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NANO SCIENCE AND ENGINEERING IN MECHANICS AND MATERIALS

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Abstract. The transcendent technologies include nanotechnology, microelectronics, information technology and biotechnology as well as the enabling and supporting mechanical and civil infrastructure systems and materials. These technologies are the primary drivers of the twenty first century and the new economy. Mechanics and materials are essential elements in all of the transcendent technologies. Research opportunities, education and challenges in mechanics and materials, including nanomechanics, carbon nano-tubes, bio-inspired materials, coatings, fire-resistant materials as well as improved engineering and design of materials are presented and discussed in this paper.

1. INTRODUCTION

Nanotechnology is the creation of new materials, devices and systems at the molecular level - phenomena associated with atomic and molecular interactions strongly influence macroscopic material properties [according to I. Aksay, Princeton]; with significantly improved mechanical, optical, chemical, electrical... properties. Nobelist Richard Feynman back in 1959 had the foresight to indicate “there is plenty of room at the bottom”. National Science Foundation [NSF] Director Rita Colwell in 2002 declared “nanoscale technology will have an impact equal to the Industrial Revolution”.

In the education area in order to do competitive research in the nanotechnology areas, engineers should also be trained in quantum mechanics, molecular dynamics, etc. The following lists some of the key topics across different scales. The author has been advocating a summer institute to train faculty and graduate students to be knowledgeable in scales at and less than the micrometer (see: http://tam.northwestrn.edu/summerinstitute/Home.htm)

- 10^{-12} m QUANTUM MECHANICS [TB, DFT, HF…]*
- 10^{-9} m MOLECULAR DYN. [LJ...]; NANOMECHANICS; MOLECULAR BIOLOGY; BIOPHYSICS
- 10^{-6} m ELASTICITY; PLASTICITY; DISLOCATION...
- 10^{-3} m MECHANICS OF MATERIALS
- 10^{-0} m STRUCTURAL ANALYSIS

MULTI-SCALE ANALYSES & SIMULATIONS…

The National Science Foundation has supported basic research in engineering and the sciences in the United States for a half century and it is expected to continue this mandate through the next century. As a consequence, the United States is likely to continue to dominate vital markets, because diligent funding of basic research does confer a preferential economic advantage (Wong, 1996). Concurrently over this past half century, technologies have been the major drivers of the U. S. economy, and as well, NSF has been a major supporter of these technological developments. According to the former NSF Director for Engineering, Eugene Wong, there are three *transcendental* technologies:

- Microelectronics – Moore’s Law: doubling the capabilities every two years for the last 30 years; unlimited scalability; nanotechnology is essential to continue the miniaturization process and efficiency.

*TB = TIGHT BINDING METHOD; DFT = DENSITY FTNAL THEORY; HF = HATREE-FOCK APPROX.; LJ = LENNARD JONES POTENTIAL

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- Information Technology [IT] – NSF and DARPA started the Internet revolution more than three decades ago; the confluence of computing and communications.
- Biotechnology – unlocking the molecular secrets of life with advanced computational tools as well as advances in biological engineering, biology, chemistry, physics, and engineering including mechanics and materials.

Efficient mechanical and civil infrastructure systems as well as high performance materials are essential for these technologies. By promoting research and development at critical points where these technological areas intersect, NSF can foster major developments in engineering. The solid mechanics and materials engineering (M&M) communities will be well served if some specific linkages or alignments are made toward these technologies.

Some thoughtful examples for the M&M and other engineering communities are:

- Bio-mechanics/materials
- Simulations/modeling
- Thin-film mechanics/materials
- Micro-electro-mechanical systems (MEMS)
- Wave Propagation/NDT
- Smart materials/structures
- Nano-mechanics/materials
- Nano-electro-mechanical systems(NEMS)
- Designer materials
- Fire Retardant Materials and Structures.

MEMs can be used as platforms for NEMS. Another product of the nanotechnology is carbon nano-tubes [CNT] which are self-assembled in deposition from C-rich vapors, consisted of honeycomb lattices of carbon rolled into cylinders; nm in diameter, micron in length. CNT have amazing properties:

- 1/6 the weight of steel; 5 times its Young's modulus; 100 times its tensile strength; 6 orders of magnitude higher in electrical conductivity than copper; CNT strains up to 15% without breaking
- 10 times smaller than the smallest silicon tips in Scanning Tunnel Microscope - STM [CNT is the world's smallest manipulator]
- CNT may have more impact than transistors
- ideal material for flat-screen TV [~2003]
- similar diameter as DNA
- bridge different scales in mesoscale - useful as bldg. blocks ~ e.g. nanocomposites; gases storage
- metallic or semiconducting
- as single-electron transistor; logic gate
- as RAM – on/off do not affect memory storage - no booting needed.

Sources:

CARBON NANOTUBES – THE FIRST 10 YEARS, *NATURE, 2001.*

MECHANICAL ENGINEERING, ASME, NOV. 2000

TECHNOLOGY REVIEW, MIT, MAR. 2002

Considerable NSF resources and funding will be available to support basic research related to nano science and engineering technologies. These opportunities will be available for the individual investigator, teams, small groups and larger interdisciplinary groups of investigators as well as centers. Nevertheless, most of the funding at NSF will continue to support unsolicited proposals from individual investigator on innovative "blue sky" ideas in all areas including nano science and engineering technologies.

2. NANOTECHNOLOGY

Nanomechanics Workshop

Initiated by the author, with the organization and help of researchers from Brown [K. S. Kim, *et al.*], Stanford, Princeton and other universities, a NSF Workshop on Nano- and Micro-Mechanics of Solids for Emerging Science and Technology was held at Stanford in October 1999. The following is extracted from the Workshop Executive Summary. Recent developments in science have advanced capabilities to fabricate and control material systems on the scale of nanometers, bringing problems of material behavior on the nanometer scale into the domain of engineering. Immediate applications of nanostructures and nano-devices include quantum electronic devices, bio-surgical instruments, microelectrical sensors, functionally graded materials, and many others with great promise for commercialization. The branch of mechanics research in this emerging field can be termed nano- and micro-mechanics of materials, highly cross-disciplinary in character. A subset of these, which is both scientifically rich and technologically significant, has mechanics of solids as a distinct and unifying theme. The presentations at the workshop and the open discussion precipitated by them revealed the emergence of a range of interesting lines of investigation built around mechanics concepts that have potential relevance to microelectronics, information technology, bio-technology and other branches of nanotechnology. It was also revealed, however, that the study of complex behavior of materials on the nanometer scale is in its infancy. More basic re-

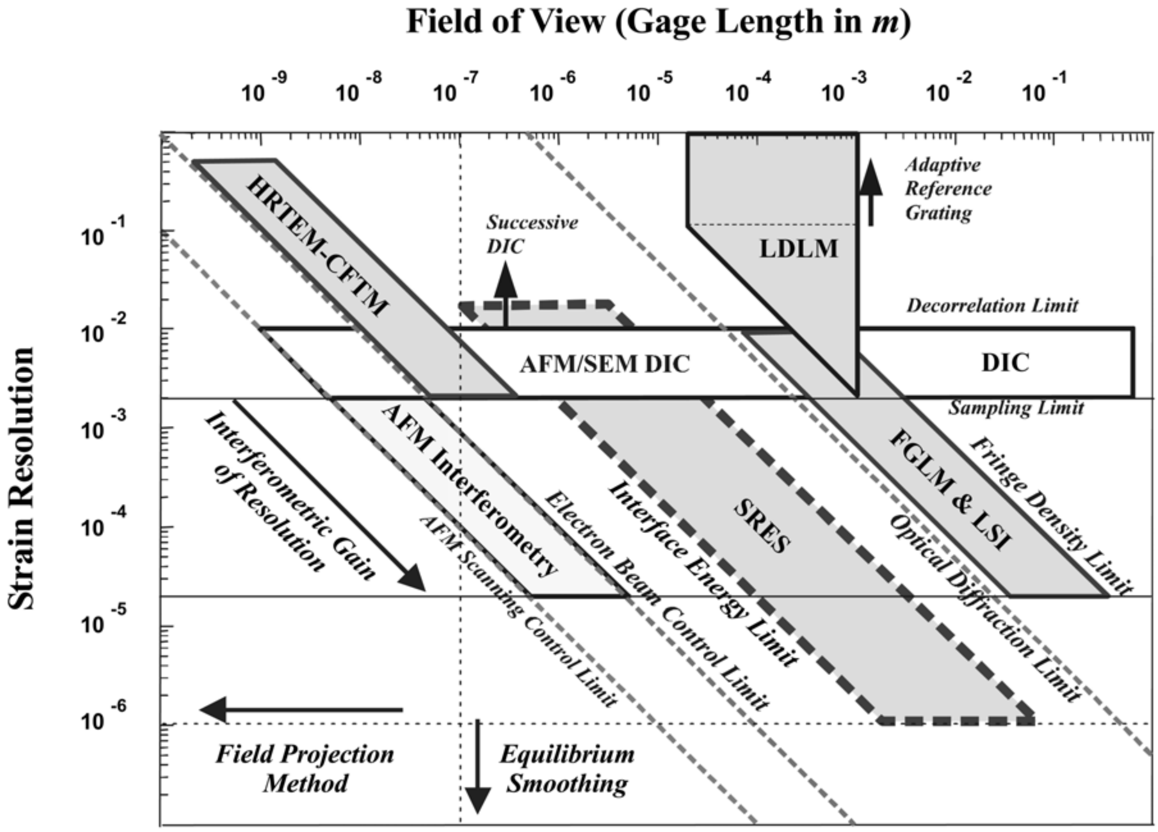

Fig. 1. Instruments and techniques for experimental micro and nano mechanics [courtesy of K. S. Kim of Brown University] where HRTEM High Resolution Transmission Electron Microscopy, SRES – Surface Roughness Evolution Spectroscopy, CFTM – Computational Fourier Transform Moire, FGLM – Fine Grating Laser Moiré, AFM – Atomic Force Microscopy, LSI – Laser Speckle Interferometry, SEM – Scanning Electron Microscopy, DIC – Digital Image Correlation, LDLM – Large Deformation Laser Moire.

search that is well coordinated and that capitalizes on progress being made in other disciplines is needed if this potential for impact is to be realized.

Recognizing that this area of nanotechnology is in its infancy, substantial basic research is needed to establish an engineering science base. Such a commitment to nano- and micro-mechanics will lead to a strong foundation of understanding and confidence underlying this technology based on capabilities in modeling and experiment embodying a high degree of rigor. The instruments and techniques available for experimental micro- and nano-mechanics are depicted in Fig. 1, courtesy of K. S. Kim of Brown University.

One of the key instrument in nanotechnology is the atomic force microscope [AFM]. However the limitation is:
AFM SCAN SPEED ~100HZ [TAKES ~30 MIN. FOR A SMALL IMAGE OF 20,000 PIXELS].

To improve the speed and performance of the atomic force microscope, more optimal control of the cantilever and more robust software to acquire and process the data as well as other improvements are needed. A portable AFM has also been developed by IBM recently.

The potential of various concepts in nanotechnology will be enhanced, in particular, by exploring the nano- and micro-mechanics of coupled phenomena and of multi-scale phenomena. Examples of coupled phenomena discussed in this workshop include modification of quantum states of materials caused by mechanical strains, ferroelectric transformations induced by electric field and mechanical stresses, chemical reaction processes biased by mechanical stresses, and changes of biomolecular conformality of proteins caused by environmental mechanical strain rates. Multi-scale phenomena arise in situations where properties of materials to be exploited in applications at a certain size scale are controlled by physical processes occurring on a size scale that is orders of magnitude smaller. Important problems of this kind arise, for example, in thermo-mechanical behavior of thin-film nanostructures, evolution of surface and bulk nanostructures caused by various material defects, nanoindentation, nanotribological responses of solids, and failure processes of MEMS structures. Details of this workshop report can be found by visiting http://en732c.engin.brown.edu/nsfreport.html.

Nanoscale Science and Engineering Initiatives

Coordinated by M. Roco (IWGN, 2000), NSF recently announced a multy year program [NSF 03-043; see: www.nsf.gov] on collaborative research in the area of nanoscale science and engineering (NSE). This program is aimed at supporting high risk/high reward, long-term nanoscale science and engineering research leading to potential breakthroughs in areas such as materials and manufacturing, nanoelectronics, medicine and healthcare, environment and energy, chemical and pharmaceutical industries, biotechnology and agriculture, computation and information technology, improving human performance, and national security. It also addresses the development of a skilled workforce in this area as well as the ethical, legal and social implications of future nanotechnology. It is part of the interagency National Nanotechnology Initiative (NNI). Details of the NNI and the NSE initiative are available on the web at http://www.nsf.gov/nano or http://nano.gov.

The NSE competition will support Nanoscale Interdisciplinary Research Teams (NIRT), Nanoscale Exploratory Research (NER), Nanoscale Science and Engineering Centers (NSEC) and Nano Undergraduate Education (NUE). In addition, individual investigator research in nanoscale science and engineering will continue to be supported in the relevant NSF Programs and Divisions outside of this initiative. This NSE initiative focuses on seven high risk/high reward research areas, where special opportunities exist for fundamental studies in synthesis, processing, and utilization of nanoscale science and engineering. The seven areas are:

- Biosystems at the nanoscale
- Nanoscale structures, novel phenomena, and quantum control
- Device and system architecture
- Nanoscale processes in the environment
- Multi-scale, multi-phenomena theory, modeling and simulation at the nanoscale
- Manufacturing processes at the nanoscale
- Societal and educational implications of scientific and technological advances on the nanoscale.

The National Nanotechnology Initiative started in 2000 ensures that investments in this area are made in a coordinated and timely manner (including participating federal agencies – NSF, DOD, DOE, DOC [including NIST], NIH, DOS, DOT, NASA, EPA and others) and will accelerate the pace of revolutionary discoveries now occurring. Current request of Federal agencies on NNI is about $710 million. The NSF share of the budget is around $220 million [on NSE, part of NNI].

3. CHALLENGES

The challenge to the mechanics and materials research communities is: How can we contribute to these broad-base and diverse research agendas? Although the mainstay of research funding will support the traditional programs for the foreseeable future, considerable research funding will be directed toward addressing these research initiatives of national focus. At the request of the author [KPC], a NSF research workshop has been organized by F. Moon of Cornell University to look into the research needs and challenges facing the mechanics communities. A website and report with recommendations of research needs and challenges available (see *Mechanics*, AAM, 32 (78) (2003)).

Mechanics and materials engineering are really two sides of a coin, closely integrated and related. For the last decade this cooperative effort of the M&M Program has resulted in better understanding and design of materials and structures across all physical scales, even though the seamless and realistic modeling of different scales from the nano-level to the system integration-level (Fig. 2) is not yet attainable. ***The major challenges are the several orders of magnitude in time and space scales from the nano level to micro and to meso levels.*** The following list summarizes some of the major methods in bridging the scales, top down or bottom up, and their limitations.

- **FIRST PRINCIPLE CALCULATIONS - TO SOLVE SCHRODINGER'S EQ. *AB INITIO*, e.g. HATREE- FOCK APPROX., DENSITY FUNCTIONAL THEORY,…**
  – COMPUTIONAL INTENSIVE, O(N^4) – N is the number of orbitals.
  – UP TO ~ 3000 ATOMS
- **MOLECULAR DYNAMICS [MD] pico sec. range – DETERMINISTIC, e.g. W/ LENNARD JONES POTENTIAL**

MATERIALS		STRUCTURES		INFRASTRUCTURE
nano-level	micro-level	meso-level	macro-level	systems-level
(10^{-9})	(10^{-6})	(10^{-3})	(10^{+0})	(10^{+3}) m
Molecular Scale	*Microns*	*Meters*		*Up to Km Scale*
*nano-mechanics	*micro-mechanics	*meso-mechanics	*beams	*bridge systems
*self-assembly	*micro-structures	*interfacial-structures	*columns	* lifelines
*nanofabrication	*smart materials	*composites	*plates	*airplanes

Fig. 2. Physical scales in materials and structural systems (Boresi & Chong, 2000).

– MILLIONS TIMESTEPS OF INTEGRATION; TEDIOUS
– UP TO ~ BILLION ATOMS FOR NANO-SECONDS

- **COMBINED MD & CONTINUUM MECHANICS [CM], e.g. MAAD[Northwestern U.]; LSU; BRIDGING SCALE; …**
  – PROMISING, but bridging time and space scales is the constraint...
- **INTERATOMIC POTENTIAL/CM – HUANG [U. of Illinois – UC]: EFFICIENT;MD STILL NEEDED IN TEMPERATURE, STRUCTURAL CHANGES, DISLOCATIONS…**

In the past, engineers and material scientists have been involved extensively with the characterization of given materials. With the availability of advanced computing and new developments in material science, researchers can now characterize processes and design and manufacture materials with desirable performance and properties. One of the challenges is to model short-term nano/micro-scale material behavior, through meso-scale and macro-scale behavior into long-term structural systems performance, Fig. 2. Accelerated tests to simulate various environmental forces and impacts are needed (NSF, 1998). Supercomputers and/or workstations used in parallel are useful tools to solve this scaling problem by taking into account the large number of variables and unknowns to project micro-behavior into infrastructure systems performance, and to model or extrapolate short term test results into long term life-cycle behavior (NSF, 1998; Chong, 1999). Twenty-four awards were made totaling $7 million. A grantees' workshop was held recently in Berkeley and a book of proceedings has been published (Monteiro *et al.*, 2001).

Biomimetics or bio-inspired materials are to learn from nature's millions of years of evolution and optimization to see how to design and built stronger and high performance materials. An excellent example of nature's design is the nacre [or the shell of the red abalone], which has the nanostructured morphology and exceptional mechanical properties with just 2% of protein-binding agent. Katti, et al, did a finite element modeling of nacre 2001. Researchers at Northwestern University and elsewhere are also investigating different aspects of nacre.

Tremendous progress is also being made in micro and nano sensors. Researchers at University of California – Berkeley have been working on "smart dust" sensors – with a target of a size of a cube 1mm on each side, capable of sensing [e.g. cracks in materials] and transmitting wirelessly the data collected. Researchers at IBM – Zurich and Basel have developed the artificial nose to detect minute analytes and air quality in the air [Fig. 3].

Researchers at NIST and other places have been building nano-clay filled polymers with natural clay

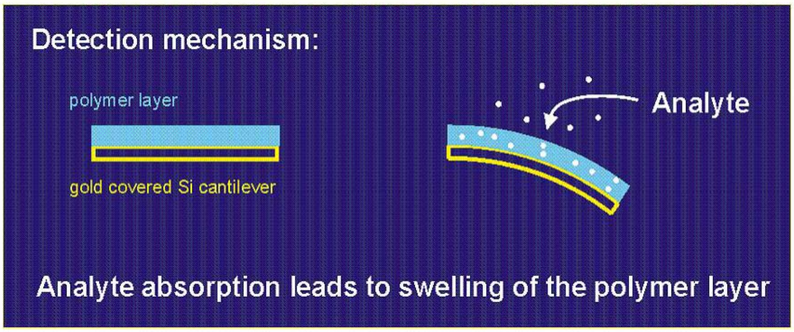

Fig. 3. Cantilever detection mechanism [IBM – Zurich].

form platelet [less than 1 nm in thickness] and 1 to 5% by volume. These nano-clay filled polymers can dramatically improve fire resistance as well as mechanical properties. Metal oxide nanoparticles have also been used in coatings for protection of UV light, self-disinfecting surfaces, solar cells, indoor air cleaners, etc. In general, nanocomposites possess superior properties.

4. SUMMARY, ACKNOWLEDGMENTS AND DISCLAIMER

An overview of research opportunities and challenges of nanotechnology in mechanics and materials, including nanomechanics, carbon nano-tubes, bio-inspired materials, coatings, fire-resistant materials as well as improved engineering and design of materials are presented and discussed.

The author would like to thank his colleagues and many members of the research communities for their comments and inputs during the writing of this paper. Information on NSF initiatives, announcements and awards can be found in the NSF website: www.nsf.gov. Parts of this paper have been presented elsewhere (Chong, 2002; 2003). Information pertaining to NIST can be found on its website: www.nist.gov. The opinions expressed in this article are the author's only, not necessarily those of the National Science Foundation.

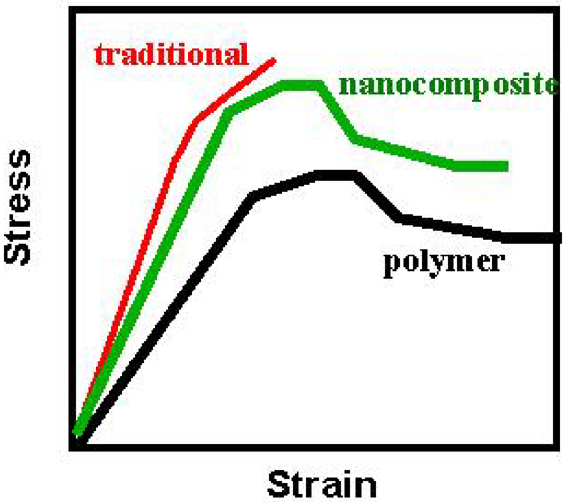

Fig. 4. Below shows the stress-strain characteristics of nano-composites [L. Schadler, RPI].

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