Presentation/Publication Information:
An invited talk to be given by Deepak Srivastava of the Computational Nanotechnology task at the monthly Silicon Valley Computer Club gathering on 17th March, 1999 at 8, Almandra Lane, Los Altos, CA. A copy of the presentation is attached.

Acknowledgments:
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Abstract:
An invited talk to review the status of the progress in Nanotechnology, based on publicly available, already presented and/or published material. The copy of the slides are enclosed. No abstract was required or submitted for this presentation.
Carbon based Nanotechnology Review

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- Concept: Feynman’s postulate
- Vision: Molecular Assemblers
- Progress in Microtechnology

Collaborators:
- Madhu Menon — University of Kentucky
- Dan Hren — North Carolina State University
- Rod Nash — University of Washington, St. Louis
- K. I. Cho — Stanford University

Research Focus

Nanotube - Nanomechanics

- Nanotubes are extremely strong highly elastic nanofibers
  - high value of Young modulus over 1.2 TPa
- Dynamic response of nanotubes to holistic deformation
  - axial compression, bending and torsion

Axial Compression

Bending

Torsion

- redistribution of strain
  - sharp buckling leading to bond rupture
SEM images of MWNTs dispersed on a V-ridge substrate

(a) Before Reaction

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


Research Focus II
Carbon based Electronics

Experimetal Status

Individual Single Wall Nanotubes as Quantum Wire
S. J. Tans et al., Nature (April, 97)

- Nanotube Nanodevice - showing localized rectifying behavior in the IV characteristics
  P. G. Collins et al., Science (October, 97)

- IV Characteristics and Electronic Structure (DOS) of structurally nanotubes
  J. W. G. Wilden et al., Nature (January, 98)
  T. W. Oyama et al., Nature (January, 98)

- Single nanotube-molecule transistor at room temp.
  S. J. Tans et al., Nature (May, 98)

- Nanofabricating cutting of nanotubes with STM
  L. C. Venema et al., Appl. Phys. Lett. (Nov, 97)
sections

Carbon Nanotube Electronics Band Structure (basics)

Hexagonal Lattice of a Graphene Sheet (~Chirality)

First Brillouin zone for an armchair tube.

Chemical vector $a_2$

Topological Defect: Hetero-Junctions I

2-point Nanotube Heterojunctions

Molecular Electronic Switches

Chico et al. Phys. Rev. Lett. 96
Charlier et al. Phys. Rev. B 96
Lambert et al. Chem. Phys. Lett. 96

We studied the effect of capping the tubes and relaxing the junctions with a quantum DFT/BNNM method.
Topological Defects: Heterojunctions II

J-terminal "T-tunnel" Junctions of Nanotubes

Topological Defects: Heterojunctions III

Pathways to Three-Dimensional Molecular "Networks"

Metal-Semiconductor-Metal
"Y" Tunnel Junction - A four-terminal nanotube heterojunction

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


These are "ideal" junctions and we don't know how to make these...

Some work is in progress to conceptualize and test "real" junctions.

CxByNz Nanotubes and Junctions I

- Hand gap engineering over a larger range should be possible:
  - BN = -5.5 eV
  - BC$_3$N = -2.0 eV
  - C = -0.1 eV
  - BC$_3$ = -0.5 eV
- A variety of junctions, quantum dots and superficies should be possible
- Should be more robust

- Example: Composite (10,0) nanotube
  - 0.34 eV/atom
  - 0.46 eV/atom
  - 0.17 eV/atom

C  BN  BC$_3$  N

Topological Defects: Heterojunctions II

B doping of Carbon Nanotube

Random  Island (BC3)  Superlattice (BC3)

0.000  -0.018  -0.016 eV/atom

Phase separation of doped and undoped regions is thermodynamically stable!

- BN/C Junctions

- Interface Energy = 2.5 eV/N
- Stable interfaces should be possible!
Comments:

- Proposed "new" nanotechnology materials and devices.
  - multiple nanotube junctions and networks
  - H, N doping, interfaces and tips

Tested feasibility of "new" concepts:
- Conformational strain driven mechanical - kink chemistry is certainly a new way to do site specific reactions on side-walls.
- Feasibility of H storage in nanotube based material

Future possibilities are bright:

Mechanical

Chemical

Electronic

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