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

Research Focus

-  Nanomechanics/Materials
-  Carbon Based Electronics
-  Nanodevice/Materials Applications
-  BeC60 Nanotubes
-  Nanotube-Motor
-  Nano-Lithography
-  H2 Nanotube in nanotube

Nanotube - Nanomechanics

- Nanotubes are extremely strong, highly elastic nanofibers
  - high value of Young modulus swat — 1.2 TPa
- Dynamic response of nanotubes to ballistic deformation
  - axial compression, bending and torsion
  - redistribution of strain
  - sharp buckling leading to local rupture
**NanoTube-Nanomechanics**

Energies of Mechanical Deformation:

- Compression
- Beating
- Tension

**NanoMechano-Chemistry I**

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

**NanoMechano-Chemistry II**

- Torsionally twisted SWNT equilibrated in an H bath

**NanoMechano-Chemistry III**

- Mechanism of Strained induced chemisorption
- Unstrained
- Bound
- DOS
- Bound after H absorption
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 interfacial properties

Nano Mechano-Electronics II

Example: bending and torsion of armchair (1,10) nanotube

Bending

Torsion

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. G. Collins et. al. Science (October, 97)

- UV Characteristics and Electronic Structure (DOS) of structurally nanotubes
J. W. Wilder et. al., Nature (January, 98);
T. W. Odom et. al., Nature (January, 98)

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

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

Topological Defect: Hetero-Junctions I

2-point Nanotube Hetero-junctions
Molecular Electronic Switches

We studied the effect of capping the tubes and relaxing the junctions with a quantum STBSE 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.

- 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\textsubscript{x}B\textsubscript{y}N\textsubscript{z} Nanotubes and Junctions I

- Band gap engineering over a larger range should be possible:
  - BN: -5.5 eV
  - BC\textsubscript{3}N: -2.0 eV
  - C: -0.1 eV
  - BC\textsubscript{3}: -0.5 eV
- a variety of junctions, quantum dots and superfibers should be possible
- should be more robust

- Example: Composite (10,0) nanotube
  - 0.1 eV/atom
  - 0.36 eV/atom
  - 0.17 eV/atom

C\textsubscript{x}B\textsubscript{y}N\textsubscript{z} Nanotubes and Junctions II

- B doping of Carbon Nanotube

- BN/C Junctions
  - Interface Energy = 2.6 eV
  - BN - C Interface Energy = 0.3 eV:C-B bond
  - 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