An Interdisciplinary International Collaboration in Nano-structured Property and Nano-scale Contouring Measurement Research and Education

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ABSTRACT: *Nanotechnology is promised to make profound impact on human life in coming decades. In order to do competitive research in the nanotechnology, engineer educations need to include fundamental courses such as meso-mechanics and molecular dynamics. Nanoscience and engineering is inherently interdisciplinary. Therefore, fundamental courses and interdisciplinary training are imperative. Since no country enjoys earlier leads in this arena, international collaboration is central to bring about critical momentum for breakthrough. This paper will describe an interdisciplinary international team effort in nanotechnology.*

Nanoscale material structure offers distinct behavior that cannot be explained by traditional models and theories. The author has conducted theoretical and experimental studies to investigate the size dependent properties of the nanostructure. Collaboration with the United States Air Force provides support and perspective in characterizing nanomaterial. A novel computational methodology that is more computationally efficient, better reflect the physical reality, and conductive for the observation of deformation mechanism has been developed.

The effort in nanoscale property characterization is further integrated with other disciplines to make the nanocale curve measurement and fabrication possible. In the recent development of measurement and fabrication using scanning probe microscopy (SPM), major focus has been on point-to-point path. Contouring measurement and machining has the advantages of high efficiency and enhanced precision. However, research on contouring nano-scale measurement and fabrication is lacking. The interdisciplinary program represents a concerted effort that integrated the development of nano-stage and control algorithm, investigation on tribological phenomenon and property characterization, and fabrication study to achieve the ultimate goal of contouring. The construction and control of nano-position stage is essential for contouring. Understanding the tribological property at nano-scale is central for repeatable and durable operation of nano-scale stage. The mechanical property characterization of a thin film provides vital information for the fabrication study. Investigation on fabrication is fundamental for the concurrent measurement and fabrication with high precision. Synergy among academia, industry and government agency plays a pivotal role in this endeavor for nanotechnology education and research.

The efforts in fundamental engineering education and interdisciplinary training have led to an innovation computational methodology. The developed computational method has broad applications in nanoscale modeling and simulation. The author will solicit future collaborative partners during session presentation and workshop.

1 INTRODUCTION

Nano technology is one of the transcendent technologies that are the primary drivers pf the 21th century and the new economy. [WONG, E. 1996][CHONG, K. P. 2004] In order to do competitive research in the nanotechnology, engineer educations need to include fundamental courses such as meso-mechanics and molecular dynamics. [CHONG, K. P. 2004] Nanoscience and engineering is inherently interdisciplinary. A focus on interdisciplinary effort is imperative. Since no country enjoys earlier leads in this arena, international collaboration is central to bring about critical momentum for breakthrough.

The following sections will include an international effort for the nanomaterial characterization. Discussions on molecular dynamics and atomic static approach are included. An interdisciplinary team effort to enable nano-scale contouring measurement and fabrication will be followed.

2 NANO MECHANICAL CHARACTERIZATION

Nanoscale material structure offers distinct behavior that cannot be explained by traditional models and theories. The thin film is such an important basic element for advanced functional materials and devices that knowledge concerning its mechanical properties becomes more and more important. Materials beyond sub-micrometer dimensions, like thin films, are readily employed now. However, mechanical properties like hardness and elastic modulus obtained from the bulk material are usually used for the thin film because of experimental difficulties. It is obvious that mechanical properties may vary locally for a material if they are measured over nanometer dimensions. The determination of in situ mechanical behavior for nano-scale materials is inevitable for the development of science and technology on this scale. A better understanding of nano-scale physical property can lead to unique nanostructures and innovative nonosystems for a wide range of applications.

Nanoindentation is a new means of determining mechanical properties through analysis of the load-depth curve obtained during nano-scale indentation. [DHIHETTY, J., HAY, W., CHEN, & PADMANABHAN, P. 1998][LUCAS, B. N., OLIVER, W. C. & SWINDEMAN, J. E. 1998][HAY, J. L., O'HERN, M. E. & OLIVER, W. C. 1998][HAY, J. C. & PHARR, G. M. 1998][LUGSCHEIDER, E., BARIMANI, C. & LAKE, M. 1998][LU, W. & KOMVOPOULOS, K. 2001][KLAPPERICH, C., KOMVOPOULOS, K. & PRUITT, L. 2001] Although it is the small-scale counterpart of the traditional hardness test, it is far from being understood at the small level. A number of commercial machines are available nowadays, machines called "nanoindenters," which has the ability to measure loads and displacements with resolutions better than 1 μN and 1 nm, respectively. [BHUSHAN, B., 1995] In conventional hardness tests, the quantity "hardness" is defined as the maximum load divided by the area of the residual impression. Nano-scale studies are a new branch of science in which even basic definitions must be established. The most common current definition of "nano-hardness" during nanoindentation is maximum load divided by contact area at that load, with contact area calculated from analysis of the load-depth curve based on the Hertizian contact theory of continuum mechanics. However, the validity of this new definition remains a source of controversy. Some studies have attempted to measure nano-hardness based on the classical area of residual impression, but accurate determination of the size of nano-indentation has proven difficult to measure experimentally. [BHUSHAN, B., 1995] Additionally, it has been suggested that the analysis of the load-depth curve based on Hertz contact theory breaks down at the indentation depth of nanometer regime. Hence, computer simulation of nanoindentation is of increasing interest as a means to circumvent the problems of experimental measurement.

Molecular Dynamics

Molecules have the potential energy that is attributed to the static and dynamic Coulombic forces of electrically charged particles comprising the molecules. The potential energy determines the intermolecular forces, thereby is the cause of molecular motions. In molecular dynamics, the molecules are allowed to move naturally under the influence of intermolecular forces. The positions and velocities of each molecular are followed in time by solving the classical equation of motion, such as Newton's equation, using standard numerical methods. The macroscopic properties are then calculated by averaging the appropriate function of molecular positions and velocities over time. Since much time is consumed calculating the force between atoms because of the need to consider all of the surrounding atoms for any one atom at each integral time. A bookkeeping scheme will be used to improve the inefficiency. The pair potential energy such as Morse and Lennard-Jones, and many body potential such as Embedded Atomic Methods (EAM) and tight bonding are widely used to simulate the intermolecular interactions.

Atomic Statics

Although Molecular dynamics can simulate the phenomena at a molecular level, it requires extensive computing time. Based on the fact that in condensed systems, atoms or molecules always oscillate around the minimum-energy positions. If we just compute the changes of the minimum-energy positions

that are the mean positions of each oscillating atom, then computation in this way is quasi-static, thereby greatly reducing the computing time. First, the interatomic potential energy is assumed to be described as the sum of the potentials which depend only on the distance of the atoms. During the process of simulation, the atoms in the material always move to the minimum-energy positions under the equilibrium condition. Thus, we can establish a computationally more efficient procedure based on the nonlinear finite element formulation.

We consider the arbitrary two atoms ‘ i ‘ and ‘ j ‘ to be two nodes, and their potential to be one element. Assume that the atom ‘ i ‘ is located at the position (x i ,y i) with displacement u i , v i in the x, y directions, respectively. Then by defining the nodal displacement vector {u}I j and the corresponding nodal force vector {F}I j =(f i, g i , f j , g j) T for the ‘ i ‘ and ‘ j ‘ atoms, the total pair potential energy is formulated as

$$E_{ij} = \phi(r_{ij}) - \{u\}_{ij}^{T}\{F\}_{ij} \tag{1}$$

Where $\phi(r_{ij})$ is the pairwise potential, while ri j is the atomic distance between the two atoms so that its differential with respect to {u}I j is

$$d\,r_{ij} = [B]d\{u\}_{ij} \tag{2}$$

Then the principle of minimum energy enforces the minimization of Ei j with respect to {u}I j such that

$$\frac{\partial E_{ij}}{\partial \{u\}_{ij}} = \left(\frac{\partial \phi}{\partial r_{ij}}\right)[B]^{T} - \{F\}_{ij} = \{0\} \tag{3}$$

Equation (3) is the element equilibrium equation that represents the equilibrium of forces acting on the atoms ‘ i ‘ and ‘ j ‘ and when the equilibrium equation is achieved by iteration procedure, it would converge to zero with an acceptable tolerance.

Then according to the usual assembly procedure of the finite element formulation, element equation (3) is assembled to obtain the total system equation

$$\sum_{i \neq j}\left(\frac{\partial \phi}{\partial r_{ij}}\right)[B]^{T} - \{F\}_{ij} = \{f\}_{\text{internal}} - \{F\}_{\text{external}} = \{0\} \tag{4}$$

After imposing the boundary conditions and constraints, the Newton-Raphson iterative technique will be adopted to solve the equilibrium equation (4) using a suitable displacement control scheme. Then, the whole equilibrium path of the simulation process can be obtained.

International Collaboration

There has been considerable recent interest in the mechanical characterization of thin film systems and nano-scale material using depth-sensing indentation tests. The validity of test results for hardness and modulus depends largely upon the analysis procedure used to process the raw data. An international collaboration with United States Air Force (AFOSR) provides for support and perspective to establish a more efficient atomic approach as described in the section of atomic statics instead of MD simulations. With this approach, we can simulate the indenter indenting the thin film in a reasonable speed and consequently better reflect the mechanical behavior of the indentation. Figure 1 illustrates the copper atom configuration of the thin film considered in the present investigation. [JENG, Y. R. & TAN, C. M. 2003][JENG, Y. R. & TAN, C. M. 2003] Furthermore, the mechanism of the elasto-plastic deformation can be examined more easily without the fluctuant motion of atoms. Figure 2(a) shows the curve of load (force experienced by the indenter) versus indentation depth for an entire nanoindentation cycle. Figure 2(b) shows the deformed configuration of the indented thin film. The hydrostatic stress and the deviatoric stress at the maximum indentation depth and after the indentation cycle are presented in the contour subplots of Figure 3. [JENG, Y. R. & TAN, C. M. 2002][JENG, Y. R. & TAN, C. M. 2003] In the future, the established atomic approach can also be employed to study residual stress in thin films, scratch resistance and film adhesion, and, in some cases, van der Waals type surface forces. Once it becomes possible to understand and control feature size, it will also become possible to enhance material properties and device functions beyond what we currently know how to do or even consider as feasible.

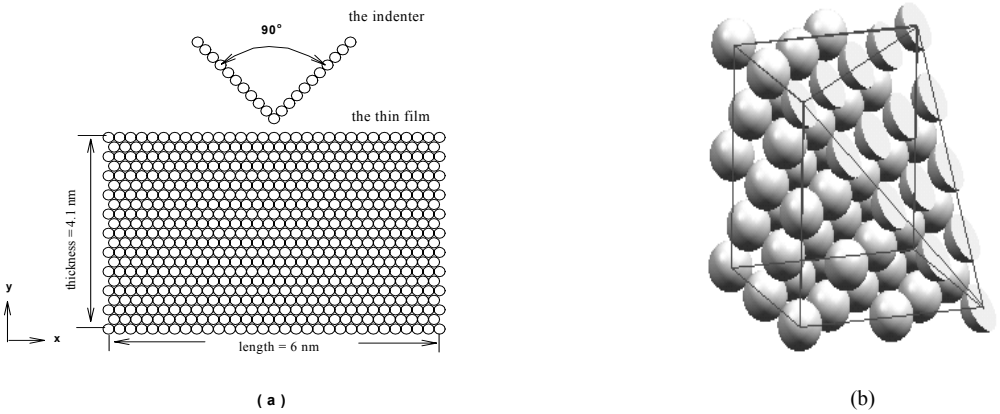

Figure 1. (a) Atomistic model used in present nanoindentation simulation. (b) Three-dimensional illustration of monocrystalline fcc copper thin film.

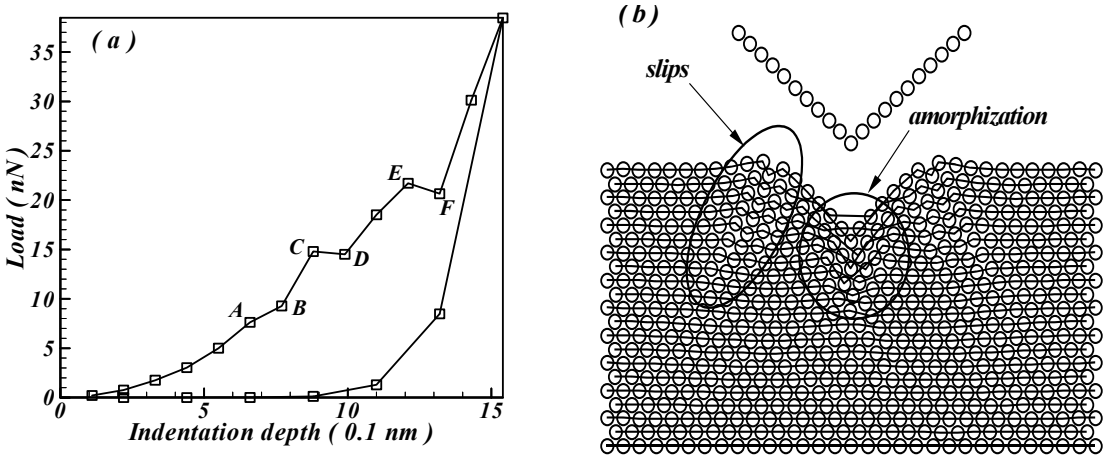

Figure 2. (a) The Load versus Indentation depth curve of the nanoindentation cycle. (b) The configuration of the deformed thin film after the nanoindentation cycle.

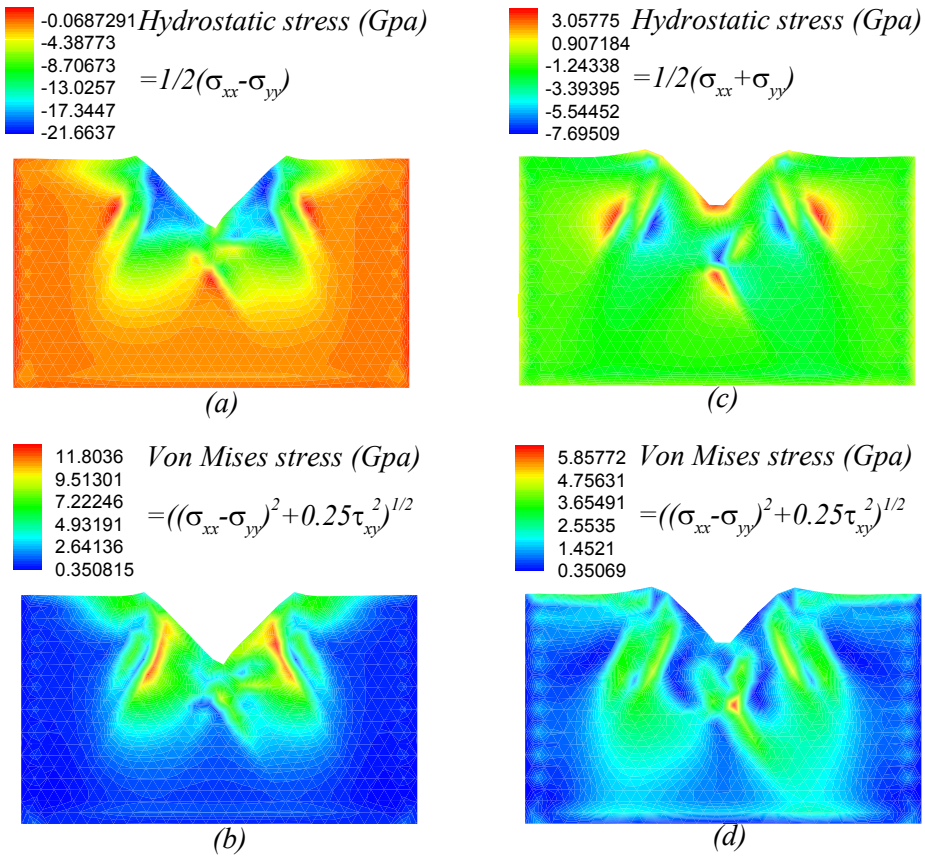

Figure 3 The hydrostatic and von Mises stress evaluated at the maximum indentation depth and after the nanoindentation cycle are drawn in flooded contour subplots (a) ~ (d).

Ignoring the thermal vibration of atoms in the condensed matter, we establish a more efficient approach based on the nonlinear finite element formulation instead of molecular dynamics method. The deformation evolution in the nanoindentation of the thin film was simulated via the proposed method. Several parameters are selected to examine their influences on the deformation behavior or the quantity hardness in the nanoindentation of the thin film. From our simulations, the following conclusions can be reached:

(1)Our study shows that the current approach is less time-consuming than the conventional MD simulation.

(2)The plastic deformation is the consequence of the instability of the crystalline structure in our static finite element structural analysis. Furthermore, the occurrence of the instability can be monitored by the non-positiveness of the tangent stiffness matrix of the crystalline structure.

(3)Two types of plastic deformation mechanisms are observed in our simulation results: the slip and the amorphization. The slip is the nucleation and propagation of the dislocation and the amorphization is that the arrangement of the atoms is disordered.

(4)The Von Mises shear stress is a good indicator of the dislocation emissions observed in the simulation.

(5)The quantity nano-hardness varies with the maximum indentation depth and the geometry of the indenter. It correlates with the deformation evolution of the nanoindentation.

(6)The rule of thumb that the maximum indentation depth should be less than 10% of the thickness of the film is examined. From our simulation results, it turns out to be a little conservative.

(7)In virtue of slip vector analysis, we have shown the phenomenon of dislocations emission induced in nanoindentations on (001) Cu surface.

Nano-scale Contouring Measurement and Fabrication

Scanning probe microscopy (SPM) has made profound impacts on nanotechnology. In the recent development of measurement and fabrication using SPM, major focus has been on point-to-point path.

Contouring measurement and machining has the advantages of high efficiency and enhanced precision. However, research on contouring nano-scale measurement and fabrication is lacking. Therefore an integrated project entitled, "Study on the key technology for nano-scale curve machining and measurement system," aimed to develop contouring measurement and fabrication through coherent team effort and innovative approach has been under way.

The research program represents a concerted effort that integrated the development of nano-stage and control algorithm, investigation on tribological phenomenon and property characterization, and fabrication study to achieve the ultimate goal of contouring. The construction and control of nano-position stage is essential for contouring. Understanding the tribological property at nano-scale is pivotal for a reliable interface to achieve repeatable and durable operation of nano-scale stage and static and dynamic friction needed for contouring control. The mechanical property characterization of nano structure material provides vital information for the fabrication study. Investigation on fabrication mechanical is fundamental for the concurrent measurement and fabrication with high precision. Consequently, this research program includes three research subprojects as follows:

Subproject (I): Nanotribology behavior and Mechanical Property at Nano-Scale

Subproject (II): Research on the Fabrication Mechanism of Nano-scale Curve

Subproject (III): Development And Control of Nano-Scale Stages And Its Application To Nano-Pattern Measurement

Each subproject is both essential and unique. All the subprojects are inter-related. Figure 4 shows the interrelationship between each subproject. As described in the Table 1, the project integration is pivoted to reach the ultimate goal. The coherent team effort will provide pioneering findings and achieve a platform contouring measurement and fabrication at nano-scale.

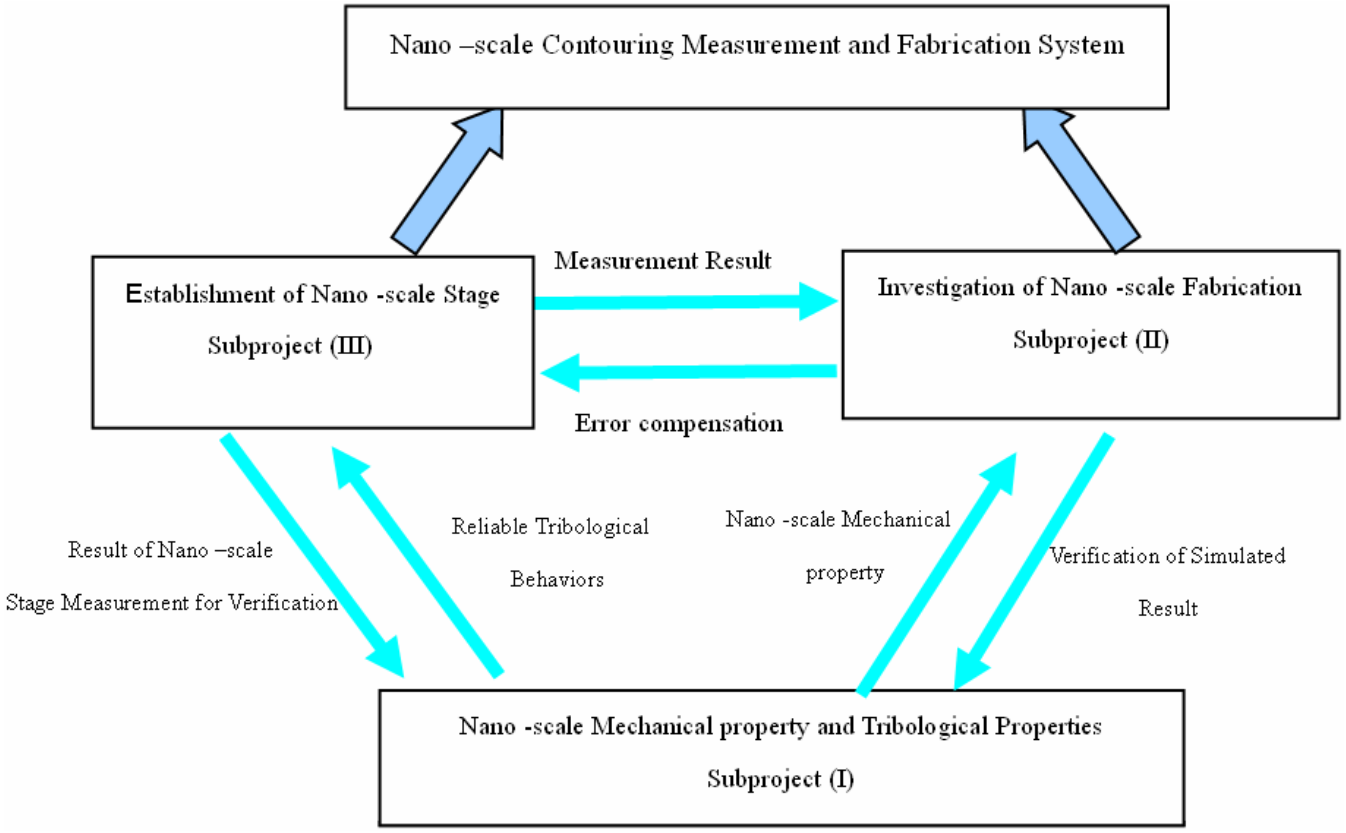

Figure 4. Overall Structure and Interrelationship between each subproject

Table 1. Merits of Project Integration

	Before Project Integration	After Project Integration
Subproject (I): Nanotribology behavior and Mechanical Property at Nano-Scale	Lack of verification for the mechanical property and tribological behavior obtained.	Provide the mechanical property needed in subproject (II) for nano-machining. Provide the reliable tribological behavior that is pivoted for the nano-scale stage and static and dynamic friction that is centrol for contouring control. In turn, the result from subproject (II) and (III) can be used for refinement and verification
Subproject (II): Research on the Fabrication Mechanism of Nano-scale Curve	Cannot solve the effect of thermal drift and hysteresis	Subproject (III) can provide compensation technique for thermal drift and hysteresis to improve accaurcy.
	Lack of mechanical property of nano structure material.	Subproject (I) can provide stess-strain relation for nano-machining.
Subproject (III): GDevelopment and control of nano-scale stages and its application to nano-pattern measurement	Without the consideration of the effect of force induced from nano-machining for the design and control of the positioning stage	Provide a nano-pattern working stage to subproject (I) and (II). In turn, subproject (II) will provide the simulated result of nano-scale curving machining to improve the accuracy of positioning and contouring. Provide of the prediction of the thermal induced error and compensation technique to subproject (II).

3 CONCLUDING REMARKS

The author has trained and motivated students through engineering courses in nano-mechanics and nano-material. These efforts lead to the development of an innovative computational approach. An international collaboration research on characterization of nano-scale material using this computational approach has been exciting and fruitful. An interdisciplinary team effort to achieve the ultimate goal of contouring nano-scale measurement and fabrication has been under way.

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