Dean’s message

In each century, one or two technological breakthroughs emerge that are so novel, so fundamental in their impact on our world, that they are regarded as transformative. Nanotechnology may very well be the defining applied technology of our time. One nanometer measures $10^{-9}$, or one-billionth of a meter. Because nanotechnology involves the manipulation of matter at the atomic or cellular level, it holds the potential to change everything we do, from drug delivery and imaging to self-cooling garments, solar cells and semiconductors to quantum computers. The possibilities appear endless.

Nanotechnology is the revolution of the 21st century, and we at UConn are engaged in a wide range of research aimed at better understanding how nanotechnology may be integrated into diverse applications to improve our lives. We are fortunate to reside in a state that is both supportive of, and in fact leading, technological developments in this fundamental area. In early 2008, Connecticut Governor M. Jodi Rell announced that the State would support $5 million in nanotechnology-oriented industry-university partnerships at Yale University and the University of Connecticut. Amid this supportive, highly collaborative atmosphere, we at UConn view nanotechnology as a pivotal part of our larger research foci, which include our Eminent Faculty Initiative in Sustainable Energy and our selection as the lead research institution in a newly formed DHS network of Centers of Excellence in Transportation Security.

We invite you to examine the following presentations, which were delivered during a half-day forum on nanotechnology here at UConn. Through these overviews, you will gain a snapshot of activities ongoing at UConn and glimpse a sliver of the future.

Sincerely,

Mun Y. Choi
Dean, School of Engineering
University of Connecticut
Acknowledgements

We wish to express our sincere thanks to UConn President Michael Hogan and Provost Peter Nicholls, for their ongoing support. In addition, we thank the following individuals, whose support made this forum possible: Greg Anderson, Elliot Ginsberg, Robert Mansfield, Harris Marcus, Stephen Andrade, Louis Manzione, Carl Nett, Lisa Troyer, Donna Cyr, Michael Newborg and Mansoor Khan. We would also like to thank our SoE Advisory Board members Tom Martin and Steve Heath for attending the workshop.

We wish to thank our researchers for their enthusiasm and scholarly excellence, amply demonstrating their leadership at the forefront of nanotechnology.

In addition, we thank our attending faculty members, undergraduate and graduate students for their strong support in making this event a success.

Finally, we would like to thank our able staff members whose efforts contributed toward the success of this forum: Noreen Wall, Orlando Echevarria, Chris LaRosa, Donna Thibault and Diane Perko.
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Nanotechnology in Manufacturing: Areas of Interest

UCONN SOE Nanotechnology Research Forum
Robert E. Mansfield, Jr., Brig Gen, USAF (RET)
Director, National Center for Aerospace Leadership
5 March 2008
Opportunities in Aerospace and Defense

• National Nanotechnology Initiative: 13 Agencies involved
  – NSF, DoD & DOE ~ 70% R&D spending
    • DoD largest over all: $450M in ’07; $487M (est) in ’08; $431M (proposed in ’09)
    – There are growing investments in Nano-manufacturing (1 of 8 investment areas)
      • $48.1M in ’07; $50.2M in ‘08; $62.1M in ’09
  • Manufacturing at the nano-level is vital; but important too is the ability to machine, maintain and apply nano-materials and coatings.
    – Investigation and investment in this area needed to transition manufacturing base
  • Aerospace and Defense are looking for materials that:
    – Are more durable; lighter; stronger; smaller; conductive; adaptive and reconfigurable (responsive to external stimuli)
    – Accelerate information processing
Areas of Interest at CCAT

Transformation of manufacturing processes as well as impacts on maintenance, repair and overhaul (MRO)
- Laser based surface engineering at the micro and nano levels
- Surface finishing/machining for enhanced durability and tribology
- Metrology for assured performance

Enhancement of materials characteristics
- Durability (composites and coatings)
- Multi-functional performance (thermo/chemical/structural/electrical)

Devices for in-process control and system performance
- Embedded sensors/diagnostics
- Component and system performance optimization

Potential Areas of Collaboration
Building Momentum - Connecticut’s Nanotechnology Strategy

UConn School of Engineering Nanotechnology Research Forum

March 5, 2008

Steve Andrade
Battelle Technology Partnership Practice
Why Nanotechnology Matters ...

– Nanotechnology viewed by many as leading the next industrial revolution.

– Critical driver for creating and retaining jobs in Connecticut

**Economic Impact**

– Direct: By 2014, Lux Research estimates a $2.9 trillion impact affecting nearly every type of manufactured good.

– Key innovation driver for emerging and established companies.

– Key competitive driver for industry:
  - Alter supply chains
  - Alter cost structures
  - Alter replacement and servicing

“The impact of nanotechnology on the health, wealth and lives of people could be at least as significant as the combined influences of microelectronics, medical imaging, computer aided engineering and manmade polymers developed in this century.”

National Science & Technology Council, 2000
already more than 200 nanotech-based products in the marketplace

- Electronic displays and computer chips & processors
- Consumer products such as wrinkle free pants, sun screens, air filtration, sports rackets and waxes to protect cars
- Improved drugs for cancer treatment and cholesterol, wound healing, diagnostics and medical instruments

Source: __________
Nanotechnology is Critical for Connecticut’s Economic Competitiveness

• Broad reach across Connecticut’s existing and emerging manufacturing base – from aerospace to pharmaceuticals and medical devices to industrial electronics to renewable energy.
  – Estimated that 15.4% of mfg revenues in Connecticut will involve nanotechnology components by 2014 – equivalent of approximately 30,000 jobs.

• Growing numbers of emerging and established Connecticut companies putting nanotech to work:
  – Established companies: UTC, ATMI, Mott Corporation
  – Emerging companies: GenCell, MysticMD, Genomas
## Closer Look at Implications of Nanotechnology by Selected Industries: Impacts on Connecticut

<table>
<thead>
<tr>
<th>Selected Product Categories</th>
<th>Connecticut Position Today</th>
<th>2014 Sales Revenue Incorporating Nanotech</th>
<th>Expected Developments</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Aerospace</strong></td>
<td>Very Large Employment (30,956 jobs in 2006) Highly Specialized (420% US avg)</td>
<td>37% (equivalent of 11,453 CT jobs)</td>
<td>More of an enabling technology used for structural composites, new functional coatings, batteries/fuel cells, advanced sensing. May impact the supply chain significantly.</td>
</tr>
<tr>
<td><strong>Industrial Machinery</strong></td>
<td>Large Employment (16,860 jobs in 2006) Specialized (42% higher than US avg)</td>
<td>8% (equivalent of 1,349 CT jobs)</td>
<td>Advanced nano-processing and other nano-tools are a key area for advancing new nanotech company formation. Nanotech tools market could exceed $2.7 B by 2014.</td>
</tr>
<tr>
<td><strong>Industrial Electronics and Instruments</strong></td>
<td>Large Employment (11,710 jobs in 2006) Specialized (37% higher than US avg)</td>
<td>75% (equivalent of 8,783 CT jobs)</td>
<td>Logic chips patterned on nanolithography techniques, memory chips based on nanomaterials, nanostructured chip cooling systems, nanocomposite RF/EMI shielding. Key opportunity for nano-intermediates to arise in 2010-2014 period.</td>
</tr>
<tr>
<td><strong>Pharmaceuticals</strong></td>
<td>Large Employment (9,404 jobs in 2006) Highly Specialized (156% US avg)</td>
<td>23% (equivalent of 2,163 CT jobs)</td>
<td>Advance delivery of therapeutics with major impact in 2010-2014 period. Similar to biotech, Pharma outsourcing nano-research to universities and emerging companies.</td>
</tr>
<tr>
<td><strong>Ships and Submarines</strong></td>
<td>Significant Employment (8,114 jobs in 2006) Highly Specialized (316% US avg)</td>
<td>25% (equivalent of 2,029 CT jobs)</td>
<td>Nanocoatings, polymer fuel cell components, high temperature superconducting wire for motors, nanoparticulate fuel additives, nanosensors</td>
</tr>
<tr>
<td><strong>Medical Devices</strong></td>
<td>Significant Employment (7,823 jobs in 2006) Specialized (69% higher than US avg)</td>
<td>30% (equivalent of 2,347 CT jobs)</td>
<td>Nanocomposite materials, nanocoatings, nanosensors.</td>
</tr>
</tbody>
</table>
One out of three jobs in leading industries based on the use of Nanotechnology in 6 years

Nanotech’s Impact by 2014 in Key CT Industries

Nanotech’s footprint = 27,990 out of a current base of 84,507 jobs
Key Milestones in Connecticut Nanotech Development Efforts

• Five year journey …. Building a roadmap consensus and moving an action plan forward:

2003
• CT Nano Initiative formed (CNI)

2004
• State support for nanotech assessment
• Battelle study on CT Competitive Position

2005
• Legislative support for nano-education & action plan PA 05-198 & SA 05-13
• Formation of statewide nano advisory council
• Action Plan drafted

2006
• PA 06-530 enacting Action Plan
• $500,000 annual appropriation line item
• Pilot initiatives designed

2007
• Nano innovation grants piloted
• Nano Education Consortium efforts underway
• Nano univ-industry fellows initiative piloted
• CT Nanoscale Sciences Center design study
Connecticut Nanotechnology Advisory Council

• **Mission:** To provide advice and support in the development and implementation of strategies to advance nanotechnology development in the state.

• **Convened by** the Governor’s Office for Workforce Competitiveness.

• **Members:** 25 representatives from business, higher education, state and nonprofit development organizations.

• A forum and a voice to advance the agenda

• For further information: [www.nanoworkforce-ct.org/](http://www.nanoworkforce-ct.org/)
Initiatives Underway in Connecticut to Advance Nanotechnology

✓ Nanotechnology Innovation Grants
  – Developed & managed by the CT SBIR Office @ CCAT
  – Small Business seed grants to advance near-term nanotechnology product development
  – Market guidance by large primes to addressing a defined opportunity
  – First pilot on fuel cells for unmanned underwater vehicles – 3 funded projects recently completed

✓ Nanotechnology Education Consortium
  – Under auspices of the Department of Higher Education – development of a statewide 4 course nanotechnology minor
  – 2 layer courses; plus three tracks:
  – 9 higher education institutions involved in shared curriculum development

✓ University-Industry Fellowship Bridge
  – Developed & managed by the CT SBIR Office @ CCAT
  – Connects Connecticut industry with leading-edge nanotechnology developments and talent at research universities
  – Supports graduate students and post-docs addressing a nanotech topic developed in consultation between industry and university
  – 5 pilot projects now underway

➤ Signature Connecticut Center for Nanoscale Sciences
  – Critical missing ingredient from Connecticut Nanotech Action Plan – will require a state, university, industry & federal partnership
  – Provide critical “go to” facility for Connecticut for focused research and applications development
  – Shared use across universities and industry
  – Triple hitter – advance research, commercialization and education
Open Innovation – Initial Collaboration Phase

Initial Phase: CT Industry – University Collaboration on Pre-Commercialization Research

Agent & Process Manager: CT SBIR Office

KEY

- FLOWS
  - Talent
  - Technology
  - Funding

Diagram showing the flow of projects and collaborations between universities, colleges, prime contractors and large companies, innovative small firms and entrepreneurs, and the CT SBIR Office at CCAT. The state support office is also connected to these organizations.
Nanotechnology Small Business Innovation Grants

Projects conducted from February through August, 2007.

• GenCell, Southbury, CT. “Nanocatalyst Reformer in Fuel Cell Stack.” Results to date: Demonstrated technical feasibility of concept; further testing and development required. Initial revenues generated.

• Mott Corporation, Farmington, CT, with CT Global Fuel Cell Center at UConn. “Porous Metal Electrode Assembly.” Results to date: Developed processes to produce more economical and higher performing PEM fuel cells; further development and testing needed.

• MysticMD, Groton, CT with CT Global Fuel Cell Center at UConn. “Membrane Electrode Assembly.” Results to date: Developed a hybrid nanotube supported catalyst with less platinum.

Each firm is now proceeding with further technical and market development efforts to advance these technologies further toward commercialization.
University-Industry Fellowship Bridge Program

A Talent Bridge using the vehicle of applied research projects with industry guidance
Program developed & managed by the CT SBIR Office @ CCAT
5 pilot projects competitively awarded at UConn and Yale with CT companies. $250k provided by OWC (Oct 2007 thru June 2008)

• R. Magnusson, UConn- Dymax, Torrington, CT: “Development of nanoscale imprint technology for efficient fabrication of resonant photonic-crystal devices.”
• M. Shaw, UConn-Anchor Science, Branford, CT: “Conductive Nanoparticle-filled membranes structured for optimum performance”
• G. Sotzing and J. Stuart, UConn- Teleflex Medical, Coventry, CT: “Stabilized Bioactive Nanofiber Composites.”
• S. Suib, UConn - Precision Combustion, North Haven, CT: “Nano-Size Platinum and Platinum Alloy Catalysts for Improved Combustion.”
Education Consortium Initiative

15 member Education Consortium Team--representatives from 9 institutions and Dept of Higher Ed.

A First – a statewide nanotech minor, certified by the CT DHE:

2 “layer” courses plus 2 additional courses from one of three specialization tracks:

- nano-electronics
- nano-biology
- materials and nano-composites

Each course to include safety, environmental & ethics component

Goal: encourage as many colleges and universities in Connecticut to adopt this curriculum.

Next: intro curriculum for K-12, thru Ct Career Choices, other channels
A Critical Gap Remains Between the Vision and Reality of Nanotech Development in Connecticut

Connecticut’s Nanotech Vision
“Connecticut will be recognized as a leading state in the development and application of nanotechnologies to advance new products by existing and newly formed companies anchored by a set of well-established nanotechnology research and education assets across its public and private colleges and universities.”

Today’s Reality ... A Critical Missing Ingredient
- Connecticut is being outflanked by other states because of the lack of “go to” facilities for state-of-the-art nanoscale characterization, prototyping, modeling and testing
- These nanotech facilities are magnets for attracting and retaining top researchers, emerging nano companies and industry-university collaborations

The Gap
Connecticut Lacks “Go To” Signature Facilities in Nanotechnology

• A 2007 technical review, conducted by an national nanotech expert on behalf of the Ct Advisory Council, found that Connecticut’s two leading research universities – UConn and Yale – possess “adequate” facilities for a modest basic research program, but fall well short of “go to” signature facilities that will provide a competitive advantage for researchers, education programs and companies seeking to advance new product innovations.

Specific Gaps in Nanoscale Instrumentation Found in Connecticut

• Advanced state-of-the-art high-resolution imaging and characterization
• Full line of sample preparation equipment
• Structural simulation and molecular modeling tools
• Sufficient clean room and fabrication lines for prototyping
• Tools for studying the structure and chemistry of surfaces and interfaces
Design of CT Center for Nanoscale Sciences and Applications

**Key Program Aspects**

- Access to advanced atomic scale characterization and imaging instrumentation
- Availability of pilot scale prototyping for nanotechnology components and devices
- Expert eminent faculty advancing application of advanced instrumentation
- Pro-active outreach programs providing a single point of contact and technical assistance
- Significant levels of matching funds to state investments
Proposed Approach for Shared Use Facilities

• Co-Investment strategy by State with Yale and UConn
  – Multi-faceted activities… instrumentation, technical support, eminent faculty and pro-active outreach

• Build upon base of existing facilities
  – UConn’s nanotech facilities at Institute of Material Sciences, Center for Cell Analysis & Modeling and School of Engineering
  – Yale’s Institute for Nanoscience and Quantum Engineering (YINQE) … including major new clean room fabrication facility.

• Focus on developing “go to” shared use facilities for advancing Connecticut’s position in fuel cell systems, sensors & detectors and drug discovery & development.

• Ensure access for broad base of Connecticut colleges and universities as well as industry

• Seek federal and private industry investments
Focus of Investments for Connecticut’s Center for Nanoscale Sciences

Specific Investments will include:

- **Advanced tools for comprehensive characterization and high resolution imaging**, such as scanning/transmission electron microscopes, focused ion beam sample preparation, field emission scanning electron microscope, etc.

- **Fabrication tools**, such as E-beam writers

- **Modeling and simulation tools**, involving hardware and software

- **Faculty expertise, user support and ongoing maintenance**

Goal is to create complimentary, yet somewhat unique facilities at Yale and UConn
CT Nanotech Advisory Council Has Identified an “Emerging” Formula to Launching of Connecticut Centers for Nanoscale Sciences

- Projected total cost of ~ $40 million to launch across new equipment and five years of operating support
- “Competitive” level of a state investment -- $20 million
  - Largely targeted to new equipment as co-investments with Yale and UConn
  - **But critical that some level of state support be for operating funds for technical support and pro-active outreach**
  - Governor’s budget provides a start with an investment level of $5 million in capital and additional $500,000 in operating support

- Sources of Investment:
  - $10 - $20 million in direct supporting university investments from Yale and UConn … primarily faculty recruitment, industry support
  - Expectation of remaining funds ~$10-20 million from Federal grants and appropriations; foundations; others over next 5 years
  - Also more than $20 million in leveraged university investments at Yale and UConn

- Formation of an Oversight Committee to guide implementation
Contact:

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Technology Partnership Practice
Battelle
Voice: (508) 669-5560
E-mail: andrades@battelle.org
www.battelle.org/tpp
Developing Energy and Sensor Technologies with Microbes, Nature’s First Nanotechnologists

Ismael I. Nieves\(^1\), Ranjan Srivastava\(^2\) and Kenneth M. Noll\(^3\)

\(^1\)Dept. of Civil and Environmental Engineering
\(^2\)Dept. of Chemical, Mechanical and Biomolecular Engineering
\(^3\)Dept. of Molecular and Cell Biology
Bacteria-catalyzed electrical sources

microbial fuel cells, biobatteries, biosensors
Electrical output from bacterial cells is too low for large-scale applications.
Mass transport limitation is minimal

Measured output from bacterial cells to mediator
448 µA

ANODE

Reduced mediator

Oxidized mediator

Bacterial cell

CO₂ + H⁺

sugar

Measured output from bacterial cells to anode
120 µA
Electron transfer out of cells is rate limiting.

29.4 s\(^{-1}\)  \[\text{ANODE} \quad \text{e}^{-} \quad \text{Reduced mediator} \quad \text{Oxidized mediator} \quad \text{Bacterial cell} \quad \text{sugar} \quad \text{CO}_2 + \text{H}^+\]  0.00232 s\(^{-1}\)
Microbial fuel cells to power small electronic devices

Bacterial cell

Sugar → ANODE → H²O

CO₂

e–

O₂

e–

H₂O

H⁺
Microbial fuel cells as biological sensors

Bacterial cell

External analyte

Sugar

CO₂

e–

ANODE

O₂

e–

CATHODE

H₂O

H+
Alternative fuels from bacteria

Hydrogen from biomass

Thermotoga

Waste management facility

Genomics
Genetics
Biochemical analyses
Advantages of High Temperature \( \text{H}_2 \) Production

- Facilitates the breakdown of complex organic substrates
- Fewer fermentation byproducts
- Precludes intrusion of typical microbial contaminants from biomass feedstocks
- Higher entropy argues for increased \( \text{H}_2 \) production

Acetic Acid Byproduct: Can it be used as a fuel? For fuel cells? For \( \text{H}_2 \) production?
Microdiesel: *Escherichia coli* engineered for fuel production

Rainer Kalscheuer, Torsten Stölting and Alexander Steinbüchel
Westfälische Wilhelms-Universität

Agricultural waste biomass → Microdiesel

Fatty acids → Fatty acid ethyl esters

Sugar → Ethanol
A Novel Method for Micro Injection: Rotationally Oscillating Drill (Ros-Drill ©) Design and Control

Prof. Nejat Olgac
Mechanical Engineering Department, UCONN

Designing Minimally Invasive Mercury-Free μ-drill for Micro Injection
I. Rotationally Oscillating Drill (Ros-Drill©)

Flowchart of the controller program

START

Set sampling time
Set encoder
Set controller

Start button pressed

Y

Measure $T_0$, $T_1$, $A$, $f$

N

Drive the motor

Calculate trajectory

Store trajectory points

Store $T_0$, $T_1$, $A$, $f$

Calculate trajectory

Duration elapsed

N

Stop button pressed

N

Y

Y

Record trajectory points

Controller (PLC)

Driver

Feedback

Encoder

DC Motor

Pipette Holder

Bearings

Coupling

Tubing

Reference
Controlled Rotational Oscillations

Ros-Drill pierces the oocytes by using Rotational Oscillations.
Prototype and Experimental Setup

User Interface

Drill

Pipette holder

Coupling

Micro-motor

Pipette

Bearings

Tubing
Biological Experiments ICSI on mice & Transgenic Drosophila
Summary

- A minimally invasive mercury-free rotationally oscillating $\mu$-drill is designed and tested.

- Transformative impact in the areas
  - ICSI on mice
  - Harvard, U.C. Davis
  - UCONN Animal Science Department
  - Gene injection in fruit flies
  - Indiana University
  - Stem cells sub-cellular substance transfer.
Sponsor

National Institutes of Health (NIH)

For more information:

Advanced Laboratory for Automation
Robotics and Manufacturing

www.engr.uconn.edu/alarm
Advanced Laboratory for Automation Robotics and Manufacturing

www.engr.uconn.edu/alarm
Deformation-induced synthesis of nanostructured metallic materials
Rainer J. Hebert, Girija Marathe, Jyothi Suri, Arif Mubarok, Dharma Maddala

Ongoing Nanoresearch:

Severe plastic deformation processing of bulk nanolaminate materials

Phase stability under driven conditions

Example of Al nanocrystal induced during intense deformation of amorphous Al88Y7Fe5 at room temperature
We try to find answers to questions such as:

- How does the phase stability of amorphous and nanocrystalline materials change under driven conditions (driven: mechanical forcing in our case, electron/ion beams, radiation, electromagnetic fields, ... in general)?

- How can existing theories (based on thermally activated processes) be modified to include driven effects?

- How does the microstructure and the mechanical behavior of elements change at extreme deformation levels and in confined geometries?

Experimental techniques we use:

- Deformation: Dynamic tensile/compression, shear testing, surface wear, accumulative roll bonding

- Analysis: Thermo- and thermomechanical analysis, elastic constants, electron microscopy, mechanical testing (nanoindentation)
**Importance of Research:**

**Applications:**
- Bulk metallic glasses used as coating materials, super strong, corrosion resistant materials
- Nanocrystal dispersions for softmagnetic applications
- High strength sheet, explosive materials

**Materials Science:**
- Deformation behavior of non-crystalline condensed phases
- Phase stability of metastable phases under driven conditions
- Plasticity in confined geometries:

*Cu-Ni multilayer*

T. Foecke, D.E. Kramer,
Int J Fracture119/120 (2003) 351
**Challenges/partnerships:**

1. Collaboration with modeling experts (MD-, DFT simulations)
2. Specialized analysis techniques: scattering experiments (EXAFS, EBSD, “high-end” TEM)
3. Related work:
   - *Multilayers:* geology (multilayer), applied mechanics
   - *Amorphous alloys:* - Collaborations with researchers focusing on deformation of amorphous soft matter
     - Renewed interest in radiation effects on alloys
Dielectric, Pyroelectric and Piezoelectric Response of Ultra-Thin Films of Functional Oxides

S. Pamir ALPAY
Materials Science and Engineering Program, CMBE Department and
Institute of Materials Science

UCONN - School of Engineering
Nanotechnology Research Forum
March 5, 2008, Storrs CT
Degradation of Properties

Possible Reasons:

- Compositional and microstructural inhomogeneities
- Defects
- Internal stresses

Highly Tunable, Temperature Insensitive Ferroelectric Films for Tunable Applications

Description

Joint Tactical Radio System (JTRS) Manpack and Handheld Radios with active tunable ferroelectrics. High tunability (>70%), low loss tangent (<0.01), and temperature insensitive dielectric constant over a 100°C temperature range.

Status

✓ Multiple theoretical tools developed.
✓ Excellent correlation between experimental results.
✓ Theoretical analysis now capable of predicting the tunability as a function of layer thickness and choice of substrate.
✓ Film deposition parameters optimized for BST on commercial metallized Si-wafers

Benefits

◆ Temperature insensitive active device through compositional grading
◆ Si IC compatible
◆ Replacements for more costly non-silicon compatible technologies.
Optimization of Pyroelectric Response of Thin Film Ferroelectrics

Description
Theoretical results indicate a strong dependence of the pyroelectric response of ferroelectric thin films on internal stress levels. Preliminary results show tremendous potential for improving the pyro-response by tailoring internal stresses.

Status
✓ Preliminary theory for epitaxial ferroelectric films developed.
✓ Excellent correlation between experimental results.
✓ Significant deterioration in pyro-properties in the presence of internal tensile stresses.
✓ Theoretical analysis now capable of predicting the pyroresponse as a function of layer thickness and choice of substrate.

Benefits
✓ An order of magnitude increase in the pyroresponse via engineering the stress state.
**Description**

A new class of graded ferroic materials and their active counterparts, transponents, have been developed as the analogues of the transistor. Preliminary experiments, theory, and prototypes show tremendous potential for these new devices.

**Features**

- **Transpacitors**: low cost, ultra-pyroelectric detectors, strain sensors, energy recovery.
- **Transductors**: low cost, magnetometers, position, speed, angle, sensors.
- **Translastics**: actuators, smart muscles.
- **Transponents**: biological, mechanical, optical devices and structures.

**Status**

- Graded ferroelectrics and transpacitors experimentally demonstrated; results replicated by international community.
- Preliminary theory for graded ferroics initiated.
- Broad patents submitted and granted to Delphi.

**Benefits**

- Low-cost, active sensors and actuators
- Can be integrated with silicon, IC compatible
- Replacements for more costly non-silicon compatible technologies.
Algorithms and Architectures for Nanocomputing

Rajasekaran, Ammar, Greenshields, Kim, Mandoiu, Shi, Wu
Advantages of Nanocomputing

- Nanocomputing offers the promise of decreasing the size and gate propagation delays by 2-3 orders of magnitude compared to semiconductor based computers.
Several aspects of nanocomputing are of interest to scientists. For instance, effort is on to synthesize DNA molecules that can function as diodes. From these building blocks one could construct complex bio-circuits. It is conceivable that a hybrid consisting of biocircuits and electronic circuits will work the best. People have also developed DNA computers.
Protein-Based Associative Memory Processors (PBAMP)

- Protein molecules that can serve as associative memory elements have been identified.
- An example is the bacteriorhodopsin protein.
- A substrate coated with a thin film of this protein acts like a hologram with associative memory. Matching applications are many.
- A hologram can also be thought of as a convolution operation.
Bacteriorhodopsin

- Cell member of *Halobacterium salinarium*
- Light-transducing Protein, which converts light energy to chemical energy
- Very high efficiency
- Very small size
- Endure high temperature and intense light
PBAMP Contd.

- We can think of a PBMAP as a computer where convolution is a basic operation (that can be done in one unit of time).
- If convolution can be done in one unit of time, then the following can also be done in one unit of time: multiplying two polynomials, matrix multiplication, prefix sums, sorting, etc.
- Thus PBAMP is a powerful parallel machine!
- Even on the very powerful theoretical Parallel Random Access Machine (PRAM), sorting cannot be done in $O(1)$ time!
Open Problems

- What other basic operations can we achieve using biological entities?
- Build a computational model based on these operations
- Develop efficient (sequential and parallel) algorithms on these models
More Open Problems

- Nanocomputing offers massive parallelism. However, the number of faulty units in a chip could be considerable and hence we need fault tolerant models and algorithms.

- Conceive of commercial applications that can exploit the massive parallelism.

- How do we design trillion-device chips?
Chemical Characterization at High Spatial Resolution: Spectroscopy in the TEM

Jonathan Winterstein, Joysurya Basu and C. Barry Carter
Department of Chemical, Materials and Biomolecular Engineering
University of Connecticut
Research Motivation

Why Cerium Oxide?

- Multiple current and future applications: catalysis-automobile catalytic converters, fuel cell electrolytes, polishing media
- Applications are related to electrochemical properties

\[
\text{La}_2\text{O}_3 \overset{\text{CeO}_2}{\rightarrow} V_0^{**} + 2\text{La}_\text{Ce} + 3\text{O}_0
\]

\[
2\text{CeO}_2 \overset{\text{CeO}_2}{\rightarrow} 2\text{Ce}_\text{Ce}' + V_0^{**} + \frac{1}{2}\text{O}_2 + 3\text{O}_0
\]

Why TEM?

- Resolution: Sub-nm spatial resolution, sub-1 eV energy resolution with EELS
- Cutting-edge TEM spectroscopy: Chemical characterization with atomic resolution

\[
\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{SrTiO}_3
\]

Bosman et al, PRL, 2007

\[
\text{Bi}_{0.5}\text{Sr}_{0.5}\text{MnO}_3
\]

Muller et al, Science, 2008
Recent Research Example: Doped Cerium Oxide Nanoparticles

Ceria nanoparticles doped with La, Gd and Fe have been produced with a low-temperature, aqueous-based synthesis route.

Aberration-corrected STEM-EELS for valence-state mapping (with A. Herzing and I. Anderson at NIST)

In situ reduction of Ce by beam damage

In the future: valence-state mapping by EFTEM
Cerium Oxide Nanoparticles: Representative Spectra

Future Research Questions:

- Can \textit{in situ} TEM data be turned into properties measurements?
- Can these particles do something useful? Can we fabricate a SOFC electrolyte, split water or catalyze a reaction?
- What about interfaces with other materials (e.g. metal nanoparticles and perovskites) and polycrystals?
Environmental Challenges of Nanoparticles and Research Opportunities

A brief overview by Baikun Li and Ross Bagtzoglou

Environmental Engineering Program
Carbon Nanotubes

- Used for coating Microbial Fuel Cell (MFC) electrodes in order to enlarge surface area and enhance bacterial adhesion & associated electricity generation.
Fate of Nanoparticles

- The fate of nanoparticles in the wastewater stream and (in particular) through the treatment process has received very little attention.
- Challenges: 1) to remove these nanoparticles efficiently. 2) to understand their impacts on bacteria (used in the treatment) in wastewater treatment process.

Figure 2 - Microscopic analyses to detect floc formation problems in operation phases.
Fate of Nanoparticles (Cont’d)

- Chaotic mixing is a possible answer to the efficient or enhanced treatment of wastewater with nanoparticles in order to remove them as much as possible (Bagtzoglou & Oates, 2007; Bagtzoglou et al. 2006)

From Téla et al. (2005)


Fig. 3. Shape of a dye (fluorescein) droplet (of initial diameter about 1 cm) after stirring on the surface of a thin layer of glycerol in a Petri dish. The stirring protocol is that of the experiment by Villenave and Duplat [21]; a number of parallel cuts is made by a rod through the fluid in two directions in an alternating manner. Experiment carried out by J.M. Jiménez, K.G. Szabo, T. Tél, and M. Wells at the von Kármán Laboratory of Eötvös University, Budapest.
Chaotic Mixing in a Bio-Reactor and Enhanced Sorption
Fate of Nanoparticles (Cont’d)

- The ultimate fate of nanoparticles in the hydrosphere (after they enter it post treatment process) and how they propagate in the groundwater, rivers, and lakes has not been studied fully yet. Can their transport be modeled as colloids?
Hierarchical Assembly of Low-dimensional Nanostructures for Energy, Environment and Sensing Applications

Puxian Gao

Department of Chemical, Materials and Biomolecular Engineering
& Institute of Materials Science
University of Connecticut

03/05/2008
Hierarchical nanostructures assembly

I. Vapor phase deposition
II. Solution based synthesis

1) II-VI semiconductors: ZnO, ZnMgO, ZnCdO, ZnS, ZnSe, CdTe, etc.
2) III-V semiconductors: GaAs, AlN etc.
3) Complex functional oxides: ABO3
Sustainable Energy and Environment

Power Source_ Hearts to Nanodevices and Nanosystems

1) Solar cell
2) Thermoelectricity
3) New Catalysts
Large scale nanowire sensors
There are claims for high carrier mobility for quasi-1D devices (diameter < 50 nm). How can we measure such small devices?

If there were no noise
Stochastic resonance could bring some balance to all walks of life.

Use random noise to increase sensitivity.
Simulation: Data + Noise: Sample (1fF): Average

Hazer's Reconstruction
Simple Averaging

Average of 5x10^4 traces acquisition with 1 fF resolution
Simulation for 10 aF equipment resolution

Averages of 1000 traces

Stochastic Resonance

μ = 0 aF
ε_{avg} = 3.1 aF

μ = 4.2 aF
ε_{avg} = 0.17 aF

ambient fluctuation

μ = 54 aF
ε_{avg} = 1.4 aF

μ = 300 aF
ε_{avg} = 8.3 aF

Stochastic resonance
ambient fluctuation level

ε_{onset} (aF)
σ_{fluctuation} (aF)

10^3 traces
5x10^4 traces
$L_{\text{poly}} \sim 140 \text{ nm}$  $W_{\text{eff}} \sim 50 \text{ nm}$  $I_d \sim 0.8 \text{ mA/\mu m (}V_d = 2.8 \text{ V)}$

- $\Delta C_{g-s/d}$ (aF)
- $\Delta G_{g-s/d}$ (pS)
- $V_g$ (V)

- Calibration pads
- Raw data

- $m_0$
- $m_1$
- $m_2$

- $C_{\text{inv}}$

- $C_{\text{inv}}$ (aF)

- $I_d$ (\(\mu\)A)
- $\mu_{\text{eff}}$ (cm$^2$/V.s)

- $Q$ (# of e-)

- $V_d = 2.8 \text{ V}$
- $0.1 \text{ V}$

- $L_{\text{poly}} \sim 140 \text{ nm}$  $W_{\text{eff}} \sim 50 \text{ nm}$  $I_d \sim 0.8 \text{ mA/\mu m (}V_d = 2.8 \text{ V)}$
Noise + repeated measurements → Precision

Non-linear nature of FET → Accuracy +

No resolution limitation for stable devices
Nanoscale Property Measurements & Mapping

Bryan D. Huey

Institute of Materials Science and Chemical, Materials, & Biomolecular Engineering

• Atomic Force Microscopy allows nanoscale measurements by probing surfaces with a sharp tip

• Nanomechanics: AFM and living cells (and optics)

• Electronic Properties: Ferroelectrics (and High Speed AFM)
AFM and living cells

- In situ optics and AFM provide a unique opportunity for coupled measurements.

Effects of EGF Exposure on HaCaT cells with 95% confidence interval

Elastic Modulus of Cells (Pa)

- 1.0 kPa
- 0.64 kPa
- 0.47 kPa
- 0.40 kPa

Length of Exposure to 25 ng/mL EGF (hours)

N = 47
N = 24
N = 24
N = 24

with B. Aneskievich (Pharmacy), and D. Knecht (MCB)
Ferroelectrics

- Applied in dielectrics and high density / low power / ‘instant-on’ memory devices (FeRAM).
- Still uncertainty about nanoscale/nanosecond properties.
- Study with high speed AFM.

\[ \text{Piezoactuation (} z_i \text{)} = -d_{zz} \times V_{\text{applied}} \times \theta \]
Mapping Dynamics

- Fast and local measurements are useful...
- But mapping provides new insights.
- Mechanical, electric, and magnetic fields can also be rapidly imaged.

**Hysteresis Loops**

**Switching Mapping**

**Switching Voltage**

**High speed switching**

**Pixel piezoresponse (au)**

**Vdc (Volts)**

**switched area (%)**

-0.2 0.4 0.6 0.8
time (msec)

0 25% 50% 75% 100% switched area (%)
Quantum Dot Gate FETs and Memory Devices: Modeling and Processing of Nanoarchitectures

F. C. Jain, E. Heller*, F. Papadimitrakopoulos, L. Wang, 
J. Ayers, and J. Chandy
Department of Electrical and Computer Engineering, UConn,
* RSoft Design Group, Ossinings, NY 10562

Supported by ONR Contracts and NSF Grants
Students: M. Gogna, F. Alamoody, E. Suarez, P-Y. Chan,
S. Karmakar, P. Gogna, R. Velampati** and A. Rodriguez**
Technical Support from: J. Fikiet and T. Zera
ID-VG Plot of a 3-State QD FET

Two layers of SiO_x-coated Si quantum dots

3-State QD FET

ID-VG Plot showing threshold shift

Floating Gate (SiO_x-coated Si quantum dots)

QD gate nonvolatile memory
Quantum Simulation of 3-State Behavior
Circuit Simulation of QD-FET Comparator and 3-state Inverter

QD-FET Comparator

QD-FET CMOS Inverter
FROM PROTEINS TO NANO-MACHINES

Kazem Kazerounian and Horea Ilies
Department of Mechanical Engineering
University of Connecticut
National Science and Technology Council (NSTC)

Addendum to the President’s 2006 Budget Request submitted to the US Congress

- ... the ability to create, control and manipulate organized matter at nanoscales will lead to an industrial and technological revolution.

- ... one of the strategic national priorities identified in the NSTC report is the development of “new mathematical and simulation capabilities and tools with high spatial and temporal resolution to guide experimental investigations” at nanoscale.
From Proteins to Nano-Machines

- Nano-machines: the next industrial revolution?
  - In vivo carriers for pharmaceutical substances;
  - Robots, grippers;
  - Switches and sensors
  - ...

- Proteins
  - nature’s time tested (and refined) solution
  - Prōtos: first or primary (of prime importance)
  - Conformational proteins are essentially (binary) switches;
  - highly parallel processes;
From Proteins to Nano-Machines

- Challenges:
  - nano-seconds timescales
    - physical observations are very difficult
    - computational issues
  - very large non-linear systems
  - simulating the effects of external stimuli
    - force models
    - multiphysics
  - protein folding is (arguably) the “problem of the century”
From Proteins to Nano-Machines

- What do we do?
  - Algorithms from robotics to minimize the potential energy (Protofold);
  - Develop *ab initio* protein folding for
    - Analysis, and
    - Design;
  - Path planning through high dimensional energy landscapes
    - New propensity maps;
  - Workspace analysis.
Nanomaterials in sensing/biosensing

Yu Lei

Department of Chemical, Materials & Biomolecular Engineering

- With the development of nanotechnology in recent years, considerable attention has been paid to use novel nanomaterials to achieve fast, sensitive, and selective determination of chemical and biological species.

Metal oxides glucose sensor/biosensor

Isoelectric point (IEP) of ZnO ~9.5 and GOx IEP~4.2,
Operating pH 7.4

ZnO nanorod
Metal oxides in sensing/biosensing

(a) ZnO nanocomb

(b) CuO nanosphere

(c) CuO fishbone

(d) CuO sisal-like
SWNT Sensors for Organophosphates and Explosives
Non-Woven SWNT Film based sensor

- Non-woven single-walled carbon nanotube films were synthesized by the floating chemical vapor depositions (CVD) using ferrocene as the catalyst in a quartz tube.
- The as-prepared SWNT film shows excellent mechanical property and conductivity.
Nanofiber based sensor/biosensor

Theron et al 2001
Carbon Nanotube Synthesis by Open-Air Chemical Vapor Deposition

Kingham Kwok, Andrew C. Lysaght, Jeffrey J. Lombardo, and Alex P. Cocco

PI: Wilson K. S. Chiu

Chiu Research Laboratory
Department of Mechanical Engineering
Open-Air Carbon Nanotube Synthesis

- Open-air synthesis
- Selective deposition
- High growth rate
- Continuous process
- Successfully deposited coatings

Experimental Apparatus
Carbon Nanotube Growth

Deposition Model

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$A_n$</th>
<th>$\beta_n$</th>
<th>$E_{a,n}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Gas Phase Reactions:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>r1 $\text{CH}_4 + \text{H} \leftrightarrow \text{CH}_3 + \text{H}_2$</td>
<td>$2.2 \times 10^4$</td>
<td>3.0</td>
<td>8750</td>
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<tr>
<td>r2 $\text{CH}_3 + \text{H} \leftrightarrow \text{CH}_2 + \text{H}_2$</td>
<td>$9.0 \times 10^{13}$</td>
<td>0.0</td>
<td>15100</td>
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<tr>
<td>r3 $\text{CH}_2 + \text{H} \leftrightarrow \text{CH}_1 + \text{H}_2$</td>
<td>$1.0 \times 10^{18}$</td>
<td>-1.56</td>
<td>0.0</td>
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<tr>
<td>r4 $\text{CH}_1 + \text{CH}_2 \leftrightarrow \text{C}_2\text{H}_2 + \text{H}_1$</td>
<td>$4.0 \times 10^{13}$</td>
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<td>0.0</td>
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<tr>
<td>r5 $2 \text{H} + \text{H}_2 \leftrightarrow 2 \text{H}_2$</td>
<td>$9.2 \times 10^{16}$</td>
<td>-0.6</td>
<td>0.0</td>
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<tr>
<td>r6 $2 \text{H} + \text{M} \leftrightarrow \text{H}_2 + \text{M}$</td>
<td>$1.0 \times 10^{18}$</td>
<td>-1.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

**Surface Reactions:**

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$A_n$</th>
<th>$\beta_n$</th>
<th>$E_{a,n}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>sr1 $\text{S} + \text{H} \rightarrow \text{H}(s)$</td>
<td>$1.0 \times 10^{13}$</td>
<td>0.0</td>
<td>0.0</td>
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<tr>
<td>sr2 $\text{H}(s) + \text{H} \rightarrow \text{S} + \text{H}_2$</td>
<td>$1.3 \times 10^{14}$</td>
<td>0.0</td>
<td>7.3</td>
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<tr>
<td>sr3 $\text{S} + \text{CH}_3 \rightarrow \text{CH}_3(s)$</td>
<td>$5.0 \times 10^{12}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>sr4 $\text{CH}_2(s) + \text{H} \rightarrow \text{S} + \text{CH}_3$</td>
<td>$3.0 \times 10^{13}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>sr5 $\text{S} + \text{C}_2\text{H}_2 \leftrightarrow \text{C}_2\text{H}_2(s)$</td>
<td>$8.0 \times 10^{10}$</td>
<td>0.0</td>
<td>7.7</td>
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<tr>
<td>sr6 $\text{S} + \text{CH}_4 \rightarrow \text{C}(s) + 2 \text{H}_2$</td>
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<td>**</td>
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<tr>
<td>sr7 $\text{S} + \text{C}_2\text{H}_2 \rightarrow \text{C}_2(s) + \text{H}_2$</td>
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<tr>
<td>sr8 $\text{CH}_3(s) + \text{H} \leftrightarrow \text{CH}_2(s) + \text{H}_2$</td>
<td>$2.8 \times 10^{7}$</td>
<td>2.0</td>
<td>7700</td>
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<tr>
<td>sr9 $\text{CH}_2(s) + \text{H} \leftrightarrow \text{CH}(s) + \text{H}_2$</td>
<td>$2.8 \times 10^{7}$</td>
<td>2.0</td>
<td>7700</td>
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<tr>
<td>sr10 $\text{CH}(s) + \text{H} \leftrightarrow \text{C}(s) + \text{H}_2$</td>
<td>$2.8 \times 10^{7}$</td>
<td>2.0</td>
<td>7700</td>
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<tr>
<td>sr11 $\text{C}_2\text{H}_2(s) + \text{H} \leftrightarrow \text{C}_2\text{H}(s) + \text{H}_2$</td>
<td>$9.0 \times 10^{6}$</td>
<td>2.0</td>
<td>5000</td>
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<tr>
<td>sr12 $\text{C}_2\text{H}_1(s) + \text{H} \leftrightarrow \text{C}_2(s) + \text{H}_2$</td>
<td>$9.0 \times 10^{6}$</td>
<td>2.0</td>
<td>5000</td>
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<tr>
<td>sr13 $\text{C}(s) + \text{NT} \rightarrow \text{S} + \text{C(NT)}$</td>
<td>$1.3 \times 10^{12}$</td>
<td>0.0</td>
<td>31104</td>
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<tr>
<td>sr14 $\text{C}_2(s) + \text{NT} \rightarrow \text{S} + 2 \text{C(NT)}$</td>
<td>$1.3 \times 10^{12}$</td>
<td>0.0</td>
<td>31104</td>
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</table>

Modified Arrhenius equation:

$$k_{f,n} = A_n T^{\beta_n} e^{-\frac{E_{a,n}}{R_n T}} \quad k_{r,n} = \frac{k_{f,n}}{K_{C,n}}$$

Species generation:

$$R_i = \sum_n \left( \delta_r - \delta_f \right)_{n,i} \left( k_{f,n} \prod_k C_{k,n,k}^{\delta_{f,n,k}} - k_{r,n} \prod_k C_{k,n,k}^{\delta_{r,n,k}} \right)$$

** Denotes “cracking” mechanism:

$$k_{f,n} = S \frac{P}{\sqrt{2 \pi m_{\text{mix}} k_b T}} \frac{A^*}{\rho_s^2 C_{\text{tot}}}$$
Deposition Arrhenius Plot:

Nanostructured Resonant Leaky-Mode Photonic Devices

Robert Magnusson
Nanophotonics Device Group
Department of Electrical & Computer Engineering
University of Connecticut

Presented by: Mehrdad Shokooh-Saremi

SoE Nanotech Forum
3 March 2008
Guided-mode resonance or leaky-mode resonance

Interaction of waveguide modes and diffracted waves in periodic nano-patterned layers and photonic crystals.

Active and potential applications

- Narrow-band reflection/transmission filters
- Wide-band reflection/transmission filters
- Tunable filters, EO modulators, and switches
- Mirrors for vertical cavity lasers
- Wavelength division multiplexing (WDM)
- Polarization independent elements
- Narrow-/wide-band Reflectors
- Narrow-/wide-band Polarizers
- Security devices
- Laser resonator frequency selective mirrors
- Non-Brewster polarizing mirrors
- Laser cavity tuning elements
- Spectroscopic biosensors
- Tunable display pixels
- Solar cell absorption enhancement
Example 1: Single-layer broadband reflector

Single-layer reflectance spectrum with R=100% across 500 nm bandwidth and rendition of internal magnetic-field structure at resonance.
Example 2: Widely-tunable nanostructured leaky-mode resonant pixels

NEMS: Tunes 100 nm by 115 nm lateral shift; 2-3 pixels cover visible region

\[ \Lambda = 385 \text{ nm} \]
\[ \theta = 0 \text{ degrees} \]
\[ F_1 = 0.15 \]
\[ F_3 = 0.1 \]
\[ d = 200 \text{ nm} \]
\[ n(\text{Si}_3\text{N}_4) = 2.1 \]
Example 3: Silicon/glass single layer polarizer experiment

- Fabricated polarizer has high transmittance (>97%) for TE-polarization and low transmittance (<3%) for TM-polarization.

- Bandwidth: ~40 nm

- Experimental extinction ratio ~97:1 at l = 1510 nm.
Rational DNA Sequence Design for Molecular Nanotechnology

Ion Mandoiu, CSE Department

- DNA is well-known as the carrier of information in living organisms

- Synthetic DNA is becoming a commodity
  - Custom oligonucleotides (up to 160-200 bases)
  - Synthetic genes (<$1/bp, up to 45Kb)
  - **Synthetic genomes** (M. genitalium 580Kb)

<table>
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<tr>
<th>Watermarks</th>
<th>0K</th>
<th>50K</th>
<th>100K</th>
<th>150K</th>
<th>200K</th>
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<th>350K</th>
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<td>1999 Transposons</td>
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<td>Synthetic DNA Cassettes</td>
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<td>Protein Coding Genes</td>
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<td>Structural RNAs</td>
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</tbody>
</table>

Complete Chemical Synthesis, Assembly, and Cloning of a *Mycoplasma genitalium* Genome


*SCIENCE* VOL 319 29 FEBRUARY 2008
Many Emerging DNA Applications

- DNA computing
- DNA mediated assembly of CNTs
- DNA self-assembly
- Molecular detection

Tag Set Design Problem

**Tag Set Design Problem:** Find a maximum cardinality set of DNA tags such that

1. Tags hybridize strongly to complementary antitags
2. No tag hybridizes to a non-complementary antitag

**Hybridization Models**

- **Hamming distance model**, e.g., [Marathe et al. 01]
  - Models rigid DNA strands
- **Longest common subsequence model**, e.g., [Torney et al. 03]
  - Models infinitely elastic DNA strands
- **c-token model** [Ben-Dor et al. 00]:
  - Duplex formation requires formation of nucleation complex between perfectly complementary substrings
  - Nucleation complex must have weight $\geq c$, where $\text{wt}(A)=\text{wt}(T)=1$, $\text{wt}(C)=\text{wt}(G)=2$ (2-4 rule)
Cycle Packing Algorithm [MT06]

Experimental results for l=20

<table>
<thead>
<tr>
<th>c</th>
<th>LP Approx</th>
<th>Cycle Packing</th>
<th>% Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>3</td>
<td>17</td>
<td>466%</td>
</tr>
<tr>
<td>5</td>
<td>9</td>
<td>40</td>
<td>344%</td>
</tr>
<tr>
<td>6</td>
<td>26</td>
<td>72</td>
<td>176%</td>
</tr>
<tr>
<td>7</td>
<td>75</td>
<td>178</td>
<td>137%</td>
</tr>
<tr>
<td>8</td>
<td>220</td>
<td>383</td>
<td>74%</td>
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<tr>
<td>9</td>
<td>641</td>
<td>961</td>
<td>49%</td>
</tr>
<tr>
<td>10</td>
<td>1854</td>
<td>2344</td>
<td>26%</td>
</tr>
</tbody>
</table>

1. Construct c-token factor graph $G$
2. $T \leftarrow \emptyset$
3. For all cycles $C$ defining periodic tags, in increasing order of cycle length,
   - Add to $T$ the tag defined by $C$
   - Remove $C$ from $G$
4. Perform an alphabetic tree search and add to $T$ tags consisting of unused c-tokens
5. Return $T$

- **Ongoing work**: temperature programming, oligo design for gene synthesis
- **Acknowledgements**: D. Trinca, UCONN Research Foundation, NSF CAREER Award IIS-0546457
High Performance Modeling and Simulation of Nanoscience and Nanotechnology

Ammar, Rajasekaran, Greenshields
Motivation

- Developments in computational methods could lead to rapid advances in many research areas including nanoscience and nanotechnology.
- Nanosystems are highly complex and require intensive computation, sophisticated algorithms, and simulations running on state of the art supercomputers.
- One reason why we have failed so far to make a good case for increased funding in supercomputing is that we have not yet made a compelling case.
**Computationally Intensive Problems for modeling and simulation of nanosystems**

- Fast Fourier Transform
- Dense Linear Algebra
- Sparse Linear Algebra
- Monte Carlo Simulations
- Optimization / solution of nonlinear systems (simulated annealing)
- Particles methods, Structured Grid and non-structured Grid
Our Approach

- Develop sequential algorithms that are superior to existing ones.
- Develop innovative parallel algorithms for different architectures.
- Search for a balanced system (unified algorithms) that can perform well for a variety of problems that will meet future scientists’ and engineers’ needs.
- High performance simulation of complex systems with nanoscale computing architectures.
- High performance modeling and simulation to study different phenomena in nanosciences and nanotechnology.
Advances in technology are making massive data sets common in many scientific disciplines including nanoscience and nanotechnology.

Data mining: finding useful information in these data sets. Data mining methods are well recognized analytic tools for finding potentially useful patterns and dependencies in massive dataset.

Parallel and distributed algorithms are required to handle the high computational complexity of the data mining process.

High performance algorithms and architectures supporting data mining methods are needed before they can be deployed in nanosciences and nanotechnology.
Image Mining

- Mining nanostructure images: An approach to study the properties of the material at the nanoscale level.
- Similarity between the images. Features such as size and height of nano-particles and inter-particle distance are important in image similarity. But there are no precise notions of similarity or well defined similarity measures.
- Common solutions: the Pixels Flow Functions (PFF) to detect changes in images by projecting the pixel values vertically, horizontally and diagonally.
- Local-Global Graph (LGG), for evaluating modifications in digital images and defining patterns and determining structural associations (relationships).
- Our roadmap is to develop innovative high performance image mining algorithms
Available expertise

- A wide varieties of high performance algorithms
- Less Talk to reduce communication cost among parallel processors and achieve linear speed up.
- Multi-core architectures (multi-threading)
- Mapping (static and dynamic) algorithms to architecture under for different operating conditions with possibility of failure
- Image processing techniques
- Performance evaluation and analysis methods
- Real-time applications
Nano-Engineering for Hydrogen Storage Applications

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Department of Chemical, Materials and Biomolecular Engineering
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Volume of 4 kg of Hydrogen Stored in Different Ways (250 Mile Range)

- Mg$_2$NiH$_4$
- LaNi$_5$H$_6$
- H$_2$ (liquid)
- H$_2$ (200 bar)
The hydrogen release rate is diffusion-controlled and thus very slow. In contrast, hydrogen uptake is very fast because of cracking and spallation of the product layer from the reactant core.
Nano-Engineering and Mechanical Activation to Enhance Hydrogen Uptake/Release Kinetics

1. Nano-engineering to decrease the diffusion distance.
2. Increasing the composition gradient to enhance diffusion via advanced catalysts.
3. Increasing the diffusion coefficient to augment the diffusion rate via mechanical activation and doping.
Grand Challenges for Advanced Hydrogen Storage Materials

1. **Novel materials:** high storage capacities (> 10 wt% H$_2$) and fast hydrogen uptake/release rates at temperatures below 100$^\circ$C.
2. **Nano-engineering:** narrow size distribution of nanoscale hydrogen storage materials.
3. **Advanced catalysts:** rapid hydrogen uptake and release so that 2 kg H$_2$ per min for refueling below 100$^\circ$C with a plateau pressure of a few bars can be achieved.

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Crystallization of Nanocrystalline Silicon Nanowires Through Self-Heating

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Electrical and Computer Engineering
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Electrical Stressing Conditions

Sudden application of 30 V
→ Breakage before current could be measured.

SEM: a smooth wire texture
single-crystal formation?
1 μs, 30 V
$I_i (@1V) = 30 \mu A$
$I_f (@1V) = 46 \mu A$

melting of different length wires with 1μs, 30 V

1 μs, 30 V
$I_i = 18 \mu A$
$I_f = 29 \mu A$

1 μs, 30 V
$I_i = 22 \mu A$
$I_f = 41 \mu A$

1 μs, 30 V
$I_i = 22 \mu A$
$I_f = 44 \mu A$
1 μs, 30 V  
$I_i (\@1V) = 20 \mu A$  
$I_f = 41 \mu A$  
partially melt & re-solidified

1 μs, 40 V  
$I_i = 21 \mu A$  
$I_f = 51 \mu A$  
fully melt & re-solidified

2.5 x current increase after stress
Initial = 13 $\mu$A ($V_{ds}$ = 1 V)  $V_{Pulse}$ = 30 V (1 $\mu$s)

Final = 40 $\mu$A ($V_{ds}$ = 1 V)

Repeated pulses with sufficient cool-down time did not change conductivity.

Wire broke after 10 pulses with 0.5 ms period

Formed a thin ribbon

+V

ground

smooth

granular (no change)

(Jaggedness on the edges is due to vibrations during SEM imaging)

Close-up SEM of a wire zoomed in at + terminal end after repeated pulses
DC Voltage Sweeps – Heating Asymmetry

0 to + 40 V

V+  0 V

W = 340 nm

0 to - 40 V

V-  0 V

W = 310 nm

Hot spot forms close to negative terminal!
$$I_{th} = 300 \, \mu A, \, 1 \, \mu s$$

$$L_{wire} = 5 \, \mu m,$$

$$W_{wire} = 250 \, nm,$$

$$thick_{wire} = 80 \, nm$$

~ 0.7 \, \mu m

Temperture (K)

Position (\mu m)

$T_{melt}$

$pad$

$wire$

$pad$

Distance and Magnification:

WD = 10 mm

Aperture Size = 30.00

Mag = 42.71 K X

EHT = 9.91 kV

Pixel Size = 8.3 nm

Signal A = Si

Date: 8 Aug 2013

Signal B = Fe

56.48
Summary

• Electrical stress as a fabrication technique
• Extremely smooth surfaces
• SEM observation of asymmetric melting and re-solidification processes (DC optical observation of asymmetric heating)
• Rich physics: coupled charge, heat and mass transport
• Device applications
  – thermoelectric devices
  – high performance TFTs
  – solar cells
  – phase change memory, filament memories
Nano-OptoElectronic Integrated Circuits

G.W.Taylor, ECE Dept.

Electronic + Optoelectronics

- OE oscillators
- OE Flip Flops
- OE counters

Optoelectronic Functions
- Transmit, Receive, Modulate, Filter

Detection, Sensing & Imaging

Digital Logic
- ALU’s
- Registers, etc

Linear circuits
- LNA’s etc

Electrical In

GaAs Substrate

Electrical Out

Optical In

Optical Out

Mar. 5, 2008
Nano Technology

• All devices based upon Molecular Beam Epitaxy on GaAs

• All devices (O & E) utilize a Modulation Doped Quantum Well Interface as the active region

• Nano-electrical feature size is submicron FET gate length

• Nano-optical feature size is submicron DFB grating element

• One epitaxial growth and one fabrication sequence required

• Fabrication technology based upon sputtered refractory metals, RIE, PECVD, ion implantation, RTA, E-gun dielectrics, alloy contacts
III-V O & E Integrated Device Capability

**Electronic**
- NHFET
- pBicFET (bipolar)
- Thyristor (dual input nonlinear thresholding device with memory)

**Optical**
- Photo-NHFET (detector)
- Absorption/Phase Modulator
- Photobipolar (detector)
- Directional Coupler
- Linear Optical Amplifier
- O/E switch – thyristor functions as detector or DFB laser with E→O and O→E switching between states
Thyristor Operation Linear & Logarithmic

Three Terminal Thyristor (20 um) With Different Current Injection

Two Terminal

Three Terminal
Photo Bipolar
Applications

• Optical Communications – single chip transceivers

• Wireless Communications-high speed AD conversion

• Radar - Optically interconnected and controlled T/R modules

• Computers-Optical I/O and digital EO functions

• Sensing – 2D imaging for visible, NIR, LWIR, VLWIR, THZ

• Single photon counting (quantum encryption)

• Long wavelength lasers/detectors for FSO communications
Information-Theoretic Analysis of Defect Tolerance in Nanocomputing Systems

Lei Wang and Faquir Jain
Department of Electrical and Computer Engineering
University of Connecticut

Graduate students: Jianwei Dai, Niral Patel, Shuo Wang, Weiguo Tang

This research is supported by NSF CCF 0621947.
Open problems in the emerging nanocomputing paradigm:

• What is the performance limit imposed by excessive non-idealities inherent in nano/molecular substrates?
• How can we achieve reliable computing with performance approaching the fundamental limit?
• Where are the new opportunities of information processing by exploiting the nonclassical properties of nano/molecular devices?

Our approach to address these problems:

- Architecture
- Implementation independent

- Information Transfer Rate $R$

- Information Transfer Capacity $C$

- Computational Substrates
  - Implementation defects, transient errors, variations

- Information Theoretical Analysis

- Research Tasks
Nanoelectronics as An Information Processing Medium

Nanowire crossbar structure

Information processing channel model

Crosspoint

Input

Output from AND gate arrays

Output from OR gate arrays

Pull-up Arrays

AND gate arrays

Pull-down Arrays

Pull-up Arrays

Pull-down Arrays

OR gate arrays

Output from AND gate arrays

Output from OR gate arrays

X

p = 1

X_{e}

Y

0

1

p = 1

p = 1

X

p = 1 - p_{d}

X_{e}

Y

0

1

p = p_{d}

p = p_{d}

X

p = 1 - p_{d}

p = p_{d}

Y

0

1

p = p_{d}

p = p_{d}

p = 1

Undetermined

X

1

p = 1

X_{e}

Y

0

1

p = 1

Undetermined

X

1

p = 1

X_{e}

Y

0

1

p = 1
Determining the Performance Limit via Information-Theoretic Measures

Relationship between the fundamental limit on reliability ($Cu$) and inherent redundancy ($Nr$) in nanocomputing systems

- Entropy
  \[ H(X) = -\sum_x p(x) \log_2 (p(x)) \]
- Mutual information
  \[ I(Y : X) = H(Y) - H(y_{N-1}, \ldots, y_1, y_0 | X) \]
  \[ = H(Y) - \sum_{i=0}^{N-1} H(y_i | X) \]
- Channel capacity:
  \[ C_u = \max_{p(x)} I(X;Y) \]

RNA nanostructures for imaging and therapy

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Dept. of Chemical, Materials and Biomolecular Engineering
Biomedical Engineering Program
Systematic evolution of ligands by exponential enrichment

RNA library
$10^{12} \sim 10^{14}$

Incubate
Partition
Amplify
Repeat

target protein
Isolate EGFR Aptamer

Concentration (μM)

Bound Fraction

Library

RU Response

Time (s)

E12

RU Response

Time (s)
RNA aptamer-siRNA Nanoconstruct
Structured fuel cell membranes

w/ Robert Weiss
Composites using nano hydroxy apatite particles to boost modulus.

w/ Mei Wei, J. Olson
Nano particle alignment for fast-acting sensors

Silicone + iron particles
\( \phi = 0.03 \)
The Suib Research Group

University of Connecticut

Steven L. Suib
Board of Trustees Distinguished Professor
Yuji Hayashi Distinguished Chair in Plasma Chemistry

Chemistry Department
Institute of Materials Science
Chemical Engineering Department

The Suib Research Group Home Page
http://web.uconn.edu/chemistry/SuibGroup/suibg.html
Research Areas

Manganese Oxides

Solid State Chemistry

Catalysis

Nanotech

Ceramics

Microwaves

Craig

Shantha-Kumar

Vince

Sinue

Edward

Josie

Chris

- Synthesis
- Characterization
- Applications
OMS-2

KMn₈O₁₆·nH₂O

OMS-1

Mg²⁺₀.₉₋₁.₉₄Mn²⁺₀.₉₋₁.₄Mn⁴⁺₄.₄₋₄.₅O₁₂·₄.₅₋₄.₆H₂O

Xiongfei Shen

Structures and Compositions of Octahedral Molecular Sieves (OMS) & Octahedral Layer (OL) Materials.

β-MnOOH

(K,Na)₄Mn₁₄O₂₇·2₁H₂O

Ex⁺
The reaction time was 4 hours. The selectivity was 100 %.
* : The reaction time was 20 hrs.

Inorganic Helices

Jay Durand

Nanolines

Beatriz Hincapie


Nanopatterns

NASA
Micromachine Design for Nanomanufacturing and Micromanipulation

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March 5, 2008
Micromachine for Nanomanufacturing
Invented Microspindle

- Inner flexural cage
- Outer flexural cage
- Flexural coupling
- Flange

± 180°
What the Machine Can Do?

- Positioning resolution: 1 nm;
- Positioning range: 200 μm;
- Positioning accuracy: 10 nm;
- Stiffness: 0.4 N/μm;
- Load capacity: 5 N;
- Radial error in rotation: 1 nm;
- Axial error in rotation: 0.5 μm.
Electronics:
Increased speed, density, sensitivity
Reduced cost and power

What does smaller mean for electronics?

Interaction with individual biomolecules

Increased surface to volume ratio:
Multi input devices
→ new circuits approaches
→ increased functionality

Interesting Physics, new implementations
CMOS is still scaling! Now, with an accelerated rate.

Current industrial research ~15 nm critical dimension

1. Performance (Speed)
   Faster devices
   High packing density
2. Low power (low leakage+)
   - Good $I_{on}/I_{off}$

- Number of challenges and possible advantages at < 30 nm scale

http://www.worthey.com/images/bottleneck.jpg
Leakage Paths

- $I_1$ substrate leakage
- $I_2$ subthreshold leakage
- $I_3, I_4$ gate leakage
- $I_5$ GIDL
- $I_6$ punchthrough

Scaling Factors

- Bulk & Peripheral
  - Bulk
  - Peripheral

- $W, L_{\text{cont}},$ doping [defect], [fixed charge], $P$
- $W, 1/L,,$ doping, etc. [fixed charge]
- $W, L, f(t_{ox})$
- $W,,$ etc.
- $W,,$ etc.
- $-$
Field Effect Transistor Operation

$V$

Gate

$n^{++}$

$n^{++}$
Highly doped drain \(\rightarrow\) n\(^{++}\)-p junction
Low \(V_t\) due to high fixed charge density

**Graph 1:**
- \(W = 1.2 \mu m\)
- \(L = 0.125 \mu m\)
- \(V_{sub} = V_s = 0 V\)
- \(V_g = -1 V\)
- \(I_{ds}\) vs. \(V_{side}\)

**Graph 2:**
- \(W_{si} = 0.6 \mu m\)
- \(L_{poly} = 0.3 \mu m\)
- \(V_{side} = -1.5 V\)
- \(V_{sub} = 0 V\)
- \(V_d = 0.1V, 1V\)

**Graph 3:**
- \(V_d = 0.1V\)
- \(V_d = 1V\)
- \(I_{max}/I_{min} = 3 \times 10^4\)
- \(SS_{min} = 65 mV/dec\)
- \(I_{max}/I_{min} > 6 \times 10^{10}\)
$I_{on} > 1 \text{mA} / \mu\text{m}$

@7.5 MV/cm

$W_{eff} \sim 40 \text{ nm}$

$L_{eff} \sim 150 \text{ nm}$

$V_{side} = -1.5 \text{ V}$

$V_{sub} = 0 \text{ V}$

DIBL = 2 mV/V

SS = 83 mV/dec.

$I_{on}/I_{off} > 10^9$

$V_{g} > 0$

depletion / accumulation boundary

$n^+$ channel

Metallurgical junctions

$V_{side} < 0$
$W < 10 \text{ nm}$

$[\text{hole}] \sim 10^{19}\text{cm}^{-3}$

Increased surface to volume ratio:
- Multi input devices
- → new circuits approaches
- → increased functionality

Surface $[\text{hole}] \sim 4.5 \times 10^{12}\text{cm}^{-2}$ @ each interface

$L_{\text{gate}} \sim 0.2 \mu\text{m} \quad W_{\text{eff}} \sim 7 \text{ nm}$
In Situ TEM of Nanomaterials

Joysurya Basu, Jonathan Winterstein and C. Barry Carter

Dept. of Chemical, Materials & Biomolecular Engineering
University of Connecticut

Thanks to colleagues at NCEM
Technique

1) Choose the TEM

2) Design the specimen

1) Design/buy/modify the TEM holder

2) Record

3) process the data