Why Nanotechnology at NASA?

- Advanced miniaturization, a key thrust area to enable new science and exploration missions
  - Ultrasmall sensors, power sources, communication, navigation, and propulsion systems with very low mass, volume and power consumption are needed
- Revolution in electronics and computing will allow reconfigurable, autonomous, "thinking" spacecraft
- Nanotechnology presents a whole new spectrum of opportunities to build device components and systems for entirely new space architectures
  - Networks of ultrasmall probes on planetary surfaces
  - Micro-rovers that drive, hop, fly, and burrow
  - Collection of microspacecraft making a variety of measurements

NASA Ames Nanotechnology Program

- Started in FY 97, currently about 25 FTEs on site working on nanotechnology research: additional 12 FTEs involved in simulation, process modeling, and computational chemistry
- Research focus ranges from carbon and protein nanotubes, quantum device physics, quantum computing, data storage to optoelectronics, DNA electronics, Bio-Sensors, Bacteriorhodopsin based Data-Storage
- Largest carbon nanotube effort in the Federal government and also one of the largest in the world
  - About 60 refereed publications in the field
  - Over 100 talks in National/International Meetings
  - Two Feynmann Awards

What is Expected from Alternative Electronic Technologies?

- Must be easier and cheaper to manufacture than CMOS
- Need high current drive, should be able to drive capacitance of interconnects of any length
- High level of integration (10^6 transistors/chip)
- High reproducibility (better than ±5%)
- Reliability (operating time > 30 years)
- Very low cost (< 1 cent/transistor)
- Everything about the new technology must be competing and simultaneously CMOS scaling should fail. If these two together do not happen, the enormous infrastructure built around silicon will make it difficult for alternatives to emerge

Carbon Nanotube

CNT is a tubular form of carbon with diameter as small as 1 nm.
Length: few mm to microns

CNT is configurationally equivalent to a two dimensional graphene sheet rolled into a tube.

CNT exhibits extraordinary mechanical properties:
Young’s modulus over 1 Tera Pascal, as stiff as diamond, and tensile strength - 200 GPa.

CNT can be metallic or semiconducting, depending on chirality.
Potential CNT Applications and Challenges

<table>
<thead>
<tr>
<th>Application</th>
<th>Properties</th>
<th>Challenges</th>
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<tbody>
<tr>
<td>CNT for electronic sensors</td>
<td>High sensitivity to chemical vapors</td>
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</tr>
<tr>
<td>CNT for environmental sensors</td>
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</tr>
<tr>
<td>CNT for composites</td>
<td>High strength and stiffness</td>
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</tr>
</tbody>
</table>


CNT Synthesis

- CNT has been grown by laser ablation (pioneering at Rice) and carbon arc process (NERC, Japan - early 90s)
- CVD, high purity, purification methods
- CVD is ideal for patterned growth (e.g., microelectronic applications)
- Well known technique for nanoelectronics
- Hydrogen feedstock
- Growth needs catalyst (transition metal)
- Multishell tubes at 500-800°C
- Numerous parameters influence CNT growth

Carbon Nanotubes at Ames

CNT in Microscopy

Atomic Force Microscopy is a powerful technique for imaging, nanomanipulation, and failure analysis. Conventional silicon or tungsten tips wear out quickly, but CNT tips are robust, offer amazing resolution.

CNT Based Biosensors

- One interest is to develop sensors for nanotubes to study dynamics of cells. CNT, though long, can be functionalized at the end to form a sensor. Current study uses AFM as an experimental platform.
- The technology is also being used in collaboration with NCT to develop sensors for cancer diagnostics. Identified probe molecules that will serve as signatures of leukemic cells, to be attached to CNT.
- Current flow due to hybridization will be through CNT electrode to an ICP.
- Prototype sensors/cancer development

Computational Nanotechnology

- Large scale computer simulations based on ab initio methods enable understanding nanotube characteristics and serve as design tool.
  - Evaluation of mechanical properties
  - Evaluation of electronic properties
  - Electron transport in CNT devices
  - Functionalization of the nanotubes
  - Design of electrical and mechanical devices
  - Evaluation of storage potential (H₂, Li)
Protein Nanotubes

- Heat shock protein (HSP 60) in organisms living in high temperatures ("extremophiles") is of interest in astrobiology.
- HSP 60 can be purified from cells as a double-ring structure consisting of 16-18 subunits. The double rings can be induced to self-assemble into nanotubes.

Atomic Chain Electronics
Experiments: Nanotube based Devices

Nanotube as Quantum Molecular Wire (Nature 1997)

Nanotube Field Effect Transistor (Nature 1998)

Nanotube Hetero-Junctions (Nature 1999)
Electronic Transport in Y-Junction Carbon Nanotubes

C. Papadopoulos,1 A. Rakitin,1 J. Li,1 A. S. Vedeneev,1,2 and J. M. Xu1,3

1Department of Electrical & Computer Engineering, University of Toronto, 10 King’s College Road, Toronto, Ontario, Canada M5S 3G4
2Russian Academy of Sciences, Institute of Radioengineering and Electronics, Frunzeino, Moscow district 141130, Russia
3Division of Engineering, Brown University, Providence, Rhode Island 02912
(Received 22 February 2000)

1st experimental Step to a Three-Terminal Nanoscale Transistor.
CNT in Microscopy

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Conventional silicon or tungsten tips wear out quickly. CNT tip is robust, offers amazing resolution.

280 nm Line/Space Array of Polymeric Resist on silicon Substrate

Silicon Tip  Multi-Walled Carbon Nanotube Tip

AFM Imaging with Single Wall Nanotube Tips
Based on Phosphate bridges acting as tunnel junctions and H acting as capacitive element.

DNA coated with metals can act as interconnects.

DNA has self-assembly properties.
Example: (NYU)

Topologically Connected DNA Segments

Cube

Truncated Octahedron

DAE    DAO    DPE    DPON    DPOW

Double Cross-Over Molecules

DNA Nano-mechanical Device
DNA as Electronics Elements:

Conflicting Claims about DNA as metal or semiconductor?

Indirect measurements in the beginning led to this controversy?

Transport measurements on single DNA molecules C. Dekker (Delft)
Nature, 2000

A 10.4 nm long, double-stranded poly(G)—poly(C) DNA molecule
Metal nanoelectrodes that are separated by 8 nm

Small gap semiconductor

- Metal coated DNA serve as conductor.
Bacteriorhodopsin for Optical Data Storage
Ann Hermione and Richard Jaffe
ahermone@mail.arc.nasa.gov

• Bacteriorhodopsin (BR) contains the chromophore retinal in an all-trans conformation.

• on photoexcitation retinal isomerizes from all-trans to mainly 13-cis.

• Changes in BR’s optical properties in the excited state, such as refractive index, make it a candidate for optical data storage.
All-trans Retinal
• The lifetime of 13-cis retinal is short and when retinal returns to the all-trans form any data stored is lost.

• Mutant BR molecules have been prepared, in which retinal isomerizes to the 9-cis form with a long lifetime, making long-term data storage possible.

• Therefore, we are trying to characterize the 9-cis isomerization pathway.
Nanotechnology: Comments

- Various experimental and simulation aspects of Nanoelectronics are currently in progress
- Individual devices and characteristics need to be incorporated in NASA specific applications
- Biosensors and nanotubes for interconnects are preliminary step in that direction
Deepak Srivastava
NASA Ames Research Center
MS T27A-1 and MS 229-3
Moffett Field, CA 94034-1000

deepak@nas.nasa.gov, (650) 604-3486

http://www.ipt.arc.nasa.gov
http://www.nas.nasa.gov/~deepak/home.html
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Conventional silicon or tungsten tips wear out quickly. CNT tip is robust, offers amazing resolution.
AFM Imaging with Single Wall Nanotube Tips

2 nm thick Au on Mica

5 nm thick Ir on Mica

Si₃N₄ on Silicon substrate
280 nm Line/Space Array of Polymeric Resist on silicon Substrate

Silicon Tip

Multi-Walled Carbon Nanotube Tip
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- Current flow due to hybridization will be through CNT electrode to an IC chip.
- Prototype biosensors catheter development

- High specificity
- Direct, fast response
- High sensitivity
- Single molecule and cell signal capture and detection
Heat shock protein (HSP 60) in organisms living at high temperatures ("extremophiles") is of interest in astrobiology.

HSP 60 can be purified from cells as a double-ring structure consisting of 16-18 subunits. The double rings can be induced to self-assemble into nanotubes.
IMPORTANCE

- Conductivity of DNA has been controversial for decades.
- Electron transfer experiments (biochemistry) / Possible connection to cancer
- Transport experiments (physics)
- DNA Electronics (Device / Lithography)
ELECTRON TRANSFER EXPERIMENTS

- Oxidative damage of DNA has been linked to cancer.
- How effective is long range electron transfer in causing oxidative damage?

- Estimates of electron transfer rates span two orders of magnitude.

* Fluorescent analog of a base pair
* Intercalator

Significant dependence on base pair mismatches.
Significant dependence on intervening sequence
TRANSPORT EXPERIMENTS

Porath et al., Nature (2000) INSULATING

Fink et al., Science (1999) NO GAP!

Current ~ 1 nA

Current ~ 10 nA

Voltage (V)

Voltage (mV)

20 mV
Based on Phosphate bridges acting as tunnel junctions and H acting as capacitive element.

DNA coated with metals can act as interconnects

DNA has self-assembly properties
DNA as Electronics Elements:

about DNA as metal or semiconductor?

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www.nas.nasa.gov/~deepak/home.html
Carbon Nanotube Electronics Band Structure (basics)

Hexagonal Lattice of a Graphene Sheet – (2xunit cell)

First Brillouin zone for an armchair tube.

\[ \text{Ch} = n \mathbf{a}_1 + m \mathbf{a}_2 \] (chiral vector)

NanoSpace 98 – D. Srivastava
Computational Nanotechnology
3-terminal CNT Heterojunctions

FIG. 3. LDOS for the relaxed (9,0)-(10,0)-(9,0) structure (T2) at various cross sections indicated in Fig. 1(b). The larger contribution in the gap is due to the presence of two extra pairs of heptagon-pentagon defects at the junction.

LDOS of (10,0)-(9,0) "T-junction"

3-terminal "T-tunnel" CNT Heterojunctions for Molecular Electronics Applications

Mol Elect 2000 – D. Srivastava
Multi-wall Y-junction Carbon Nanotubes
Semiconducting Y-junction Nanotubes with Different Angles
Computational Nanotechnology
D. Srivastava, J. D. Schall, D. W. Brenner, K. D. Ausman, M. Feng
Bio-mimetic Dendritic Neurons: Carbon Nanotube

Model of 4-level dendritic neural tree that could be made of branched carbon nanotubes

D. Srivastava et. al., Comp. in Science and Engineering, IEEE, APS (2001)