Annual Report for WP7 to IUTAM

In the past a year and a half, the activities in the field of nano- and micro-scale mechanics grow explosively under high anticipation. This annual report of WP7 (Nano- and Micro-scale Phenomena in Mechanics) can only serve as a brief summary. We outline the extension of the field in the booming era of nano-science and nano-technology, and exemplify the pioneering researches that are focused on the state-of-the art developments in nano- and micro-scale mechanics.

1. New Directions in Nanoscience and Nanotechnology

With the coming of nano-revolution, the nano-inspired researches have been popular throughout the world. The nanoscience and nanotechnology have taken much of the attentions from thousands of scientists and engineers. These specialists are struggling to deal with the fantastic intellectual challenges in the new-born areas, such as nanophysics, nanochemistry, nanomechanics, nanomaterials, nanometrology, nanooptics, nanoelectronics, nanomedecine and bio-nanotechnology.

The report from the Royal Society of London entitled ‘Nanoscience and Nanotechnology: Opportunities and Uncertainties’[1] was published on 29 July 2004. This report highlighted the significance of the nanoscale, and addressed the uncertainties about the health and environmental effects of nano-particles. It also gave the consensual definitions of nanoscience and nanotechnology. Because these definitions are rather vague, many scientists immediately look forward to an exact and scientific definition of the term “nano”.

A proud history of exploring nature is partly consisted of the activities for the manipulation of a molecule or a number of atoms via sufficiently precise micro-instruments. In present, many scientists are devoted to further knowing of the naturally occurring molecular assemblies that regulate and control biological systems. By using ‘bottom-up’ nano-fabrication techniques, engineers long for producing the bio-materials and devices including molecular biomimetics system, molecular motors, unimolecular robots and bio-chip. Since numerous new-types of nanomaterials are manufactured and investigated, their remarkable properties are being understood gradually. The nanomaterials may realize our dream of finding materials with characteristics, functions and applications at smaller and smaller scales. Combining nanomaterials and information-communication technologies, technologists are able to gain a series of progresses in information storage, sensor, computer and ‘off-roadmap’ technologies, and NBIC technology.

There are a great deal of issues which emerge with the development of nanoscience and nanotechnology. Some issues are directly related to nanomechanics, and result in the following research topics: (1) mechanical properties and behaviors of nanocomposite, nanowire and nanotube; (2) plastic deformation and fracture of nanocrystalline metals; (3) size effect, surface effect and quantum effect at the nanoscale; (4) multiscale simulations bridging spatial and temporal scales; (5) nanotechnologies involve with biology, such as molecular biomimetics, protein sidechain dynamics, bio-MEMS, bio-composite; (6) contact and adhesion mechanics at the nanoscale including nano-wear and nano-tribology.

2. Progresses for Mechanics Researches in Micro- and Nano-Scales

The following examples delineate recent research progresses for mechanics research in micro- and nano-scales.

(1) Mechanics of Nanocomposite

To enhance conductivity, strength and stiffness of polymers, bundles of carbon nanotubes act as fillers in the matrix. Nanotube-reinforced composites seem to be promising in many engineering and commercial applications. Recently, Suhr et al.[2] reported strong viscoelastic behavior by implementing direct shear testing of epoxy thin films containing dense packing of multi-walled carbon nanotubes. It is soul-stirring that composites gain 1,400% increase in damping ratio of the matrix without sacrificing the mechanical strength and stiffness of the polymers.

(2) Mechanics of Nanocrystalline Metals

The investigations of nanocrystalline metals currently concentrate on discussions about plastic deformation and failure. Wang and Yang[3] established constitutive modeling for nanocrystalline metals by taking into account cooperative grain boundary mechanisms. To study the transition of yield strength of nanocrystalline metals, Jiang and Weng[4] proposed a generalized self-consistent polycrystal model. They found that the plastic deformation of polycrystal is governed by grain boundaries, when the Hall-Petch slop is negative. Hemker[5] showed that an understanding of the deformation process of nanocrystalline metals could be inspired by probing dislocation activity via x-ray scattering. Latapie and Farkas[6] observed a combination of intragranular and intergranular fracture in nanocrystalline α-Fe via molecular dynamics simulation.

The current comprehension of nanoscale plasticity mostly relies on atomistic simulations. It is widely believed that the onset of plasticity is associated with homogeneous dislocation nucleation. But a high-temperature nanoindentation experiment[7] suggested an unexpected picture of initial plasticity that involves point defects. Furthermore, Shan et al.[8] found that grain boundary-mediated plasticity becomes a prominent deformation mechanism when they observe nanocrystalline nickel films via in situ TEM. Gerberich and Mook[9] emphasized that the studies of nanoscale plasticity immediately need quantitative experimental supports.

(3) Mechanics of Nanotubes and Nanowires

The current mechanical researches of nanotubes are mostly accomplished by extending continuum theories and implementing atomic-scale experiments. Based on Flugge's theory of composite cylindrical thin-walled lattice shells, Leung and Kuang[10] investigated the infinitesimal bucking of multi-walled carbon nanotubes under combined loading of axial compression and external hydrostatic pressure. Hough et al.[11] studied the viscoelastic properties of single-walled nanotube suspensions by developing a rheological model. In addition, Ashino et al.[12] performed quantitative force measurements on a single-walled carbon nanotube via dynamic force microscopy. Dietzal et al.[13] achieved an investigation of mechanical properties of carbon nanotubes fixed at a tip apex via atomic force microscope.

Nanowires have attracted considerable interest due to their potential applications in high-density data storage and opto-electronic nanodevices. Based on nanowire bending under lateral load for an AFE tip, Wu et al.[14] measured the full spectrum of mechanical properties which range from Young's modulus, yield strength, plastic deformation and failure. It is found that Young's modulus of Au nanowires is independent of diameter, and the smallest diameter wire has the largest yield strength that is up to 100 times that of bulk materials. In contrast to bulk nanocrystalline metals, plastic deformation in Au nanowires is characterized by strain-hardening. Such results just demonstrate that dislocation mechanism (dislocation glide and pile-up) is still operative down to diameters of 40 nm.

(4) Mechanics of Thin Solid Films

The research scope has extended to investigations for nanomechanical, adhesion and nanotribological behaviors in the field of thin solid films. In the work of Charitidis and Logotheetidis [15], hardness, elastic modulus and frictional coefficient of carbon based films were obtained from indentation and nanoscratch experiments. The hardness of a-C film was measured to be equal to ~25GPa, which indicate that it can be used as protective coating material. By incorporating a discrete dislocation dynamics and atomistic studies of dislocation nucleation mechanisms, Hartmaier et al.[16] investigated the time-dependent irreversible deformation of a thin metal film. The simulation results reveal films with different thickness exhibit different deformation mechanisms, and that agrees with experimental findings.

(5) Size Effect at the Nano- and Micro- Scale

The size effects related to changes in materials internal dimensions are widely known and exploited. Researches by Uchic et al.[17] showed that dramatic size effects occurred at surprisingly large single crystal sample dimensions. It is concluded that sample spatial scales limits the length scales available for plasticity. Nicola et al.[18] introduced size effects in polycrystalline thin films via two-dimensional dislocation dynamics. Their results emphasize that strengthening of polycrystalline films depend on both film thickness and grain size.

(6) Multiscale Modeling and Simulation

The book entitled ‘Multiscale Modeling and Simulation’[19] was published at the beginning of 2004. It reviews recent progress in multiscale modeling, with a view toward constructing systematic, reliable and controlled multiscale methodologies. The heterogeneous multiscale method[20] presents a unified framework for designing efficient multiscale methods that couple macro- and micro-scale computational models. Liu et al.[21] proposed an order-N atomic-scale finite element method (AFEM) which is as accurate as molecular dynamics. Because AFEM and FEM are in the same theoretical framework, their linkage can provide a seamless coverage of multiscale computation.

(7) Contact Mechanics at the Nanoscale

Contact mechanics plays an important role in the process of designing nanodevices and optimizing nanostructured materials. Luan and Robbins[22] used molecular simulations to test the limits of contact mechanics under ideal conditions. Their results indicate that the atomics-scale surface roughness which is caused by discrete distribution of atoms leads to dramatic deviations from continuum theory.

(8) Molecular and Nanoscale Biomechanics

The following thrusts are currently very active in the field of biomechanics in micro- and nano-scales: (1) nanomechanics at the interface of soft and hard matter; (2) transporting DNA and polypeptides through carbon nanotubes; (3) folding DNA with the length of several centimeters to several nanometers; (4) mechanistic view of structure-properties relation and robustness in nanostructured biomaterials; and (5) surface effects[23].

More and more nano-scale problems in the biology, which are valuable in studies and technical applications, appeared and were researched in the past years[24]. Through the researches, new phenomena are observed and studied and new nano- or micro-structures are searched for imitating.

(a) New phenomena in nano-biomechanics

Adhesive contact of biological cells[25]. The adhesion in this case characterizes two significant differences when compared with adhesive contact between metals and between semiconductors: 1) that the modulus of cells material is less than the moduli of metals or semiconductors leads to the elastic energy variation during contact process less dominant for cell than for engineer materials; 2) the molecules band surface to surface are able to migrate within the cells wall. Through that research, new mechanism of adhesion is studied.

Package of DNA. Biologic molecules with a very long length (such as DNA) can package into a container whose length is much less than the molecules. In the viral life cycle, the DNA molecule would package into the bacteriophage which is nothing but a protein coat capsid[23]. The bacteriophage is a class of virus which infect bacteria. Researchers propose mechanic model of the packaging process to understand the force effect on DNA.

(b) New structure in nano-biologic tissue:

In the biologic materials, there are many nano-composite, bone, teeth and nacre which are composed of protein and mineral with superior strength[26]. The biologic material, such as protein, is very soft, while the mineral is very brittle. Their assembly, in the form of bones, teeth and the nacre, are both stiff and tough. The nature grants this superior property by selecting the optimal nano-structure of the protein and the mineral. Study in the structure can guide humanity to produce artifical materials.

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