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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Research Focus

- Nanobehavior/materials
- Carbon based electronics
- Nanodevice/Materials Applications
- BeCu34 Nanotubes
- Nanotube-Motor
- Nanolithography
- H2 Nucry in nanotubes

Nanotube - Nanomechanics

- Nanotubes are extremely strong highly elastic nanofilbers
  - high value of Young modulus Swat - 1.2 TPa
- Dynamic response of nanotubes to holistic deformation
  - axial compression, bending and torsion
  - redistribution of strain
  - sharp buckling leading to bond rupture
Energetics of Mechanical Deformation

Compression

- Single Wall
- Multi-Wall

16% strain

Bending

- Single Wall
- Multi-Wall

90 deg fold

Torsion

- Single Wall
- Multi-Wall

720 deg twist

Time (ps)

Predictions of enhanced chemical reactivity in regions of local conformational strain: Kinky Chemistry

Kink on a bent tube

Ridge on a twisted tube

Kinky Chemistry

Mechanism of Strained induced chemisorption

Unreacted

Reacted

DOS

Bandgap (eV)

Part (eV)
Nano Mechano-Chemistry

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

Mechanical deformations alter the electronic characteristics of nanotubes.

Nano mechanic-electronic effects are "strength" dependent on the nanotubes.

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 IV characteristics
  P. G. Collins et al. Science (October, 97)

- IV Characteristics and Electronic Structure (DOS) of structurally nanotubes
  J W G Wildor 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)

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

Hexagonal lattice of a graphene sheet (Chapell-cell)

First Brillouin zone for an armchair tube.

Topological defect: Heterojunctions I

2-point Nanotube Heterojunctions
Molecular Electronic Switches

Bent Junctions
Straight Junctions

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 DFTBMD 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 satisfy Generalized Euler's Rule about the global topology of connected networks.)
- V. Crespi, Phys. Rev. Lett. (88)

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 Juncions I

- Band gap engineering over a larger range should be possible:
  - BN: -5.5 eV
  - BC_N: 2.0 eV
  - C: -9.1 eV
  - Br: -9.5 eV
- a variety of junctions, quantum dots and superlattices should be possible
- should be more robust

- Example: Composite (10,0) nanotube
  - BN: 0.56 eV/atom
  - BC_N: 0.21 eV/atom
  - C: 0.17 eV/atom

CxByNz Nanotubes and Juncions II

- B doping of Carbon Nanotube

  Random
  Random
  Random

  Isolated (BC_N)
  Isolated (BC_N)
  Isolated (BC_N)

  C
  BC_N
  BN

  Random
  Random
  Random

  Superlattice (BC_N)
  Superlattice (BC_N)
  Superlattice (BC_N)

  C
  BC_N
  BN

- BN/C Junctions

  Interface Energy = 25 mJ/m^2
  Interface Energy = 45 mJ/m^2

  Stable interfaces should be possible!
**Comments:**

Proposed "new" nanotechnology materials and devices.
- multiple nanotube junctions and networks
- B, 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**