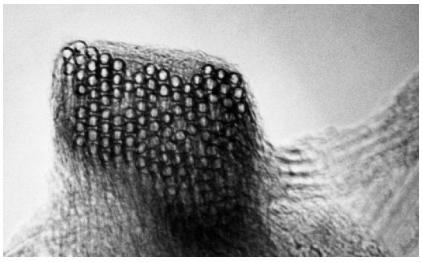


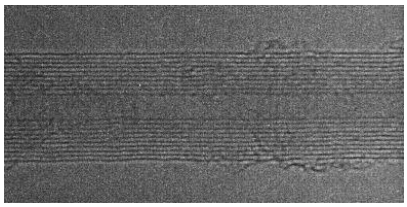
C_{60} inside C_{240} inside C_{540}

Heggie, Uni. Sussex

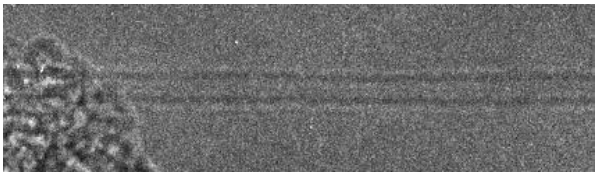
Subsequently

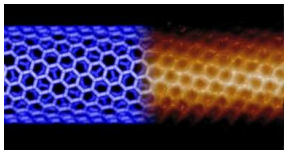
Carbon Nanotubes discovered by Sumio Iijima in 1991





TEM multi-walled tube

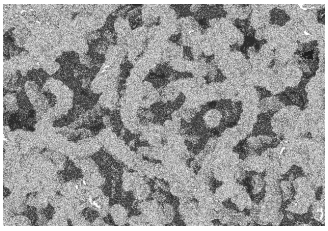




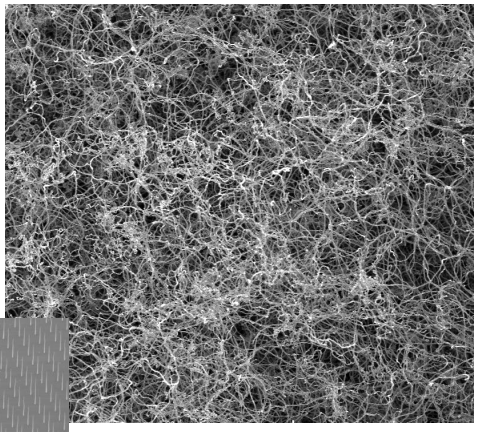
TEM/AFM single-walled tube

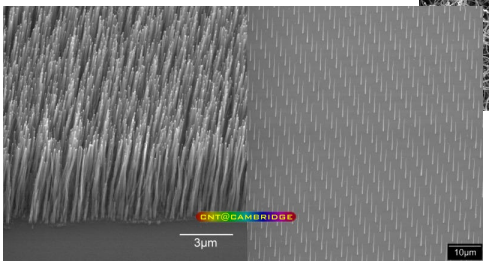
Zettl group, Berkeley
Smalley, Rice

Nanotubes



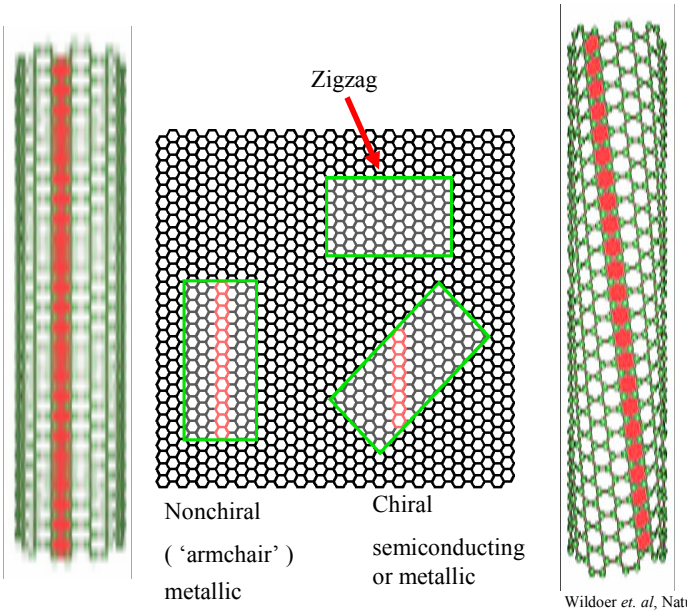
Wang, in preparation





Forro, Europhysics News (2001) Vol. 32 No. 3

Nanotubes



Nonchiral

('armchair')

metallic

Chiral

semiconducting or metallic

Wildoer *et. al*, Nature 391, 59 (1998)

Odom *et. al*, Nature 391, 62 (1998)

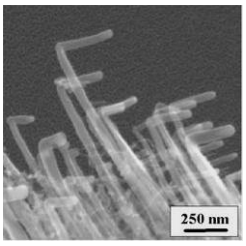
Electronics

Nanotube Quantum Wires
NASA → $11M to Rice

Motorola's 5" flat panel nanotube display. 1/8" thick

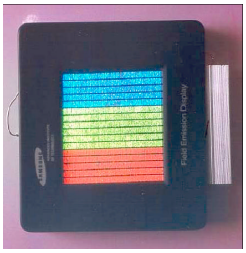
Diodes and Transistors for computing

Data storage



Jin UCSD

Springs
tips for atomic force microscopes, smaller electrical connectors in integrated circuits



Choi et al. APL, 1999

field-emission displays

Applications

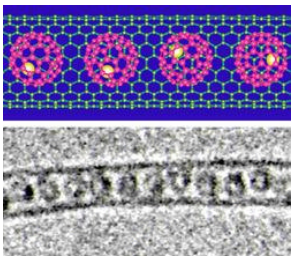
High Strength Composites

Heat exchangers

Membranes, supports

Body Armor

Molecular gears, motors etc.



Sensors- force, pressure, chemical

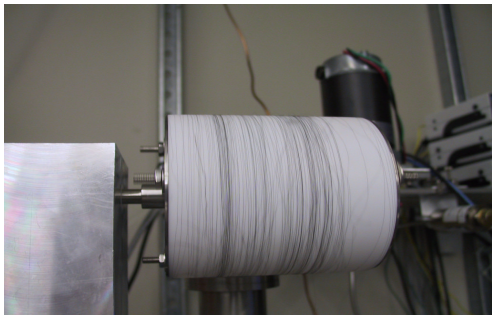
Catalysis, high surface area

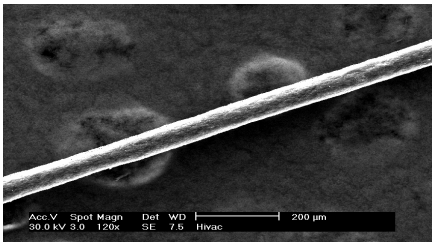
Batteries, Fuel Cells

Hydrogen, Lithium Storage

Even more out there...

Carbon nanotubes: measured at 200 GPa (54xKevlar)





Fiber Spinning in Progress Close-up

Smalley, Rice

Even more out there...

"Technically it's feasible," said Robert Cassanova, director of the NASA Institute for Advanced Concepts. "There's nothing wrong with the physics."

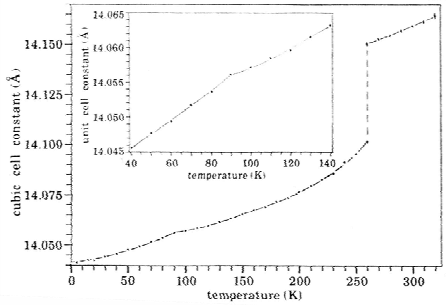
David Raitt, senior technology transfer officer for the European Space Agency, believes the question is not whether to build a space elevator, but only how long it will take.

- Artsutanov, Y. **1960**. V Kosmos na Elektrovoze, Komsomolskaya Pravda, (contents described in Lvov 1967 Science 158:946).
- Isaacs, J.D., Vine, A.C., Bradner, H., and Bachus, G.E. **1966**. Satellite Elongation into a true 'Sky-Hook'. Science 151:682.
- Pearson, J. **1975**. The Orbital tower: a spacecraft launcher using the Earth's rotational energy. Acta Astronautica 2:785.
- Clarke, A.C. **1979**. The Space Elevator: 'Thought Experiment', or Key to the Universe. Adv. Earth Oriented Appl. Science Techn. 1:39.

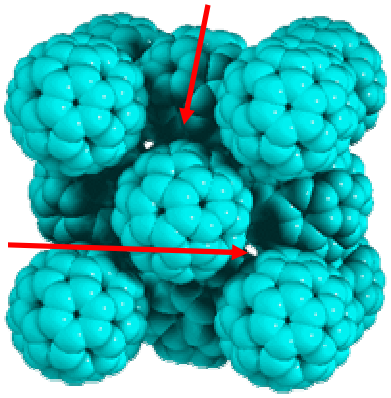
LiftPort Group, the space elevator companies, today announced plans for a carbon nanotube manufacturing plant, the company's first formal facility for production of the material on a commercial scale.

PRESS RELEASE
Date Released: Monday, April 25, 2005
Source: Liftport

Properties of C_{60}

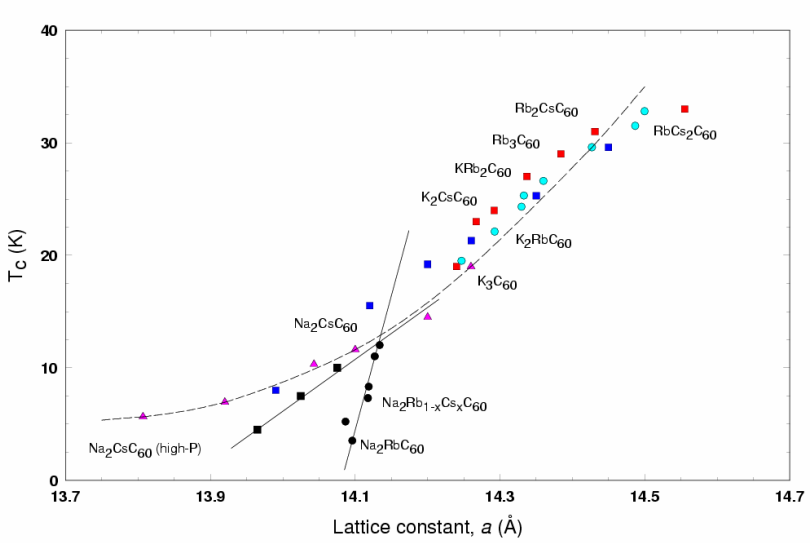


OCTAHEDRAL
2.06 Å

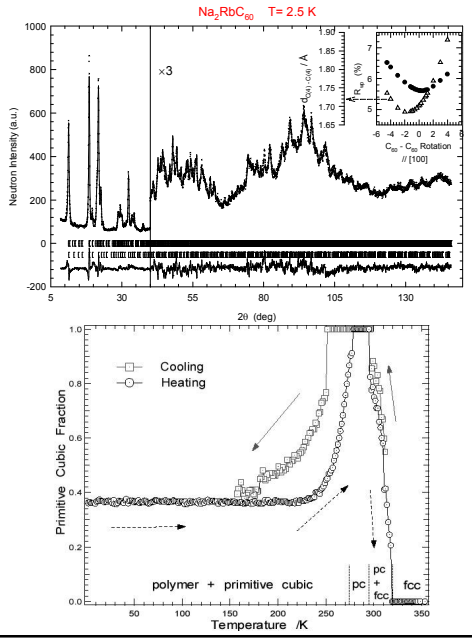


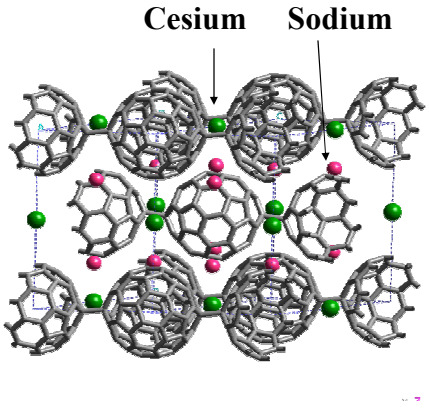
TETRAHEDRAL
1.12 Å

Alkali Metal Intercalation



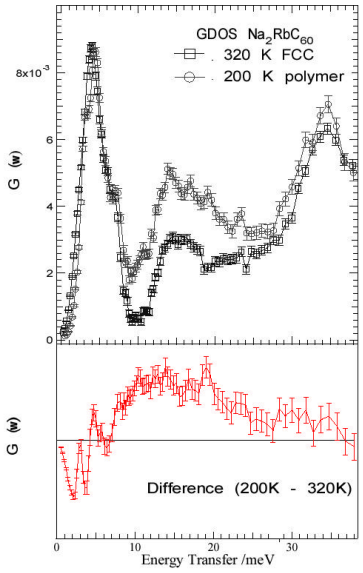
Polymer Complications





Lappas, Brown, 1999, 2000

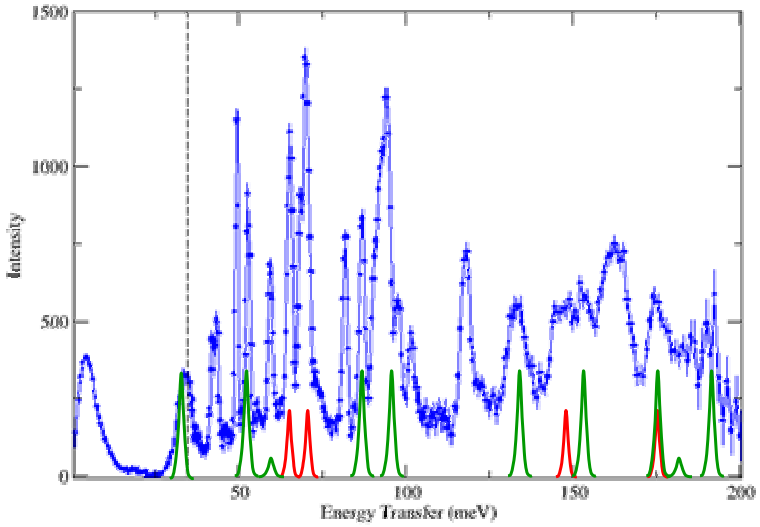
Complications



Nemes 2003, Brown, 2000

Aside: What are those peaks?

$2A_g+Au+3T_{1g}+4T_{1u}+4T_{2g}+5T_{2u}+6G_g+6G_u+8H_g+7H_u$



Nemes 2003, Brown, 2000

AIMS

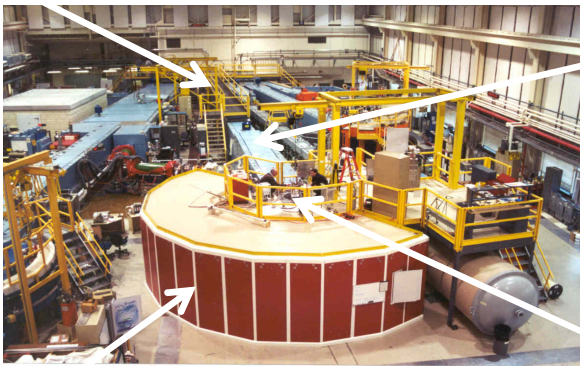
- Experience Practical TOF spectroscopy
  - sample choice
  - geometry consideration
- Learn something about the instrument
  - Wavelength / Resolution / Intensity
- Data Reduction
- Data Analysis and Interpretation
  - instrument resolution function and fitting
  - extract EISF and linewidth
  - spatial and temporal information

In particular

- Above 260 K
  - Determine the Q-dependence of the quasielastic scattering. (Extract timescales/activation energy)
- On cooling through the phase transition
  - Monitor the diffraction pattern as function of Temp.
- Below 260 K
  - Compare g(ω) to FANS data
  - Compare libration intensities to a SHO
  - Estimate the activation energy for rotational jumps

TOF spectroscopy, *in practice*

(1) The neutron guide

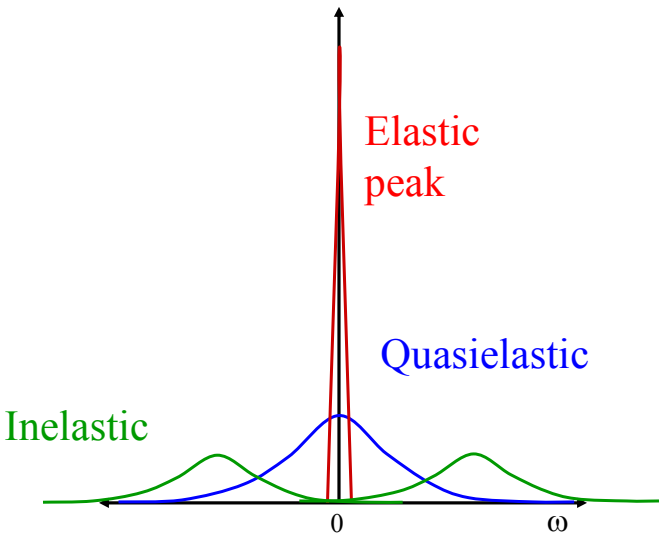


(2) The choppers

(3) The sample area

(4) The flight chamber and the detectors

Total Scattering



Types of Experiments

- Translational and rotational diffusion processes, where scattering experiments provide information about time scales, length scales and geometrical constraints; the ability to access a wide range of wave vector transfers, with good energy resolution, is key to the success of such investigations
- Low energy vibrational and magnetic excitations and densities of states
- Tunneling phenomena

- **Chemistry** --- e.g. clathrates, molecular crystals, fullerenes
- **Polymers** --- bound polymers, glass phenomenon, confinement effects
- **Biological systems** --- protein folding, protein preservation, water dynamics in membranes
- **Physics** adsorbate dynamics in mesoporous systems (zeolites and clays) and in confined geometries, metal-hydrogen systems, glasses, magnetic systems
- **Materials** --- negative thermal expansion materials, low conductivity materials, thermo-electrics, hydration of cement, carbon nanotubes, proton conductors, metal hydrides