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.

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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 Florida
- Dan Bruner — North Carolina State University
- Rod Rest — University of Washington, St. Louis
- K. L. Cho — Stanford University

Research Focus

Nanotube - Nanomechanics

- Nanotubes are extremely strong highly elastic nanofibers
  - high value of Young's modulus ~ 1.2 TPa

- Dynamic response of nanotubes to ballistic deformation
  - axial compression, bending and torsion

Axial Compression

Bending

Torsion

- redistribution of strains
- sharp buckling leading to bond rupture
Energetics of Mechanical Deformation

Compression

Semi-Energy (eV/atom)

16% strain

10 20 30

Time (ps)

Bending

90 deg fold

Time (ps)

Torsion

720 deg twist

Nitrogen Energy

Mechanism of Strained induced chemisorption

Unstrained

DOS

Bent

Bent after H adsorption

Torsionally twisted SWNT equilibrated in an H bath
Nano Mechano-Chemistry III

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


Nano Mechano-Electronics I

Mechanical deformations alter the Electronic Characteristics of Nanotubes

Nano mechano-electronics effects are "strong" dependent on the "flexibilities.

Nano Mechano-Electronics II

Example: bending and torsion of arm-chair (1,10) nanotube

Bending

Torison

Research Focus II

Carbon based Electronics

Experimental Status

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

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

- UV Characteristics and Electronic Structure (DOS) of structurally nanotubes
  J. G. Wilks et al., Nature (January, 98)
  T. W. Olson et al., Nature (January, 98)

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

- Nanofosturizing -- cutting of nanotubes with STM
  L. C. Venema et al., Appl. Phys. Lett. (Nov, 97)
Carbon Nanotube Electronics Band Structure

Carbon Nanotube Electronics Band Structure (basics)

Hexagonal lattice of a graphene Sheet = (Chiral cell)

First Brillouin zone for an armchair tube.

Chiral vector

Topological Defect: Heterojunctions

2-point Nanotube Heterojunctions

Molecular Electronic Switches

Bent Junctions

(10.0 - 16.0)

(9.0 - 15.5)

(12.0 - 11.0)

Straight Junctions

(8.0 - 7.1)

Chato 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 STBVID method.
Topological Defect: Heterojunctions II

J-terminal "T-tunnel" Junctions of Nanotubes

Topological Defects: Heterojunctions III

Pathways to Three-Dimensional Molecular "Networks"

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

- V. Crespi, Phys. Rev. Lett. (98)

There are "ideal" junctions and we don't know how to make these:

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

C_xB_yN_z Nanotubes and Junctions I

- B doping of Carbon Nanotube

C_xB_yN_z Nanotubes and Junctions II

- BN/C Junctions

Example: Composite (10,0) nanotube

- Band gap engineering over a larger range should be possible
- BN = 5.5 eV
- BC_3N = 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

0.0 eV/atom 0.05 eV/atom 0.15 eV/atom

reconstruction for in-plane F-V bond

Interface Energy = 2MgC - BN - C
Interface Energy = 0.3 eV/F bond

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 - kinked - 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