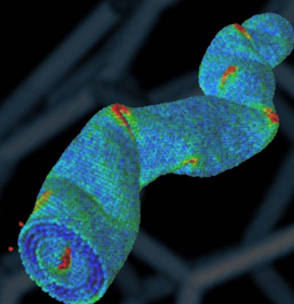
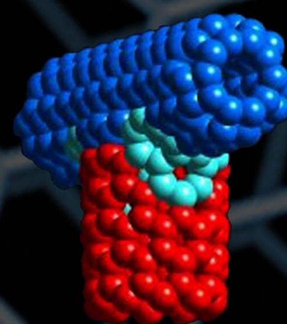
Nano and Bio Technology Research at NASA Ames

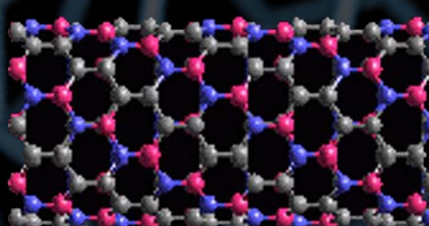
M. Meyyappan, Harry Partridge, and T.R. Govindan
NASA Ames Research Center
Moffett Field, CA 94035



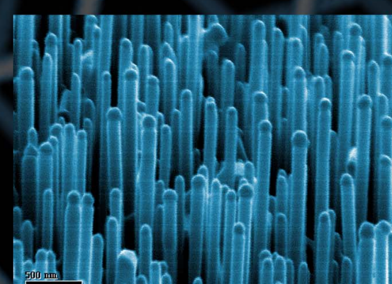
Nano-Mechanics/Materials



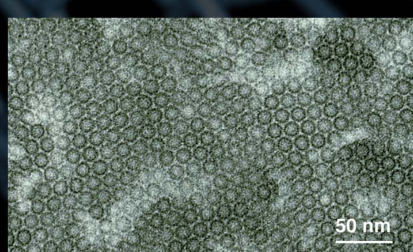
Carbon Based Electronics



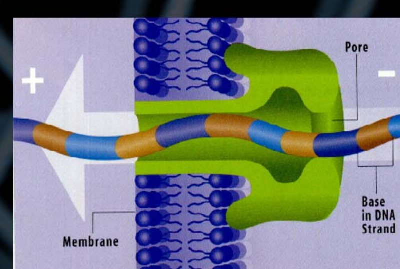
BxCyNz Nanotubes



ZnO Nanowires



Protein Nanotubes



Nanopore/Gene Sequencing

Revised: December 17, 2002

Nano and BioTechnology Research at NASA Ames

M. Meyyappan, Harry Partridge and T.R. Govindan
NASA Ames Research Center
Moffett Field, CA 94035

Abstract

This article provides an overview of nanotechnology and biotechnology research at NASA Ames Research Center and covers current results in the areas of carbon nanotube (CNT) growth and characterization and functionalization, nanotubes in scanning probe microscopy, inorganic nanowires, biosensors, chemical sensors, protein nanotubes nanotechnology in gene sequencing, computational nanotechnology, quantum device simulation, and computational optoelectronics.

I. Introduction

Advanced miniaturization is a key thrust area to enable new science and exploration missions for which ultrasmall sensors, power sources, communication, navigation, and propulsion systems with very low mass, volume and power consumption are needed. Revolutions 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, bold space architectures such as networks of ultrasmall probes on planetary surfaces, micro-rovers that drive, hop, fly and burrow, and collection of microspacecraft making a variety of measurements.

NASA Ames started an Integrated Product Team (IPT) on Devices and Nanotechnology in FY 97 to conduct basic research in the emerging field of nanotechnology as well as in semiconductor device physics, computational electronics and optoelectronics, and computational chemistry in materials processing. This effort was renamed as NASA Ames Center for Nanotechnology (NACNT) couple of years later. The Ames group has grown to a level of over fifty scientists and Table 1 lists those who are involved in nanotechnology and biotechnology research and contributed to the material presented in this article. The research focus, summarized in Table 2, covers a wide range of subjects: carbon nanotube (CNT) synthesis, characterization, functionalization, electrode fabrication sensor development, application of CNT in atomic force microscopy (AFM), inorganic nanowires for sensor and detectors, protein nanotubes, nanotechnology in genomics, development of quantum device simulator, computational optoelectronics, atomic chain electronics, and bacteriorhodapsin (BR) based holographic data storage. This article provides selected results in the above areas. A complete current publication list and reprints from the Ames group as well as descriptive project summaries can be found in the NACNT website http://www.ipt.arc.nasa.gov. This website also features a nanotechnology gallery containing videos and images [1].

Table 1.

NASA Ames Nanotechnology Research Team		
Nanotubes/Sensors	***Molecular Electronics***	***Computational Optoelectronics***
Alan Cassell	Sylvia Asano	Cun-Zheng Ning
Bin Chen	Geetha Dholakia	Jianzhong Li
Hua Chen	Wendy Fan	Alex Maslov
Martin Cinke	James Williams	***Quantum Computing, Architecture***
Brett Cruden	***Inorganic Nanowires***	Vadim Smelyanskiy
Sarah Cooper	Hou Tee Ng	Dogan Timucin
Lance Delzeit	Jing Kong	Manoj Samanta
Jie Han	Pho Nguyen	***Computational Nanotechnology***
Bishun Khare	***Protein Nanotubes***	M.P. Anantram
Jessica Koehne	Jonathan Trent	Charlie Bauschlicher
Jing Kong	Andrew McMillan	Gennady Gutsev
Jing Li	Chad Paavola	David Hash
Jun Li	Yifen Li	Natalio Mingo
Yijiang Lu	***Genomics***	Alessandra Ricca
David Loftus	Viktor Stolc	Deepak Srivastava
Cattien Nguyen	Greg Eason	Chenyu Wei
Phillipe Sarazin	Waraporn Tongprasit	Toshishige Yamada
Ramsey Stevens	Ioana Cozmuta	Liu Yang
Laura Xe	***Computational Electronics***	
	M.P. Anantram	
	James O'Keefe	
	T.R. Govindan	
	Alexi Svizhenko	

Table 2.

Research Focus	
* **Carbon Nanotubes**	• Purification
• Growth (CVD, PECVD)	• Application Development
• Characterization	* **Genomics**
• AFM tips	• Nanopores in gene sequencing
- Metrology	• Genechips development
- Imaging of Mars Analog	* **Computational Nanotechnology**
- Imaging Bio samples	• CNT - Mechanical, thermal properties
• Electrode development	• CNT - Electronic properties
• Biosensor (cancer diagnostics)	• CNT based devices: physics, design
• Chemical sensor	• CNT based composites, BN nanotubes
• Logic Circuits	• CNT based sensors
• Chemical functionalization	• DNA transport
• Gas Absorption	• Transport in nanopores
• Device Fabrication	• Nanowires: transport, thermoelectric effect
* **Molecular Electronics**	• Transport: molecular electronics
• Synthesis of organic molecules	• Protein nanotube chemistry
• Characterization	* **Quantum Computing**
• Device fabrication	* **Computational Quantum Electronics**
* **Inorganic Nanowires**	• Noneq. Green's Function based Device Simulator
* **Protein Nanotubes**	* **Computational Optoelectronics**
• Synthesis	* **Computational Process Modeling**

II. Carbon Nanotubes

Growth and Characterization

In the early days of nanotechnology research, CNTs were primarily grown by laser ablation and carbon arc techniques by various research groups across the world. Both approaches produce single wall CNT in small quantities scraped off the cooler walls of the tube. In the last few years, chemical vapor deposition has emerged as an alternative approach. CVD, a workhorse in silicon microelectronics, is ideally suited to grow nanotubes on patterned substrates if one is interested in investigating nanoelectronic devices or sensors. Ames operates two CVD reactors to grow nanotubes on substrates. The feed gas may be CO or some hydrocarbon gas, and typical growth temperatures for multiwall carbon nanotubes is 500-800° and 900° for single-walled nanotubes.

The CNT growth is catalyzed by transition metals such as nickel, iron or cobalt. The catalyst mixture can be applied to the substrate by solution chemistry followed by calcination. Parameters controlling growth appear to be numerous: nature of feedgas and composition, flow rate, temperature, type of catalyst, catalyst preparation technique, and substrate material. To date, no research group has been able to control CNT diameter or chirality. Since the number of variables involved is very large, a combinatorial chemistry approach has been used, as pioneered by Alan Cassell at Ames, for catalyst optimization in CNT synthesis [2]. Figure 1 shows a bundle of multiwall CNTs grown by this approach. Figure 2 shows a multilayer assembly of multiwall carbon nanotubes grown using CVD approach. The densities of the upper and lower layers are different and a controlled assembly would be useful in the preparation of separation membranes and composites [3].

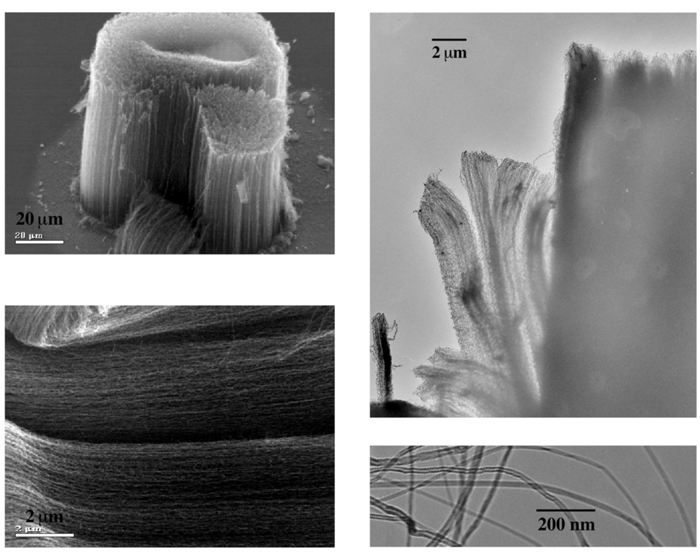


Fig. 1. Multiwall carbon nanotubes grown by CVD

We have also investigated catalyst preparation through direct ion beam sputtering which allows easy confinement of the catalyst within small patterns. It was found that adding an underlayer of Al allows increased nucleation of the nanoparticles needed for CNT growth; this metallic layer also allows tuning of the conductivity of the substrate [4].

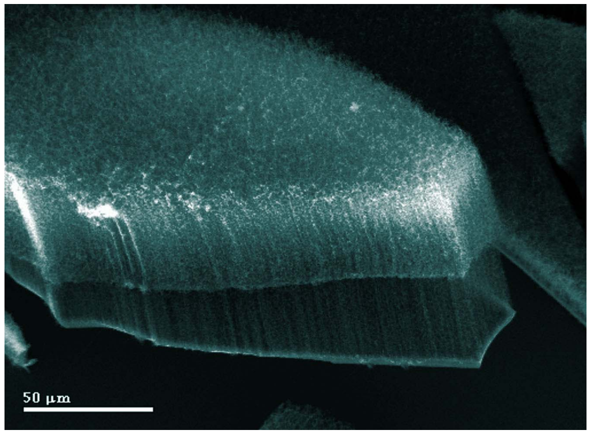


Fig. 2. Multilayer assembly of nanotubes

Figure 3 shows single wall carbon nanotubes prepared by CVD on a patterned grid using the above approach [4]. Both thermal CVD and plasma CVD are routinely used at Ames to grow SWNTs and MWNTs. Thermal CVD has allowed SWNT and MWNT growth on patterned substrates. In the case of MWNTs, continued growth over 10 minutes yields nice towers of MWNTs. These towers consist of millions of MWNTs supporting each other by van der Waals force; individual nanotubes, in high magnification, appear to grow like vines. In contrast, it is possible to obtain individual, free-standing, vertically-aligned structures with plasma CVD as seen in Fig. 4. But it is important to recognize that these structures are not MWNTs according to conventional definition, where each wall should be perfectly parallel to the central axis. The nanostructures in Fig. 4 have interior walls exhibiting a small angle with respect to the central axis. This stacked-cone shape material is preferably called multiwalled carbon nanofibers (MWNFs) to distinguish them from MWNTs. The plasma reactors used at Ames to grow these MWNTs and MWNFs is an inductively coupled reactor with an independent rf bias at the bottom electrode holding the substrate [5].

The nanotube characterization at Ames is done using scanning electron microscopy (SEM), high resolution transmission electron microscopy (HRTEM), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy and UV-vis spectroscopy.

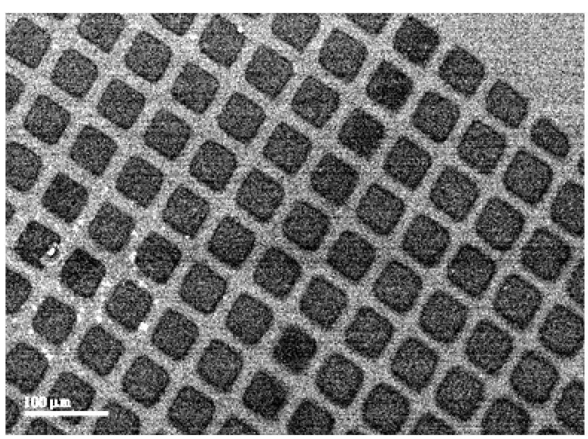


Fig. 3. Single Wall Carbon Nanotubes by CVD

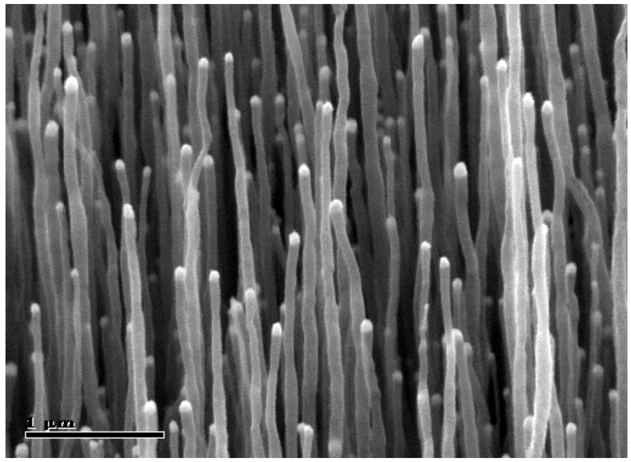


Fig. 4. Plasma CVD MWNFs

Electrode and Biosensor Fabrication

The MWNFs are ideal for developing nanoscale electrodes. They range in 20-100 nm diameter. Their density and hence, the average spacing between individual MWNFs can be varied by varying the thickness of the catalyst films. Of course, if one wishes a precise control on the spacing, then catalyst patterning by e-beam lithography would be ideal. In applications as electrodes, particularly with electrochemical approaches involving electrolytes and indicators, it is important to maintain the rigidity of the nanostructures. For this reason, gap-filling techniques were developed to fill the spacing between MWNFs with a dielectric such as SiO_2 or spin-on-glass. TEOS CVD was used to deposit SiO_2 followed by chemical mechanical polishing to planarize the top surface (see Fig. 5). Now, only the very tip of the MWNFs are exposed while the rest are buried inside the SiO_2. Electrical characterization of these tips indicate that they function as electrodes as desired [6] and hence, are suitable for attaching DNA or other chemical groups.

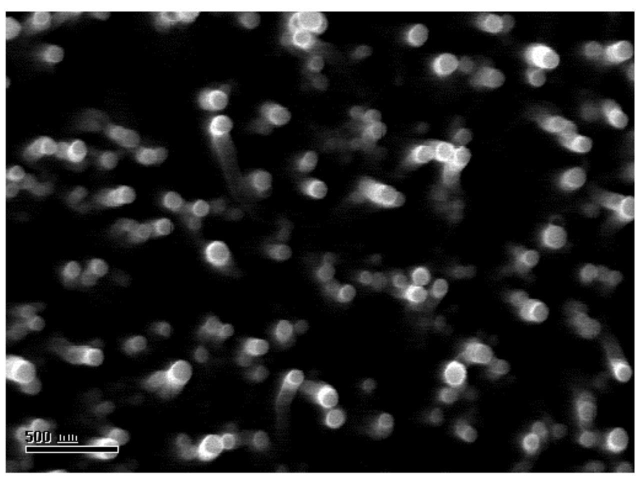


Fig. 5. SEM image of MWNFs after encapsulated in SiO_2

Jun Li and coworkers at Ames prepared the above electrode ensemble and attached DNA to the MWNF tips. The attachment is due to covalent bonding and they have also demonstrated hybridization by bringing in a complementary strand for the probe DNA molecule. In addition to the evidence from fluorescence microscopy for these events, they have also used an electrochemical indicator and obtained signals that are proportional to the amount of guanine in the target sequence.

Sensor for Cancer Diagnostics

A major area of focus in CNT applications at Ames is development of biosensors for cancer diagnostics. This work, conducted through funding from National Cancer Institute, involves development of a prototype biosensor catheter that permits detection of specific oligonucleotide sequences that serve as molecular signatures of cancer cells. The biosensor will be tested in vitro using tissue samples from patients with chronic myelogeneous leukemia and acute promyelocytic leukemia, neoplastic diseases for which molecular signatures have been well characterized. The CNT-based biosensor technology under development for cancer diagnostics will also be adapted for use in astrobiology missions, and related plans are underway. A critical element of this technology involves the ability to functionalize the tip of a nanotube array with (a monolayer of) probe molecules as described in the previous section.

Nanotubes in Catalysis

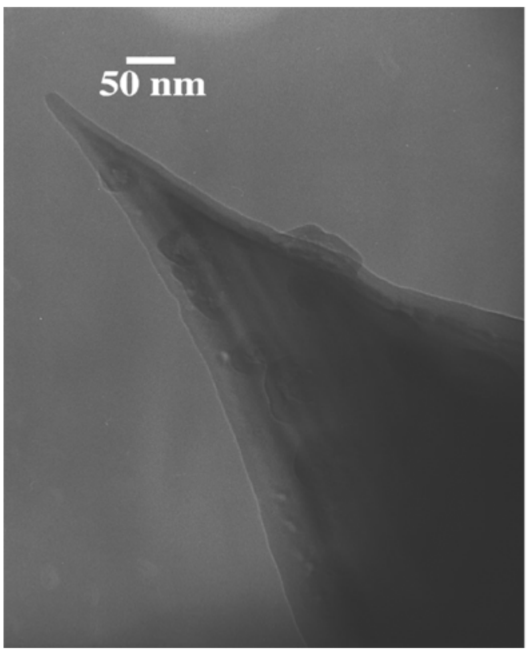
CNTs have been postulated to have a high surface area which would be useful in catalysis, gas adsorption and related applications. Though theoretical estimates put the surface area in the 3000 m^2/g range, experimental results have been well under 1000 m^2/g. Jing Li and Martin Cinke demonstrated a surface area of 1580 m^2/g for purified HiPCo SWNTs [7]. They used a two step purification process with the first step involving a debundling procedure followed by a step to clean up the metal impurities and the small amount of unwanted amorphous carbon. The large surface area based on N_2-adsorption isotherm studies have led them to investigate both physisorption and chemisorption aspects of adsorbing CH_4, NO_2, NO, CO_2, etc. onto HiPCo samples. The goal of their study is to investigate the suitability of SWNTs as catalysts or support material for waste remediation in long voyage crew cabins.

Functionalization of Nanotubes

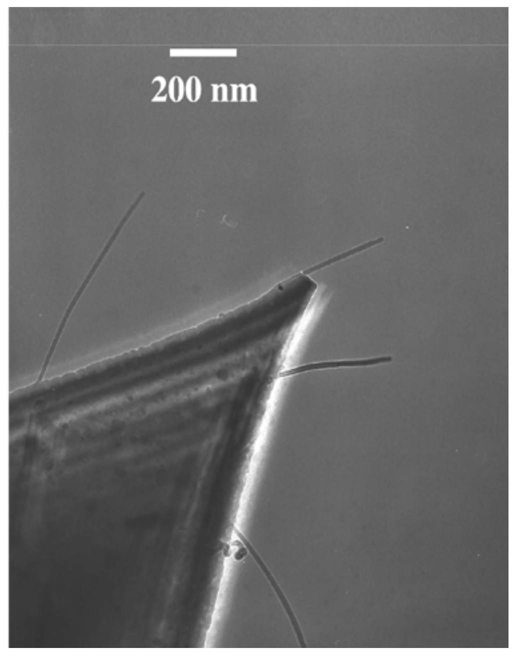
Various applications call for the need to attach chemical functional groups to the sidewall of CNTs. For example, it is believed that chemical functionalization may provide the "velcro effect" needed for incorporating CNTs in a host matrix for developing composites. Attaching fluorine along to the sidewall makes CNTs nearly insulating, changing the conductivity orders of magnitude. Regardless of the application, a common approach to functionalizationn is wet chemistry. While a wet chemistry approach is simple, it is not scalable, deals with large quantities of chemicals which need to be discarded and suffers from poor efficiency and a host of other issues which were faced by the semiconductor community 20 years ago when dealing with wet chemistry for etching semiconductors, oxides and metals. The innovation then was the cold plasma based chemistry for etching. Cold plasmas or glow discharges can be used for functionalization of CNTs as well. Khare and coworkers [8] demonstrated this approach by using a simple microwave cavity to generate a plasma that contains the requires species for functionalizations. They have demonstrated functionalization of CNTs with atomic hydrogen using a H_2 plasma and atomic fluorine with a CF_4 plasma. In all cases, a very small quantity of source gas is all what is required. Functionalization also appears to be rapid. Evidence of attaching the chemical groups was obtained from appropriate FTIR, Raman and UV signals.

CNT in Microscopy

CNT is an ideal tip for use in AFM [9,10] since it is robust and can be just a few nanometers in diameter. However, manually attaching a CNT to the tip of a cantilever can be arduous. Our group has been able to use CVD to directly grow single wall nanotubes on the AFM cantilever. Figure 6 shows an example of the effort. We have also developed an electrochemical approach to easily attach a multiwall nanotube to the AFM cantilever [10].



TEM Micrograph of Electro-deposited Catalyst on Tip of AFM Cantilever



TEM Micrograph of Shortened NT Synthesized by CVD

Fig. 6. Nanotube probe directly grown on AFM cantilever.

The AFM with nanotube tip is currently used to image and study simulated Mars dust. Figure 7 shows an image of Red Dune Sand (from Western Australia) which is a Mars analog. The CNT tip - only a few nanometers in diameter - is able to offer extraordinary resolution in imaging the dust particles. In addition, the robustness of CNT provides long lasting tips in contrast to the quick wearing of silicon tips. Our other accomplishments with CNT probes include metrology applications (for example, a profilometer) and nanoscale imaging of semiconductor surfaces. Figure 8 shows an AFM image of a thin iridium film obtained a single-walled nanotube tip. The resolution here is much better than conventional silicon tips [9]. Figure 9 compares images of a photoresist pattern obtained using a silicon tip and a nanotube tip. The silicon tip exhibits artifacts due to the pyramidal cantilever hitting the sidewall of the feature [9].

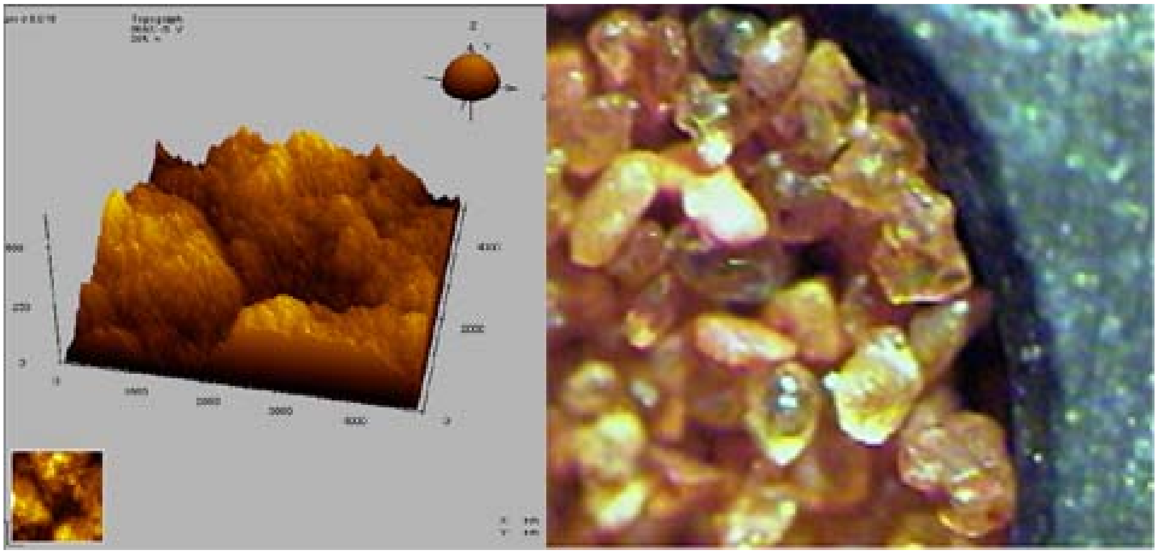


Fig. 7. AFM Image of Red Dune Sand (Mars Analog) obtained using a nanotube tip (left) compared to an image using optical microscope (right).

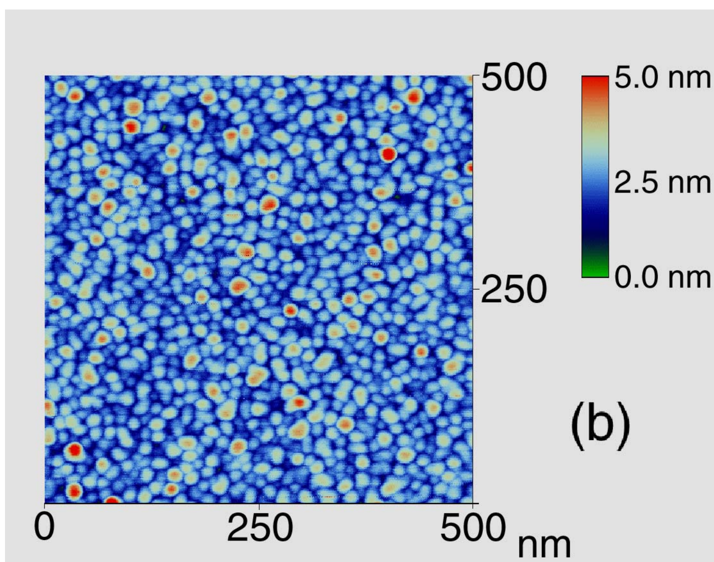


Fig. 8. AFM image of iridium film using a SWNT tip

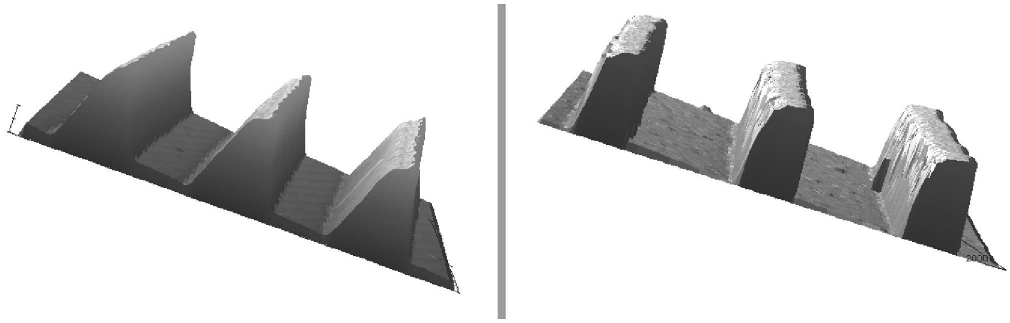


Fig. 9. Comparison of AFM images of a 280 nm line/space photolithographic pattern: silicon tip (left) and nanotube tip (right).

III. Inorganic Nanowires

Whereas the carbon nanotube research continues to address the challenge of controlling the chirality (thus creating the ability of producing metallic or semiconducting of nanotubes of specified bandgap at will), quietly a new technology is emerging based on inorganic nanowires. Materials such as Si, GaAs, InP, ZnO and other oxides have long been prepared as very thin films of 1-20 nm which propelled advances in lasers, transmitters, receivers and sensors, taking advantage of the quantum properties of these confined layers. Shrinking this by another dimension from 2-d to 1-d, it is now possible to grow most of these structures as 1-d nanowires. Hou Tee Ng at Ames has made tremendous progress in growing nanowires of ZnO and ITO. Fig. 10 shows very nicely aligned ZnO nanowires grown on a sapphire substrate. The choice of sapphire substrate is dictated by the minimum mismatch with ZnO. The bandgap of these ZnO nanowires makes them useful in developing blue lasers and blue LEDs.

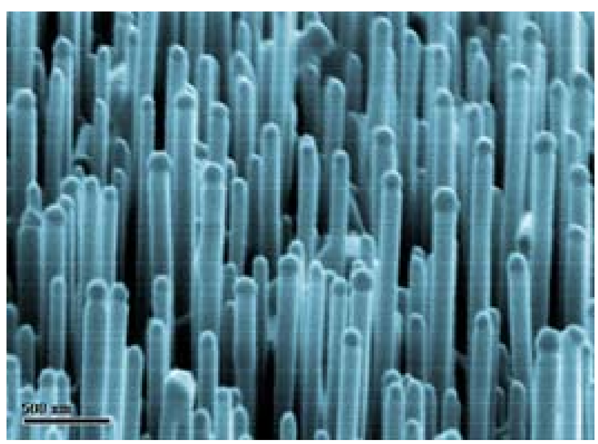


Fig. 10. ZnO Nanowires

IV. Protein Nanotubes

Jonathan Trent and coworkers at NASA Ames have been studying "heat shock protein 60" (HSP60) in organisms living at high temperatures, the so-called "thermophiles." The HSP60 can be purified from cells as a double-ring structure consisting of 16-18 subunits. The Ames group has recently discovered that the double-rings can be induced to self-assemble into tubes and then the tubes associate to form filaments [11]. The protein nanotubes shown in Fig. 11 are about 15 nm in diameter and several microns long. The nanotubes are stable up to near 100°C, depending on the pH. Currently, several applications for these protein nanotubes are being explored.

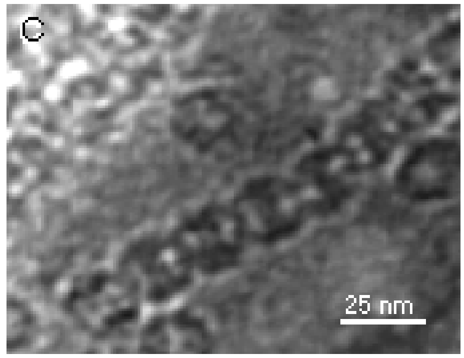


Fig. 11. Protein nanotubes

V. Nanopore technology in Gene Sequencing

Viktor Stolc and coworkers have been developing a novel nanopore technology for gene sequencing. A nanopore of the size 2-3 nm in diameter is required for this purpose, which is used in a patch-clamp mode. The apparatus consists of the pore mounted in a membrane in a cell which contains the DNA in solution. In the absence of the DNA going through the pore, there is a background current signal due to the transport of ions through the pore in response to the applied electric field across the patch clamp. When a strand of DNA passes through the pore, the background signal would be suppresses due to the blockage. Stolc and Coworkers have been trying to correlate this drop in signal to the single nucleotide in the DNA sequence. The major challenge of this technology is to generate the right size pores. Well known technologies such as focused ion beam etching generate pores a little too big to be of value (ex: 15 nm). Current efforts focus on generating small nanopores to take advantage the experimental setup that is ready at NASA Ames.

VI. Computational Nanotechnology

Extensive investigations using computational simulations on the electronics, mechanical and other properties of nanotubes have been undertaken by the Ames nanotechnology group. SWNTs exhibit remarkable mechanical properties, for example, a Young's modulus of over 1 TPa and tensile strength of about 200 GPa. They also have been unique electronic properties in that a CNT, based on its diameter and helicity, can either metallic or semiconducting. It is interesting to explore the coupling between the mechanical and electronic properties. Figure 12 shows sample results from a combination of molecular mechanics, dynamics, and tight binding simulations. The bandgap, normalized by the hopping parameter (3.1 eV) and a dimensionless radius R/Ro, is plotted against strain for various chiral tubes. For reference, the bandgap of a (10, 0) tube at 0% strain is 1 eV whereas the bandgap of silicon is 1.11 eV. The metallic

(5, 5) tube shows no variation in bandgap under tension or compression whereas other tubes show varying degree of change. The slope itself depends on the modulus of (n-m, 3) where n and m are used to define the chirality. Within each color coded group in Fig. 5, the magnitude of the change depends on the chiral angle. For example, the bandgap changes more rapidly for a (10, 0) tube compared to a (6, 5) tube. In general, there are three transitions seen in Fig. 12. The first is metal-semiconductor transition, for example, the (9, 0) tube at 1% strain. Next, the change in bandgap with strain (slope) changes sign due to quantum number change, for example, the (10, 0) tube at 10% strain. Finally, another transition is seen when the slope changes sign again due to mechanical relaxation, for example, the (10, 0) tube at 18% strain. The critical strain, defined at the transition point due to quantum number change, varies inversely with tube diameter (not shown here) which can be verified experimentally. Further details can be found in ref. 12 which also describes the effects of torsional strain on the bandgap. Reference13 describes the effect of bending on the electronic properties.

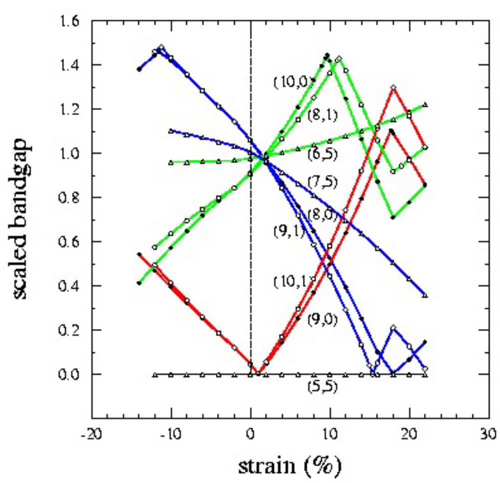


Fig. 12. Effect of strain on bandgap. Legend: n - m = 3q + 1, n - 3 = 3q, n - 3 = 3q - 1, where n, m and q are integers.

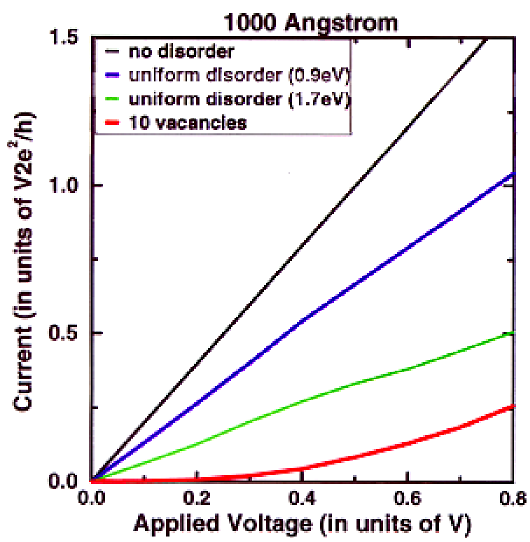


Fig. 13. Effect of disorder on CNT conductance.

A CNT is expected to be an ideal quantum wire. Ballistic transport through a nanotube would yield a low bias resistance of 6KΩ. The best measurements to date for single wall nanotubes have been shown to be in the range of 20-50 KΩ. The main reasons for the observed low conductance are defects and Bragg reflection. Theoretical work studying the effect of disorders and reflection on conductance has been carried out. Figure 13 shows computed conductance for nanotubes with uniform disorders and vacancies. Uniform disorder in CNT does not significantly affect conductance. In contrast, vacancy-type defects cause significant backscattering resulting in a conductance degradation. Further details can be found in ref. 14. Another important aspect in CNT-based electronics is the role of contacts, and theoretical investigations have been carried out to study how a carbon nanotube couples to simple metals. For good coupling, the K_f for metals must be greater than $4\pi/3a_0$ (0.17 nm^{-1} for graphite). The value of K_f for Al and Au are 1.75 and 1.21 respectively and graphite does not couple to these metals. For armchair nanotubes, this value is only 0.85$Å^{-1}$ and coupling to simple metals is very good. The armchair tube also couples better than zigzag tubes to metal. The computations show an increase in transmission with the length of the contact, as seen in experiments. Details of this study can be found in ref. 15.

The unique electronic properties of CNT have led to the fabrication of the first CNT-based field effect transistor by research groups at IBM and Delft University. The CNT-FET consisted of a SWNT in contact with source and drain contacts and modulated by a gate on the backside. The device operated at room temperature. In ref. [16], Yamada provides a theoretical analysis of the experimental data by incorporating one-dimensional quantum effects in the nanotube channel. He concludes that the lack of saturation in

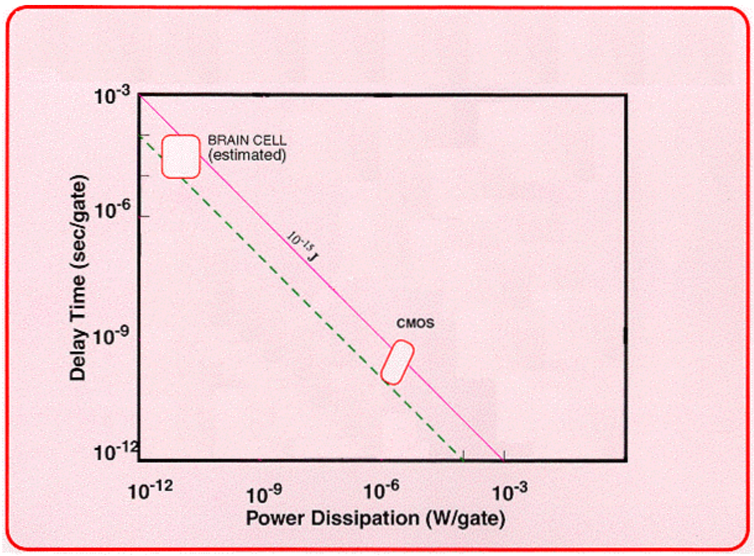


Fig. 14. Power dissipation per gate as a function of delay time

drain current as a function of drain voltage is an indication of channel carrier transport dominated by weak-localization and the electrode metal-nanotube contact influences subthreshold channel conductance vs. gate voltage. Yamada recommends a reduction in gate oxide thickness to increase the transistor gain.

While attempts to fabricate a CNT-FET are necessary first steps and allow exploration of fundamental issues and ultimate possibilities, it is critical, at this early stage, to pay attention to nanoelectronic circuit and architectures. Simple miniaturization of a CMOS-like device may not be appropriate for future nanoelectronics. Figure 14 shows switching time vs. power consumption per gate for a CMOS architecture. As device feature size and switching delay time decrease, the power consumption per gate goes up significantly and a CNT-based CMOS-like architecture is likely to face serious problems. It is interesting to note in the same plot that the brain, admittedly orders of magnitude slower, consumes significantly less power. It is possible to develop novel architectural concepts based on the unique properties of CNT, particularly metal-semiconductor, semiconductor-semiconductor, and heterojunctions [17]. Figure 15 shows nanoscale tunnel junctions for transistors which were constructed by introducing topological defects such as five (pentagon) and seven (heptagon) member rings in an otherwise all six (hexagon) based CNT [17]. Since the Y-junction proposal by Srivastava in 1997, two groups at Brown University and IISC, India independently have created Y-junctions in CVD reactors and made electrical measurements. Heterojunctions based on partial chemical functionalization and/or substitutional doping may also be possible. It is also possible to conceive of a neural tree consisting of a multiple of these Y-junctions (see Fig. 16). Deepak Srivastava envisions that these neural trees can be trained to perform complex switching and other operations just as in biological systems.

The remarkable mechanical properties of CNT are by now well known. Applications to high strength composites require extensive investigation to understand the behavior of CNT under various conditions. Nanoplasticity of SWNTs under uniaxial compression

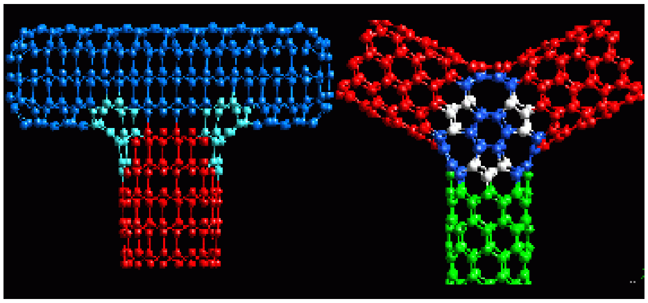


Fig. 15. Carbon nanotube "T" and "Y" junctions

was studied using generalized tight-binding molecular dynamics, and ab initio electronic structure method [18]. The bonding geometry collapses from a graphitic (sp^2) to a localized diamond like (sp^3) reconstruction under axial compression. Videoclips of this can be seen on the web under ref. [1]. The computed critical stress of about 153 GPa and the shape of the resulting plastic deformation agree well with experimental observations. Based on measurements of electrical conductivity, the thermal conductivity of SWNT has been speculated to be in the range of 1750-5800 W/m.K. which would put it in a class with CVD grown diamond. Molecular dynamics simulations at Ames has shown [19] a thermal conductivity in the range of 1000-2500 W/m.K for a (10, 10) nanotube at temperatures 100-500 deg. K. Note that this high thermal conductivity is only in the axial direction with K values in the radial direction being small. Further work is in progress to compute thermal conductivity of multiwall tubes.

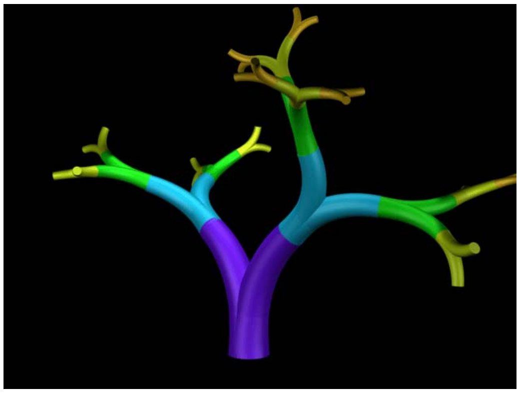
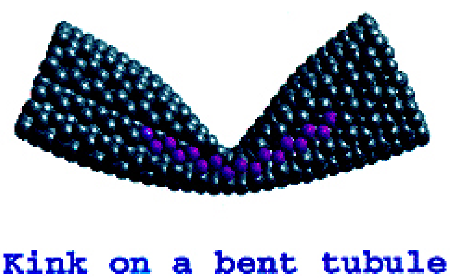


Fig. 16. Neural Tree

Several contemplated applications for CNT require functionalization of the nanotubes (both the tip and the sidewall) as mentioned earlier. Theoretical work at Ames predicts an enhanced chemical reactivity at regions of local conformational strain on the nanotubes [20]. Nanotubes which are bent or twisted show enhanced reactivity for specific sites near the distortions, as shown in Figure 17 which plots the binding energy, cohesive energy, and electronic energy for several highlighted atoms in a bent-tube. Preliminary verification of this prediction was provided by Rod Ruoff of Washington University where nanotubes laid over a V-ridge substrate were selectively attacked by nitric acid only at the sites distorted by the ridge [20].



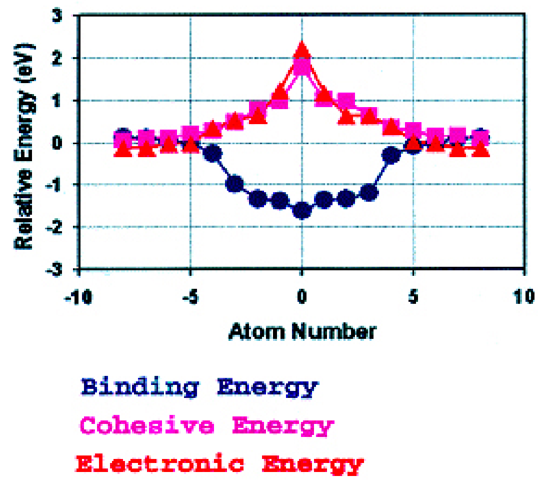


Fig. 17 Energies at various sites in a bent nanotube

The unique properties of CNT make it an attractive candidate for several nanotechnology innovations. The Ames computational nanotechnology researchers have designed a CNT-based nanogear [21, 22] shown in Fig. 18. Benzyne molecules bonded to the side of the nanotube form teeth while the nanotube forms the body about which the gear rotates. Computer simulations show that stable rotations of the driven gear are possible with the forced rotations of the powered gear. Videoclips of the nanogear rotation can be found in the website in ref. 1. The use of CNT tips in an AFM-based lithography and other applications were mentioned earlier in this report. The possibility of nanoscale etching using CNT tips has been investigated through molecular dynamic simulations. Selective atomic scale etching as well as indentation of silicon surfaces by CNT tips (mounted in an AFM) have been shown to be possible [23]. Parallelization of an array of tips has the potential to revolutionize future generation lithography. The website in ref. 1. contains videoclips of CNT etching and indentation. The possibility of storing data using H and F atoms to signify 0 and 1 bits has also been theoretically investigated [24, 25]. These atoms are sufficiently small that the interaction between adjacent data atoms on a silicon surface is small. Reference 24 speculates on how such a memory device might be constructed. A method then must be devised to differentiate

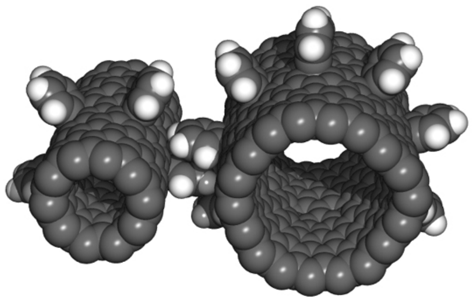


Fig. 18. A CNT-based nanogear with benzyne molecules bonded as teeth

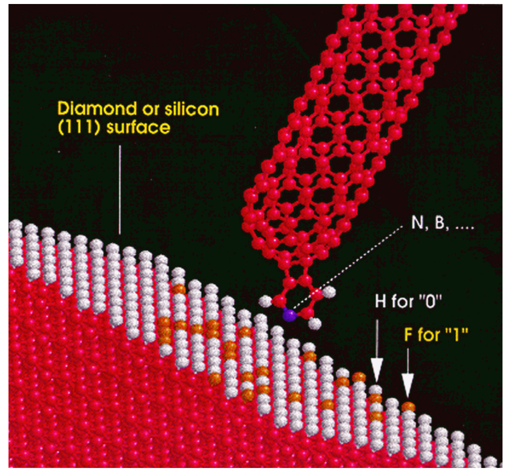


Fig. 19. Chemical data storage with H and F atoms as 0 and 1 to be read by a functionalized CNT tip.

between H and F atoms unambiguously. A suggested mechanism is to have a probe that is attractive toward one atom and repulsive to the other and ref. 25 discusses the suitability of a Sc atom and electron-rich pyridine molecule as probes (to be attached to the tip of a CNT). This type of chemical storage of data is capable of 10^{15} bytes/cm^2 storage density. Parallelization of tips again can overcome speed-related problems. . In addition to CNT, the Ames group has also been investigating boron nitride nanotubes [26], for electronics and structural applications.

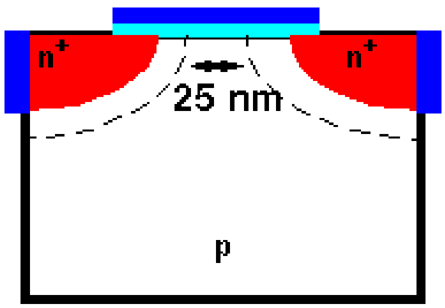
VII. Computational Electronics

The main trends in device miniaturization are relentless downscaling of CMOS technology and exploration of molecular devices. Future generation smaller and faster devices are of critical importance to powerful onboard computing, autonomous "thinking" spacecraft, and petaflop computing initiative. Modeling and simulation not only provides an understanding of how these devices work, but also can serve as a design tool in developing new generation devices. In submicron devices under consideration, the electron wavelength is comparable to device dimensions and the transit time becomes comparable to scattering time. Under these conditions, classical propagators fail. The Ames Computational Electronics group has developed a multidimensional quantum device simulator based on a Nonequilibrium Green's Function (NEGF) approach. Figure 20 shows a 25 nm-MOSFET studied using this simulator along with contours of electron density.

VIII. Computational Optoelectronics

Optoelectronics is a major enabling technology for the tera-era information technology. Information transmission, processing, and storage are key areas of active research in optoelectronics. Ames has a significant computational optoelectronics activity in progress. The goal is to develop comprehensive modeling and large scale simulation capability for studying and design of quantum optoelectronics devices.

Vertical cavity surface-emitting laser (VCSEL) is one of the most advanced and smallest semiconductor laser with light coming vertically out of the semiconductor wafer surface (see Fig. 21). It can be integrated with transistors in peta-flop computing with VCSEL-based optical interconnects, interprocessor communication, multi-gigabit Ethernet, high throughput image processing and virtual reality, and biological and chemical detection of molecules of interest in astrobiology and other space applications. Ames has developed a comprehensive model and simulation of VCSELs in 2-D space and time domain thus allowing detailed investigation of transverse modes. Figure 21 shows snapshots of computed laser intensity for a VCSEL. Other investigations include ultrafast modulation of semiconductor lasers [27] for high speed communication and compact and coherent THz sources [28].



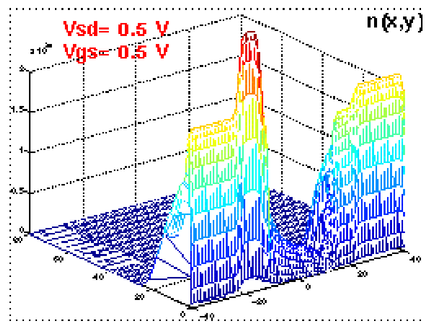
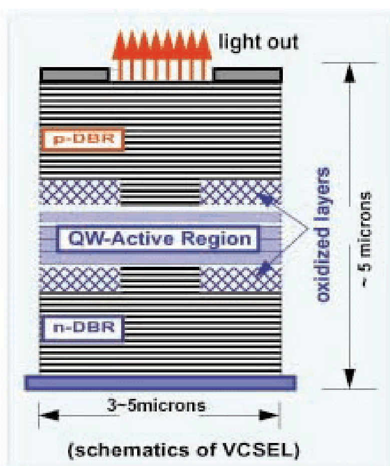


Fig. 20. Electron density contours for a 25 nm CMOS computed using a NEGF approach.



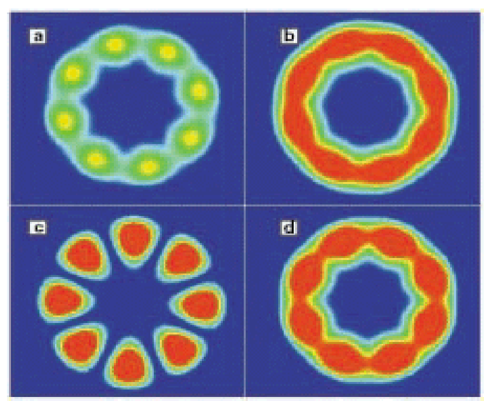


Fig. 21. 2 Dimensional VCSEL simulation showing laser intensity.

IX. Concluding Remarks

Nanotechnology - in its various forms such as nanoelectronics, nanoelectromechanical systems, ultrasmall and highly sensitive sensors, multifunctional materials, biologically inspired materials, systems and architectures, and possibly many others scientists have not yet thought of - is expected to play a strong and critical role in future space transportation and exploration. Also, the intersection of nano, bio, and information technologies provides rich possibilities for exploring useful concepts and breakthroughs. NASA Ames Center for Nanotechnology has been conducting innovative research in these areas to meet Agency's future needs. A strong computational program complements all the experimental activities.

A strong computational program complements all experimental activities. Excellence in computational sciences has long been a tradition at Ames, and Ames organizations such as Numerical Aerodynamic Simulation (NAS) Division and Computational Chemistry Branch have led the way in numerous subjects of interest to the Agency. In that tradition, a strong program in computational nanotechnology, computational quantum electronics, and computational quantum optoelectronics is being pursued. The vision for this program is to develop highly integrated and intelligent simulation environment that facilitates the rapid development and validation of future generation of electronic, photonic, and other devices, and sensors as well as materials and processes through virtual prototyping at multiple levels of fidelity.

Acknowledgement

The authors acknowledge the excellent research contributions from the staff listed in Table 1 and the web work by Amara de Keczer. The support for the nanotechnology and biotechnology work at Ames from Scott Hubbard, Jack Boyd, Steve Zornetzer, Eugene Tu, David Blake, and Mark Kliss is gratefully acknowledged.

References

1. http://www.ipt.arc.nasa.gov
2. A. M. Cassell, S. Verma, L. Delzeit, M.Meyyappan, and J. Han, “Combinatorial Optimization of Heterogeneous Catalysts used in the Growth of Carbon Nanotubes,” Langmuir, Vol. 17, pp. 260-264 (2001).
3. A. M. Cassell, M. Meyyappan, and J. Han, “Multilayer Film Assembly of Carbon Nanotubes,” J. of Nanoparticle Research, Vol. 2, pp. 387-289 (2000).
4. L. Delzeit, B. Chen, A.M. Cassell, R. Stevens, C. Nguyen, and M. Meyyappan, “Multilayered Metal Catalyst for Controlling the Density of Single Walled Carbon Nanotube Growth,” Chemical Physics Letters vol. 348, pp. 368- (2001).
5. L. Delzeit, I. McAninch, B.A. Cruden, D. Hash, B. Chen, J. Han, and M. Meyyappan, "Growth of Multiwall Carbon Nanotubes in an Inductively Coupled Plasma Reactor", Journal of Applied Physics, Vol. 91 (9), 6027-6033 (2002).
6. J. Li, R. Stevens, L. Delzeit, H.T. Ng, A. Cassell, J. Han and M. Meyyappan, "Electronic Properties of Multiwalled Carbon Nanotubes in an Embedded Vertical Array", Applied Physics Letters, Vol. 81 (5), pp. 910-912 (2002).
7. M. Cinke, J. Li, B. Chen, A. Cassell, L. Delzeit, J. Han, and M. Meyyappan, "Pore Structure of Raw and Purified HiPCo Single-walled Carbon Nanotubes", Chemical Physics Letters, Vol. 365, pp. 69-74 (2002).
8. B. Khare, A.M. Cassell, C.V. Nguyen, M. Meyyappan, and J. Han, “Functionalization of Carbon Nanotubes Using Atomic Hydrogen,” NanoLetters (2001).
9. C.V. Nguyen, K.J. Chao, R.M.D. Stevens, L. Delzeit, A. Cassell, J. Han and M. Meyyappan, “Carbon Nanotube Tip Probes: Stability and Lateral Resolution in Scanning Probe Microscopy and Applications to Surface Science in Semiconductors,"
10. R. Stevens, C. Nguyen, A. Cassell, L. Delzeit, M. Meyyappan, and J. Han, “Improved Fabrication Approach for Carbon Nanotube Probe Devices,” Applied Physics Letters, Vol. 77 (21), pp. 3453-3455 (2000).
11. T.H. Yaoi, K. Kagawa, and J. Trent, "Chaperonin Filaments: Their Formation and an Evaluation of Methods for Studying Them", Arc. Biochem. Biophys., Vol. 365 (1), pp. 55-62 (1998).
12. L. Yang, M. Anantram, J. Han, and J.P. Lu, "Band-gap Change of Carbon Nanotubes: Effect of Small Uniaxial and Torsional Strain", Physical Review B, Vol. 60(19), pp. 13874-13878 (1999).
13. L. Yang and J. Han, "Electronic Structure of Deformed Carbon Nanotubes", Physical Review Letters, Vol. 85 (1), pp. 154-157 (2000).
14. M.P. Anantram and T.R. Govindan, "Conductance of Carbon Nanotubes with Disorder: A Numerical Study", Physical Review B, Vol. 58 (8), pp. 4882-4887 (1998).
15. M. Anantram, S. Datta, and Y. Xue, "Coupling of Carbon Nanotubes to Metallic Contacts", Physical Review B, Vol. 61 (20), pp. 14219 (2000).
16. T. Yamada, "Analysis of Submicron Carbon Nanotube Field Effect Transistors," Applied Physics Letters, Vol. 76 (5), pp. 628-630 (2000).

17. M. Menon and D. Srivastava, "Carbon Nanotube "T-junctions": Nanoscale Metal-Semiconductor-Metal Contact Devices", Physical Review Letters, Vol. 79, pp. 4453-4456 (1997).
18. D. Srivastava, M. Menon, and K. Cho, "Nanoplasticity of Single-wall Carbon Nanotubes Under Uniaxial Compression,"Physical Review Letters, Vol. 83 (15), pp. 2973-2976 (1999).
19. M.A. Osman and D. Srivastava, "Temperature Dependence of Thermal Conductivity in Single Wall Carbon Nanotubes", Applied Physics Letters (2000).
20. D. Srivastava, D.W. Brenner, et al, "Prediction of Enhanced Chemical Reactivity at Regions of Local Conformational Strain on Carbon Nanotubes: Kinky Chemistry" Journal of Physical Chemistry, B., Vol. 103, pp. 4330-4337 (1999).
21. J. Han, A. Globus, R. Jaffe and Glenn Deardorff, "Molecular Dynamics Simulation of Carbon Nanotube Based Gears", Nanotechnology, Vol. 8, pp. 95-102 (1997).
22. D. Srivastava,"A Phenomenological Model of the Rotation Dynamics of Carbon Nanotube Gears with Laser Electric Fields", Nanotechnology, Vol. 8, pp. 186-192 (1997).
23. F. Dzegilenko, D. Srivastava, and S. Saini, "Nanoscale Etching and Indentation of Silicon (111) Surface with Carbon Nanotube Tips", Nanotechnology, Vol. 10, p. 253 (1999).
24. C.W. Bauschlicher, A. Ricca, and R. Merkle, "Chemical Storage of Data", Nanotechnology, Vol. 8, pp. 1-5 (1997).
25. C.W. Bauschlicher and M. Rosi, "Differentiating Between H or F and CN on C(111) of Si(111) Surfaces", Journal of Physical Chemistry B, Vol. 102, pp. 2403-2405 (1998).
26. M. Menon and D. Srivastava, "Structure of Boron Nitride Nanotubes: Tube Closing Versus Chirality", Chemical Physics Letters, Vol. 307, pp. 407-412 (1999).
27. C.Z. Ning, S. Hughes, and D.S. Citrin, "Ultrafast Modulation of Semiconductor Lasers Through a Terahertz Field, "Applied Physics Letters, Vol. 75 (4), pp. 442-444 (1999).
28. A. Liu and C.Z. Ning, "Terahertz Optical Gain Based on Intersubband Transitions in Optically Pumped Semiconductor Quantum Wells: Coherent Pump-Probe Interactions," Applied Physics Letters, Vol. 75 (9), pp. 1207-1209 (1999).