Report on the activities of the WP-7 on Nano- and Micro-Scale Phenomena in Mechanics

The annual report of WP7 (Nano- and Micro-Scale Phenomena in Mechanics) for the year 2003 is focused on the following issues: (1) an estimate of rapid growth of the subject field; (2) new contents of mechanics encountered in nano- and micro-scale phenomena; (3) current research thrusts; (4) examples of research advances; and (5) proposed activities in the future.

1. Research Trend for the Nano- and Micro-Scale Phenomena in Mechanics

It is fairly apparent that the area of Nano- and Micro-Scale Phenomena in Mechanics is booming. The area continues to grow, and the number of academics involved in this area is increasing. Several indicators are listed as follows. (1) The funding on nanoscale science and technology in the United States, Europe and Asia continues to increase; (2) Almost all universities want to hire new faculties in the nano-technology area. (3) The number of symposia on nanotechnology in major international conference continues to grow.

2. New Mechanics Contents in Nano- and Micro-scale Phenomena

The investigations devoted to the nano- and micro-scale phenomena greatly enrich the contents of theoretical and applied mechanics. These new contents include: (1) combined continuum and atomistic formulation of matters; (2) long range forces in nano- and micro-scales; (3) new avenues of field (mechanical, electric, magnetic, optical and thermal) coupling in the nano- and micro-scales; (4) enriched phenomena of scale effect; (5) multi-scale simulation as the new focus of computational mechanics; (6) a new understanding, in the cell and DNA levels, of biomechanics; (7) new technological issues such as NEMS, nanotubes, nanofluidics, nano-tribology and quantum dots.

These developments also create a stronger association of mechanics with physics, biology and material sciences. In contrast to the trend near the beginning of the 20th century when mechanics was separated from physics and combined to a large extent into engineering, the trend in the beginning of the 21st century is somewhat different.

3. Current Research Thrusts in Nano- and Micro-mechanics

The emphasis on nanoscale science and technology has shifted from fundamental science to technology. When US NSF funded its first centers on nanoscale science and technology in 2001, all five centers (Harvard, Cornell, Rice, RPI, Columbia) are on nanoscale science. When NSF awarded two new centers in 2003, the focus was on nanomanufacturing – to link nanoscale features to macroscopic products. Mechanics will play an important role here in this multiscale linkage.

The active thrusts in Nano- and Micro-mechanics include: (1) multiscale modeling technique to link nanoscale and macroscale; (2) development of continuum theories at the nanoscale (in order to overcome the time constraint of molecular dynamics); (3) technological issues associated with the development, manufacturing and reliability of MEMS and NEMS; (4) experimental technique to measure nanoscale mechanical properties; (5) design and modeling of nanostructured materials such as nano-grained materials, carbon-nanotubes and their composites, bio-inspired and bio-mimic materials, nano-structured smart materials; (6) nano-fluidics; (7) nano-tribology; (8) nano-biology such as the folding and unfolding of proteins, gene dynamics, cell adhesion, and the mechanical behavior of virus; (9) heat transfer and combustion at nano- and micro scale.

4. Examples of Research Advances

There were ample important research progresses in the year 2003 in the field of Nano- and Micro-scale Phenomena in Mechanics. Selected below are 10 examples for a brief illustration:

(1) *Mechanics of Nanotubes*. Two review articles [1,2] came out to sum up the progress in this subject. The review paper by Qian et al. [1] provides prospectives for a wide spectrum of computational issues concerning carbon nanotubes and their interaction with fluid. The review chapter by Huang and Wang [2] introduced a nanoscale continuum theory from the interatomic potential and the atomic structure of the material. Without any parameter fitting, the nanoscale continuum theory agrees well with molecular dynamics simulations in the study of carbon nanotubes properties, including pre-deformation energy, elastic modulus, fracture nucleation and defect nucleation, coupled electro-mechanical properties, coefficient of thermal expansion, and binding energy. One of the earlier contributions in the same group (Zhang et al. [3]) was the most cited paper in JAM in the year of 2002.

(2) *MD simulation for Supersonic Fracture*. From both the spatial and time scales, MD simulation suits for the investigation of dynamic fracture. The recent work by Buehler et al. [4] indicated the predictive power of MD simulation. By employing an upturn inter-atomic force potential, they simulated the supersonic crack growth in the mode II case and intersonic crack growth in the mode I case. The same concept was realized in a continuum analysis for supersonic crack growth in the mode III case [5].

(3) *Thin Film Mechanics*. The long-awaited book by Freund and Suresh [6] was published at the end of the year 2003. This comprehensive book covers most mechanics aspects for thin film materials, including stress, defect formation and surface evolution.

(4) *Nanoscale Experimentation*. Two types of experimental techniques are developed in UIUC to measure nanoscale mechanical properties. The first was developed by Saif [7] who uses MEMS to measure the properties of nanoscale devices (down to about 100nm or less). The second was developed by Yu who uses AFM to conduct the nanoscale tension, such as the tension test of carbon nanotubes

(5) *Deformation of Nano-grained Metals*. Understanding for the deformation of nano-grained metals was gained through large scale MD simulation [8] for the case of fast deformation, in which the high strain rate raised the flow stress, and consequently led to the burst of stacking faults. The grain boundary sliding also contributed to the overall deformation. Grain rotation is induced by the movement of disclination dipoles along the grain boundaries [9]. In-situ experimental observation for the deformation of nano-grained nickel is also achieved [10], and that is the most cited work in all papers published in Acta Materialia in the year 2003.

(6) *Surface Nanocrystallization*. Surface Mechanical Attrition Treatment (SMAT) is a way to induce severe plastic deformation in the surface layer of the material. The mechanics mechanism for such a process is resolved, and there are many applications for their products. For example, utilizing the high density of the grain boundary networks, one may achieve low-temperature (300C) nitriding of surface-nanocrystallized material [11], and that offers an immense opportunity to enhance the strength, as well as the resistance against wear, fatigue and stress corrosion of the machine parts.

(7) *Nano-indentation*. The size effect of nano-indentation has been a persistent challenge for nanomechanics. Nix and Gao explained the scale dependence of nano-indentation by strain gradient plasticity. Since then, there have been many works endeavored on this subject. We would like to mention an interesting work by Elmustafa and Stone [12] that is the most cited paper published in JMPS in the year of 2003. They pointed out that when the results are fitted to a strain gradient plasticity model, the data at deep indents (microhardness and large nanoindentation) exhibit a straight-line behavior closely identical to literature data; however, for shallow indents (nanoindentation data), the slope of the line severely changes, decreasing by a factor of 10, resulting in a "bilinear behavior".

(8) *Reliability and Nanoscale Failure*. A reference book “Interface and Nanoscale Failure” [13] came out in the year 2003 that contained a collection of review chapters on different aspects for the structural integrity

towards the applications in nanoscale. The issues include: reliability of interconnect structures, reliability of MEMS, crack–dislocation interaction, experimentation at the Micron and Submicron Scale, nano-moiré method and nanoscopic crack tip deformation, combined atomistic and continuum simulation for fracture and corrosion, nanoindentation, surface nanocrystallization and mechanical behavior of bulk nanocrystalline materials, and mechanics of nanotubes.

(9) *Nanoscale Mechanics of Biological Materials*
The progresses toward the understanding on the nanoscale mechanics of biological materials have been rewarding in the year of 2003. It is interesting to see that many established experts in solid mechanics (such as LB Freund, S Suresh, HJ Gao and R Phillips) shifted their research focus to the interface between the biological system and the nano-mechanics. The sectional lecture of Gao in the forthcoming ICTAM-2004 Warsaw conference will also be devoted in this topic, with concrete progress [14] in the understanding for the strength for bio-materials organized in specific nano-structures.

(10)*Large-scale MD simulation*
Large-scale parallel MD simulation has made headway in the past years. Abraham et al. [15] open the era of giga-atoms simulation that depicted in vivid details the generation of dislocation forest and the formation of the dislocation cells for a notched sample. With the help of QSC super-computer at Los Alamos National Lab, USA, the computation involving 19-billion particles [16] has been performed.

5. Expected Activities in the Future

It seems that almost all mechanics meetings/conferences have sessions on nanotechnology. The members of WP7 have been very active to visit different research groups in the world, and to attend and to organize symposia and workshops on nanomechanics-related subjects. In the future, WP7 should work together to organize some workshops or symposia on the topic area. Several future activities are listed below:

February 2004, WP7 endorsement for the proposed IUTAM symposium "Multi-scale plasticity of crystalline materials", at Eindhoven, Netherlands in 2006.
May 30 – June 04, 2004, attending IUTAM Symposium on Size Effects on Material and Structural Behavior at Micron- and Nanometer-Scales, Hong Kong, China.
August 16 – 21, 2004, attending ICTAM 2004, Warsaw, and having a WP7 meeting.
September 1 – 3, 2004, organizing IUTAM Symposium on Mechanics and Reliability of Actuating Materials, Beijing, China.

June 27 - June 30, 2005, participating on the organization of IUTAM Symposium on Mechanical Behavior and Micro-mechanics of Nanostructured Materials, Beijing, China.

Report composed by Wei YANG
Professor and Chair of WP7

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