Adaptive Hierarchical Multiscale Framework for Modeling the Deformation of Ultra-Strong Nano-structured Materials

Research Proposal to
The National Science Foundation
NSF/ Sandia Program

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1 Project Summary & Objectives

The topic of this project belongs to focus area #3 of the NSF solicitation: "Micro/Nanoscale Phenomenology and Metrology." Nano-structured materials are extremely attractive for applications requiring high strength and ductility. Two such areas are: (1) nano-layered composites for future aerospace applications demanding high strength-to-weight ratios; and (2) next-generation interconnect and packaging components in future electronic devices. While atomistic Molecular Dynamics (MD) simulations are the most reliable tools for investigating deformation phenomena at the nano-scale (in absence of electronic structure considerations, and with well-calibrated interatomic potentials), they are limited to very small volumes and short simulation times. Likewise, dislocation dynamics simulations are limited in the ability to resolve the core structure of defects and to incorporate dislocation nucleation events without ad hoc assumptions. We plan to develop an adaptive hierarchical multiscale framework (AHMF), where appropriate computational methods and physics models are selected adaptively based on error estimators. Using this framework, we plan to investigate the deformation characteristics of two classes of nano-structured materials: polycrystalline nano-twinned copper inter-connects, and multi-layer nano-composites. We will apply these new tools to the design of bcc/fcc nano-layered materials, and the development of nano-twinned Cu interconnect lines with ultra-high strength and normal conductivity so that they can act as free standing interconnects. The models will be validated with on-going experiments at UCLA, supported by a recent NSF-NIRT program.

Intellectual Merit

The mechanisms that control the dependence of the strength on the size of nano-crystals, or nano-laminates are not all understood, particularly for nano-laminates composed of duplex fcc / bcc crystal structure, and also for polycrystalline aggregates of sub-micron size copper crystals containing nano-twins. Nano-twinned Cu has ultra-high strength, but its conductivity is as good as coarse-grained Cu. Current computational methods are limited in their ability to simulate realistic nano-structured systems, because of severe requirements on the number of simulated atoms in MD, the required time-scale for comparisons with experiments, and the ability to couple atomistic simulations to continuum methods. The intellectual content of the proposed research is summarized as: (1) discovery of the physical mechanisms that control strength and ductility at the nano-scale; (2) development of a rigorous adaptive hierarchical multiscale framework, with well-quantified error estimators; (3) contributing to the challenging concept of *materials-by-design*, which will ultimately change the way materials are optimized .

Broader Impact

The proposed project has direct applications to future nano-technology in two important sectors: future aerospace materials, and next generation nano-electronics. It will expand the applications of nano materials and technology, and enhance the leading position of the US in global competition for markets in aerospace and in electronic devices. The development and applications of novel multiscale computational methods will enable the US to continue its international lead in high-speed, large-scale computational technology as well. The proposed research will also impact graduate education world-wide by the development of two graduate courses on *Multiscale Computational Methods for Nano-structured Materials*, with the first focusing on fundamentals and the the second on applications. Parts of these courses were jointly taught by Professors Fish and Ghoniem in Brazil during summer 2004, and were sponsored by NSF. The courses will be further developed on-line for US graduate students to prepare them for global competition and research.

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2 Project Description

2.1 Motivation & Background

The approach of multiscale modeling of materials relies on a systematic reduction of the degrees of freedom at natural and identifiable length scales. Connections between such scales are currently achieved either by a parameterization or by a "zoom-out"or "coarse-graining"procedure. Seamless coupling between length scales has not yet been achieved as a result of two main challenges: (i) the computational complexity of coupled simulations involving different underlying equations of motion via the coarse-graining approach, and (ii) the inherent difficulty in dealing with system evolution stemming from time scaling, which does not permit coarse-graining over temporal events. We briefly discuss here the motivation behind the current proposal.

- **Progress and Applications of Ultra-strong Materials**
  As a result of recent progress in manufacturing and engineering utilization of nano- and micro-scale engineering structures, there is an urgent need for physically-based approaches that are capable of predicting the strength, ductility and propensity of these structures to failure under mechanical and thermal loads. Examples of new and possible applications are quantum dots, multi-layered thin films for laser optics, rocket engine chamber walls, ultra-hard coatings, and a host of emerging nano-to-micro-scale sensors and actuators. Conventional continuum methods for prediction of the mechanical properties of sub-micron structures fail to describe their plastic deformation and subsequent failure.

  Information technology, especially in the microelectronics, has been a major contributor to economic growth and job generation in the U.S. Modern electronic devices are built on semiconductor wafers, mostly silicon wafers. Silicon wafer based integrated circuit devices are the drivers of current information technology. Microelectronic technology starts from a 2-dimensional area on a wafer surface and builds to 3-dimensional device structures. The making of millions and now billions of electronic circuits on a chip has resulted in the continuous shrinking of device dimension from micro to nano region. Scaling down from micro-size to nano-size devices requires revolutionary inventions rather than incremental step-by-step improvements. In today's laboratory environment, the minimum feature size of field effect transistor (FET) device is as small as 7 nm. The challenge is how to integrate a very large number of such small or even smaller transistors and circuits on a wafer, and how to connect them together with wires (interconnects). Such interconnects must have significant strength and ductility so as not to deform and fail due to the passage of a high-density current and the thermomechanical loads imposed on them.

  In a recent Science paper, Lu et al reported [1] a fascinating phenomenon that has attracted much attention. Using pulsed electro-deposition technique they synthesized pure copper samples with a high density of nanoscale growth twins, as shown in Figures 1, 2-a, and 2-b, taken from their work. The lamella thickness of the twins showed a peak to about 15 nm. The pulsed electro-deposition was carried out galvano-statically using cathodic square wave pulses by turning off the current periodically, with a duty cycle of on-time of 0.02 sec and off-time of 2 sec. The peak current density is very high at about 0.5 Å/cm^2 and the PH value in the bath is very low, about 1. The substrate used was amorphous Ni(P), which was also electroplated on an iron sheet. As Figure 2 shows, polycrystalline copper with nanoscale twins exhibits a tensile strength about 10 times higher than that of conventional coarse-grained copper, while retaining an electrical conductivity comparable to that of pure copper. This rare combination will be very valuable as a VLSI interconnect material. The ultrahigh strength will be good for the mechanical properties

of the multi-level interconnect structure and also for chemical-mechanical polishing (less dishing) in manufacturing of the dual-damascene structure. Furthermore, it can serve as a candidate for free-standing interconnects using air as dielectric insulation. The major advantage of a free standing interconnect is that there will be no thermal stress between the interconnect and air.

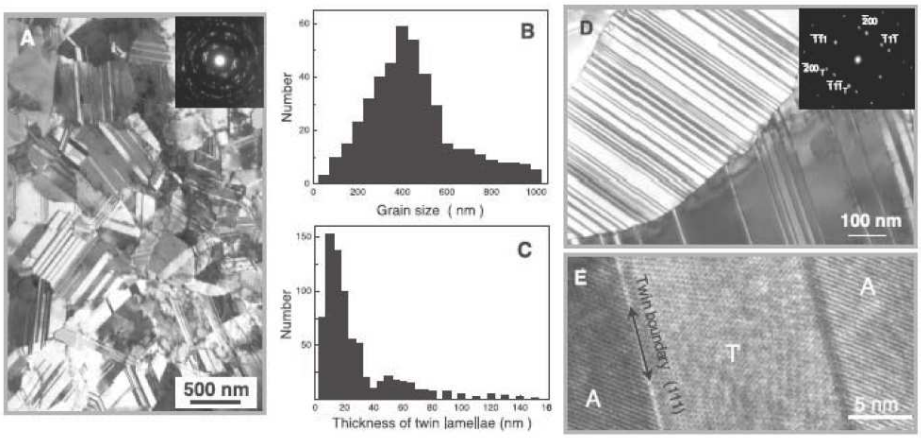

Figure 1: 1(A) A bright-field image of an as-deposited Cu. (B) Statistical distribution of grain size, (C) Statistical distribution of thickness of twin lamellae. (D) Nano twins are parallel to 111 planes. (E) High resolution of twin sequence of ATATA [1]

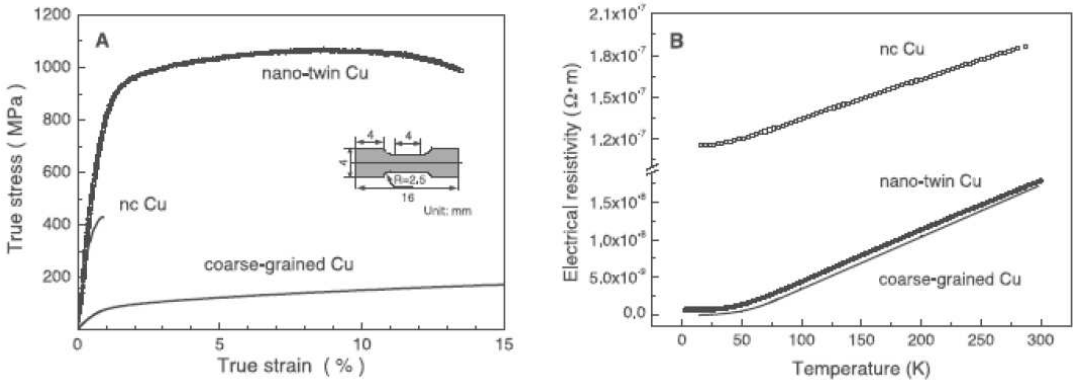

Figure 2: (a) Left, Typical tensile stress-strain curve of nano-twinned Cu, nano-grain Cu of grain size of 30 nm, and coarse-grained Cu; (b) right, measured temperature dependence of electrical resistance of nano-twinned Cu, nano-grained Cu, and coarse-grained Cu. [1]

Another area of great technological potential is the development of light-weight, high-strength structures. Nano-layered composite materials exhibit extraordinary strength characteristics, and may eventually be utilized in applications requiring high strength-to-weight ratios, such as future Aircraft and Aerospace structures. The strength of multi-layer materials is derived from the resistance of interfaces between layers to dislocation motion, as dislocations cross them from one layer to another. To design ultra-strong, yet ductile materials, one needs to understand how dislocations interact with interfaces. Resistance forces to dislocation motion can result from structural defects and/ or elastic modulus mismatch. The influence of interface structure

is attributed to several sources: lattice constant mismatch that generates coherency strains, misfit interfacial dislocations in semi-coherent and incoherent interfaces, stacking fault energy mismatch of the incoming and outgoing slip planes, slip system mismatch that forces cross-slip of dislocations across the interface, and dislocation core spreading into the interface [2, 3, 4]. Elastic modulus mismatch across the interface induces dislocation image forces, which appear to be the dominant source of resistance. Experimental data for the dependence of the nano-layer composite strength on its thickness is shown in Figure 3 [5, 6, 7]. The "inverse Hall-Petch (HP) effect"; that is the decline in strength as the nano-grain size gets smaller is evident in fcc systems; albeit the opposite behavior is observed for duplex fcc/bcc systems, as for example in the Cu-Cr and Cu-Nb cases. The role of dislocation core structure and splitting into partials during the nucleation process from grain boundaries in fcc crystals has been recently confirmed by Swygenhoven and co-workers [8], and it would be of the greatest interest to ascertain similar origins for the inverse HP effect in duplex fcc/bcc nano-systems. Before we describe proposed research tasks, we briefly outline modeling and simulation challenges that limit the attainment of digital design of these important classes of materials.

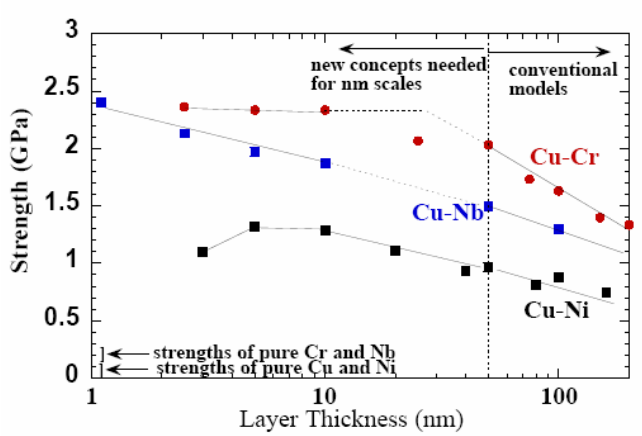

Figure 3: Dependence of Nano-layer composite strength on the layer thickness. Experimental data of Misra et al., LANL [5, 6, 7]

- **Modeling and simulation challenges**
  While idealized stress states can be used to determine an estimate of transitions from uniform to localized Confined layer Slip (CLP), it may be very advantageous to determine such transitions with more realistic stress states and dislocation geometry. In addition, most of the experimental research on multi-layer nano-composites is based on geometry and configurations that do not permit the existence of uniform stresses, but indeed involve complex nano-scale 3-D stresses and stress gradients. Such data must eventually be correlated to structures operating under a variety of mechanical load and temperature gradients, and of vastly different sizes, which again requires consideration of deformation modes in complex stress states. Dislocation behavior in multi-layers will be mainly controlled by layer differences of slip systems, mismatch strain/stress and material moduli. The main factor that requires further development at this stage is the variation of stress fields and forces from layer to layer, so as to utilize such variations as a material design parameter. Since elastic anisotropy is an important factor for the deformation of Cu, Ghoniem and co-workers extended the original work on Parametric Dislocation Dynamics (PDD) to fully anisotropic crystals [9, 10, 11]. Efficient computational methods for the elastic

field, self and interaction forces of 3-D dislocations in anisotropic elastic crystals are developed for incorporation into dislocation dynamics computer simulation codes. The elastic field of a general dislocation loop is determined by incorporating numerically-evaluated derivatives of Green's functions in the fast sum method of Ghoniem et al. [12, 13, 14]. Self-forces of dislocation loops are calculated by numerical integrations performed on the dislocation line, and several approximation methods to the full integration are also explored. The effects of elastic anisotropy in cubic crystals on the elastic field, self-forces, Frank-Read source expansion, finite-length dipoles and dislocation junctions are systematically determined. Large-scale 3-D dislocation dynamics simulations are carried out with full elastic anisotropy in Cu single crystals. We found that the dislocation microstructure and strain hardening behavior are strong functions of elastic anisotropy [9]. When a dislocation approaches an interface between two layers, within 10-20

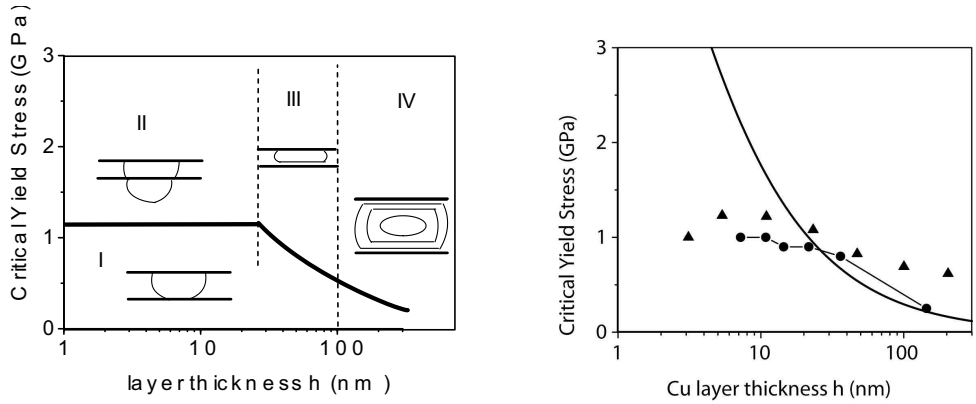

Figure 4: (a) Left, Deformation regimes for laytered nano-composites determined by DD simulations (b) Right,Yield strength of a Ni-Cu layered thin film as a function of the layer thickness. Solid line: Freund's formula, triangles: experimental results [Misra, et al.[7]], and circles: current simulation results [11]

atomic planes, the image force changes rapidly. Our model showed that when a dislocation crosses an interface from a soft to a hard layer, additional external forces must be applied to overcome an elastic mismatch barrier. The developed method extends the concept of the Kohler barrier in 2-D, and shows that the interface force barrier not only depends on the relative ratio of the elastic moduli of neighboring layers, but it also depends on the 3-D shape of the dislocation, the number of interacting adjacent layers, and on layer thickness. For layers of thickness less than approximately 100 nm, a single F-R source will determine the overall strength of the layer as a competition between confinement in the layer by image forces generated by elastic modulus mismatch, and resistance to deformation by self-forces on the curved ends of the dislocation loop. If the modulus mismatch is not too great, dislocation loops will cross from layer to layer rather than be confined within a layer. One would expect that the maximum strength be determined by the layer thickness and the ratio of elastic moduli as well. For thicker layers, F-R sources can operate many times leading to dislocation multiplication and the formation of a pile-up. In such case, the dominant deformation mode is the Hall-Petch mechanism. The results of these DD simulations are shown in Figure 4-a and 4-b. However, they are based on continuum mechanics, with all the usual approximations of singular fields, cut-off distances, etc., and have not been validated against MD simulations at comparable conditions. The primary goal of the proposed work is to develop a hierarchy of models with increased complexity, and then to dynamically map

the simplest possible member of the hierarchy into the appropriate space-time window. Model error estimators will be developed to ensure that quantities of interest are accurately resolved (compared to the reference MD solution).

Since Cu is elastically anisotropic, the elastic compliance tensor will have to be described in a common coordinate system, and thus we would have significant changes in elastic anisotropy as dislocations cross from one twin lamella into a neighboring one. Our findings described above are based on continuum elasticity and thus need to be calibrated with atomistic simulations for similar volumes, time-scales, and boundary conditions. However, the development of large-scale atomistic simulations for nano-layered composites, or for twinned polycrystals for calibration and comparison with the proposed adaptive hierarchical multiscale (AHMF) framework are not available today because of several challenging factors.

To appreciate the current difficulties with MD simulations, and the need to calibrate the AHMF at similar volumes and time-scales, we show the results of recent calculations at UCLA (unpublished). Typical MD simulation conditions are: periodic BC along the z-axis, free surface BC along x-axis, shear strain and fixed boundary conditions along the y-axis (the top and bottom layers), the simulation box contains 57,600 Cu atoms, and on a single CPU, we perform 250,000 time-steps in 3-5 days. The total simulated time is 0.25 ns, and the strain rate is 5×10^8 s^{-1}.

A schematic illustration of the simulation conditions for twinned copper nano-crystals is shown in Figure 5. Results of recent simulations of single perfect and twinned nano-crystals are shown in Figures 6, and 7, respectively. For the twinned crystal in Figure 7, small dislocation loops (green atoms) nucleate in the middle crystal as a result of higher strain energy during shear (elastic anisotropy effect), migrate towards the twin boundaries, coalesce into two Schockley partial dislocations that move in opposite directions to the crystal boundaries, and thus enable the twin interface to migrate.

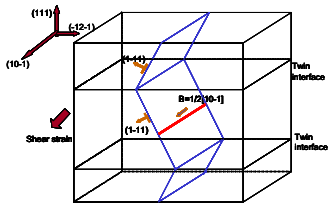

Figure 5: Schematic illustration of the simulation conditions for twinned copper nano0crystals (Lan Li, UCLA, unpublished results)

1. With realistic interatomic potentials, the number of simulated atoms is limited to less than 100,000, and thus the simulated volume is very small.
2. The total simulated time is several thousand time steps of a femto-second each. Thus, strain rate sensitive phenomena are difficult to capture. One of the key controlling factors in the twinning versus dislocation slip is the strain rate.
3. The boundary conditions of the atomistic region are generally not coupled (especially for the dynamics in 3-D simulations) with the continuum region. Recent work on coupling the atomistic to the continuum region consider quasi-static [15, 16, 17], defect-free coupling, or simulations with 2-D defects across the atomistic-continuum interface [18].

We propose to develop an Adaptive Hierarchical Multiscale Framework (AHMF) and apply it to

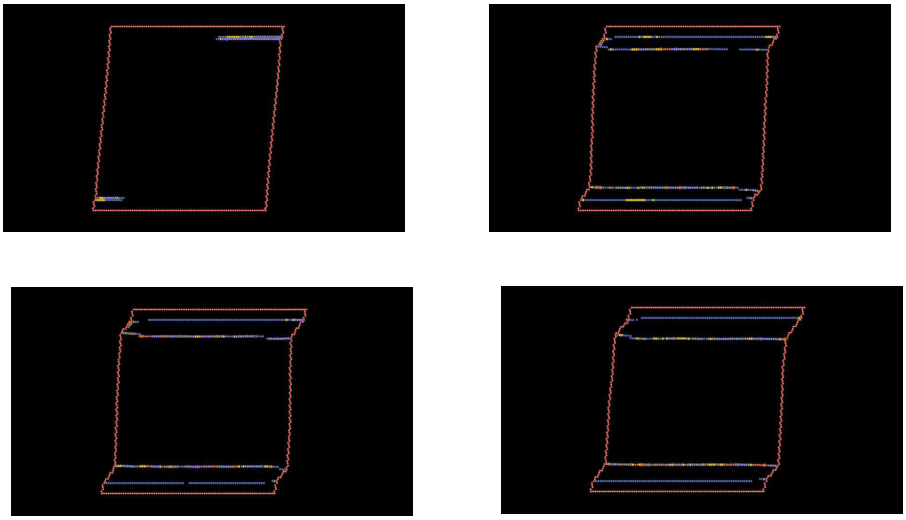

Figure 6: Results of MD simulations for a sequence of snap-shots showing the development of twins in a perfect copper crystal under shear deformation (Lan Li, UCLA, unpublished results)

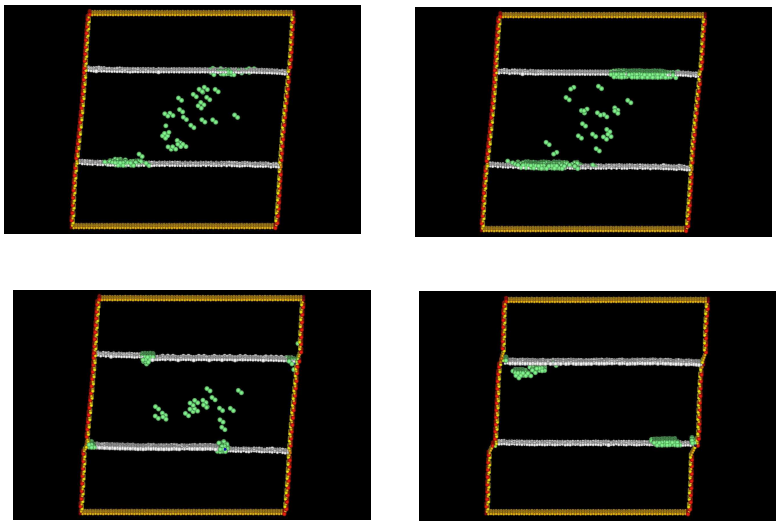

Figure 7: MD simulations of a twinned copper nano-crystal showing the process of twin boundary motion resulting from homogeneous dislocation loop nucleation

the computational design of nano-structured materials that are particularly important for future interconnect and packaging technology in the electronics sector, and for future high-strength and light weight materials for the aerospace sector. The approach combines both the physics-based and mathematics-based multiscale methods in a focused and efficient collaboration between RPI (mathematics-based) and UCLA (physics-based).To integrate education and research, we will develop an on-line course on *Multiscale Computational Methods for Nano-structured Materials*. Parts of this course was jointly taught by Professors Fish and Ghoniem in Brazil during summer 2004, and was sponsored by NSF.

Development of the proposed adaptive hierarchical multiscale framework will result in considerable insights into the physics of nano-scale plastic flow for optimizing the required high strength without spontaneous failure modes. We will address the question of how to control and manage dislocation motion in small volumes with the intent of designing ultra-strong, high conductivity, and ductile Cu interconnects. Key features of the modeling effort will include studies for the nucleation of nano-twins, dislocation motion in nano-twinned Cu, and dislocation interaction with twin interfaces. This will be accomplished with the proposed adaptive hierarchical multiscale framework consisting of the following two components: (i) a suite of hierarchical multiscale models with increased complexity including coarse-grained molecular dynamics model, atomistically informed dislocation dynamics model, local and nonlocal thermomechanical continuum models calibrated to atomistics; and (ii) dynamic mapping of an appropriate model in a hierarchy to the space-time widow based on model error estimators.

The developed tools will be aimed at computational design of ultra-strong, yet ductile materials at the nano- to micro- length scales. The models will be specifically applied to the simulation of plastic flow in ultra-strong confined layers (nano-laminates, and layered thin films), and to ultra-strong nano-twinned copper interconnects. Development of the proposed computer models will allow future material designers to engineer nano- and micro- layered composites for optimized performance by large-scale computer simulations. Such capabilities do not exist today, but significant progress has been made during the past decade to furnish necessary foundations for the proposed developments.

2.2 Proposed Research Program

2.2.1 General Approach

Both nano-layered materials and nano-twinned Cu interconnects involve deformation processes at multiple spatial and temporal scales. This disparity of scales will be addressed by constructing a hierarchy of mathematical models with increasingly more sophisticated effects. The most-comprehensive member of the sequence will be based on the molecular dynamics (MD) model. Quantum mechanical effect will not be considered in this work. An error estimate of a particular model in a hierarchy will be obtained by comparison to higher-level members (often solved approximately). A member of the sequence is considered admissibly accurate if the modeling error in the data of interest is sufficiently small. The goal is to identify an optimal member of the sequence, which is both admissibly accurate and computationally least expensive. We will consider the following members of hierarchy:

1. Thermo-mechanical continuum (TMC) model derived directly from molecular dynamics equations. The TMC description will be formulated using the Generalized Mathematical Homogenization theory recently developed for polymer melts [19], [20]. The primary objectives of the TMC model are two-fold: (a) due to its ability to represents the gross response of lattice vi-

bration (phonons), the TMC model will provide a seamless transition to the atomistic region used for modeling of discrete defects; (b) it will serve as a coarse model within the implicit coarse-grained MD model formulated based on the multigrid principles (see CGMD in 4).

2. Nonlocal thermo-mechanical continuum (NTMC) model is a generalization of the local continuum (TMC) model aimed at accounting for nonlocal effects. The NTMC description will be obtained using the Multiscale Enrichment based on Partition of Unity (MEPU) method developed in [21], [22] for polymer melts. The NTMC model will be employed to extend the range of applicability of the local TMC model to account for high gradients and a deviation from periodicity. By employing NTMC model the size of the atomistic region can be substantially reduced at the expense of increased computational cost in the continuum region. Ideally, the NTMC description will be employed at interphase between TMC and atomistic models.

3. An Atomistically-Informed Dislocation Dynamics (AIDD) method will be used to capture dynamics and interactions of dislocations. The short-comings of current DD simulations will be addressed here. Atomistic information will *inform* DD simulations of key dislocation properties, such as the cut-off distance (or core width), the range of interaction with interfaces, nucleation rates, and the generation of defect debris (point defects or defect clusters) will be passed on to the DD code . It is important to note that while TMC assumes scale separation, DD makes no such assumption. Moreover, if we revise the basic DD approach to be consistent with the thermo-mechanical continuum description derived directly from MD, then such a modified DD model will be superior in terms of accuracy to the TMC model. Whether such AIDD approach is more accurate and cost-effective than the NTMC model is remained to be seen and will be one of the goals of this project.

4. Coarse-grained molecular dynamics (CGMD) model is a coarse-graining of MD in both space and time. The CGMD description will be derived using the space-time multigrid approach recently developed in [23]. CGMD will be used to model evolution of defects and we expect that the results will sufficiently accurate at least at low strain rates.

5. Concurrent multiscale description involving two or more of the aforementioned models

2.2.2 Formulation of hierarchical multiscale model & adaptivity

(I)-Thermo-mechanical continuum

The TMC description for nano-layered and nano-twinned materials will be derived by approximating atomistic displacements in MD equations by means of multiple scale space-time asymptotic expansion of the form $\mathbf{u}(\mathbf{x}, \mathbf{y}, \tau, t, s_i) = \mathbf{u}^0 + \varepsilon \mathbf{u}^1 + \cdots$, where $\mathbf{x}$ is a differentiable continuum coordinate; $\mathbf{y} = \mathbf{x}/\varepsilon$ the discrete coordinate denoting position of atoms in a unit cell and $0 < \varepsilon \ll 1$; τ, the fast time coordinate, which tracks atomic vibrations for finite temperature applications; t the usual time coordinate; s_i, the slow time coordinates, which from the physics point of view captures dispersion effects, whereas from the mathematics point of view eliminates the secularity of asymptotic expansions. The atomistically calibrated TMC model has been validated for polymer melts and we will investigate its suitability for predicting thermomechanical response of nano-layered and nano-twinned materials.

(II)- Nonlocal thermo-mechanical continuum

The NTMC description will be obtained by enriching the kinematics of the aforementioned TMC model using partition of unity approach. Note that NTMC model is free of scale separation and periodicity assumptions inherent in TMC description. It employs hierarchical decomposition of atomistic

displacements, $\mathbf{u} = \mathbf{u}^c + \mathbf{u}^f$ where $\mathbf{u}^c$ and $\mathbf{u}^f$ are the continuum and fine scale enrichment, respectively. Fine scale enrichment will be approximated as $\sum \mathbf{H}(x)\mathbf{N}(x)\mathbf{a}$, where $\mathbf{N}(x)$ are the coarse scale element shape functions; $\mathbf{H}(x)$ the influence functions obtained from the unit cell solution; and $\mathbf{a}$ the enrichment degrees-of-freedom. The method can be interpreted as a quasi-continuum with evolving instantaneous Cauchy-Born hypothesis that takes into account localized deformation.

(III)- Atomistically informed Dislocation Dynamics

Once the TMC equations have been constructed for nano-layered and nano-twinned materials we will develop atomistically informed dislocation dynamics (AIDD) approach consistent with the thermomechanical continuum description. Also, the suitability of both the AIDD and NTMC models as coarse-grained models within the space-time multilevel method will be investigated.

Ghoniem and co-workers [12], and [13] have developed the Parametric Dislocation Dynamics (PDD) framework and have shown that if dislocation loops are discretized into curved parametric segments, one can obtain the field by numerical integration over the scalar parameter that represents the segment. If one of these segments is described by a parameter ω that varies,for example, from 0 to 1 at end nodes of the segment. The segment is fully determined as an affine mapping on the scalar interval $\in [0, 1]$, if we introduce the tangent vector $\mathbf{T}$, the unit tangent vector $\mathbf{t}$, the unit radius vector $\mathbf{e}$, as follows: $\mathbf{T} = \frac{\mathbf{dl}}{d\omega}$, $\mathbf{t} = \frac{\mathbf{T}}{|\mathbf{T}|}$, $\mathbf{e} = \frac{\mathbf{R}}{R}$. Let the Cartesian orthonormal basis set be denoted by $\mathbf{1} \equiv \{\mathbf{1}_x, \mathbf{1}_y, \mathbf{1}_z\}$, $\mathbf{I} = \mathbf{1} \otimes \mathbf{1}$ as the second order unit tensor, and $\otimes$ denotes tensor product. Now define the three vectors ($\mathbf{g}_1 = \mathbf{e}$, $\mathbf{g}_2 = \mathbf{t}$, $\mathbf{g}_3 = \mathbf{b}/|\mathbf{b}|$) as a covariant basis set for the curvilinear segment, and their contravariant reciprocals as: $\mathbf{g}^i \cdot \mathbf{g}_j = \delta^i_j$, where δ^i_j is the mixed Kronecker delta and $V = (\mathbf{g}_1 \times \mathbf{g}_2) \cdot \mathbf{g}_3$ the volume spanned by the vector basis.

$$\frac{d\sigma}{d\omega} = \frac{\mu V |\mathbf{T}|}{4\pi(1-\nu)R^2} \left\{ \left(\mathbf{g}^1 \otimes \mathbf{g}_1 + \mathbf{g}_1 \otimes \mathbf{g}^1 \right) + (1-\nu) \left(\mathbf{g}^2 \otimes \mathbf{g}_2 + \mathbf{g}_2 \otimes \mathbf{g}^2 \right) - (3\mathbf{g}_1 \otimes \mathbf{g}_1 + \mathbf{I}) \right\} \qquad (1)$$

Once the parametric curve for the dislocation segment is mapped onto the scalar interval $\{\omega \in [0, 1]\}$, the stress field everywhere is obtained as a fast numerical quadrature sum [12]. The Peach-Kohler force exerted on any other dislocation segment can be obtained from the total stress field (external and internal) at the segment. The total self- energy of the dislocation loop is determined by double line integrals. However, Gavvaza and Barnett [24] have shown that the first variation in the self- energy of the loop can be written as a single line integral, and that the majority of the contribution is governed by the local line curvature.

Furthermore, Ghoniem and coworkers [11] extended the PDD approach to anisotropic multi-layer materials. Line integral forms for the elastic field of dislocations in anisotropic, multilayer materials are developed and utilized in PDD computer simulations. Developed equations account for interface image forces on dislocations as a result of elastic modulus mismatch between adjacent layers. The method is applied to study dislocation motion in multi-layer thin films. The operation of dislocation sources, dislocation pileups, Confined Layer Slip (CLS), and the loss of layer confinement are demonstrated for a duplex Cu/Ni system. The strength of a thin film of alternating nano-layers is shown to increase with decreasing layer thickness, and that the maximum strength is determined by the *Koehler barrier* in the absence of coherency strains. For alternating Cu/Ni nanolayers, the dependence of the strength on the duplex layer thickness was found to be consistent with experimental results, down to a layer thickness of ≈ 10 nm. We propose to enrich the PDD approach for anisotropic nano-layered materials with atomistic information on the following aspects: (1) dislocation core-width, (2) cut-off distance from interfaces, (3) transmission and confinement across and on interfaces, (4) nucleation of fresh dislocations, and (5) generation of point defects and their clusters.

(IV)- Coarse-grained molecular dynamics

CGMD model is aimed at bridging diverse temporal scales. The space-time variational multigrid method [[23]], which forms the basis for the CGMD, consists of wave-form relaxation scheme aimed at capturing high frequency response of atomistic vibrations and coarse scale solution in space and time intended to resolve smooth features of the discrete medium. The waveform relaxation [[25]] decomposes the system into very small subsystems (for instance, atom-by-atom decomposition) which can be integrated in parallel and take advantage of unstructured time integrators. The coarse model correction $\mathbf{u}^f + \mathbf{Q}\mathbf{e}^C$ is calculated from the Hamilton principle on the subspace of coarse scale functions, where $\mathbf{Q}$ is the interscale transfer operator; it depends on the choice of the coarse scale model. The TMC, NTMC or DD models can serve in this capacity. Preliminary studies on polymer melts revealed that the space-time variational multigrid method is scalable in both space and time, offering a speed-up over the classical velocity-verlet integrator of more than 10 on 16-processor machine.

(V)- Concurrent multiscale description

Deformation of nano-layered and nano-twinned materials involves motion of dislocations suggesting that an optimal model may consist of a combination of aforementioned models. This type of hand-shaking can be accomplished using various domain bridging methods ([26, 27, 28, 29]) or multigrid-like methods ([30, 31, 32]). An important aspect of concurrent methods that will be addressed is matching conditions at the interface between different models. For instance, at the MD/continuum interface, MD generates phonons, which are usually not represented in the continuum region and hence might be reflected at the continuum/MD interface. This is not the case for continuum description based on the TMC and NTMC models where lattice vibration is accounted for by means of coupled thermal equation.

(VI)- Model error estimation and adaptive strategy

Selection of the appropriate member of the hierarchy will be guided by model error estimators. The error of the TMC model will be estimated by comparing the magnitude of the higher order terms neglected in the asymptotic expansion to those taken into account and by the deviation from the periodicity assumption; the error in the NTMC description will be estimated by the bifurcation analysis that would signal propagation of dislocations; the error in the AIDD model will be predicted by the proximity of dislocations to the interfaces and its ability to resolve nucleation; the error in the CGMD model will be determined by strain rate effects. Additional model error indicators will be developed as we better understand the limitations of various models and their interplay. Figure 8 depicts a diagram of such an adaptive model selection process guided by model error estimators. Note a double-arrow connecting AIDD and CGMD models, indicating that dislocation nucleation has to be resolved at the atomistic scale, but once it is formed DD model may suffice provided that dislocations to not interact with interfaces.

2.2.3 Applications

(I)-Ultra-strong Nano-Composites

In material processing techniques that result in strained-layer heteroepitaxy, strain energy in the thin film is proportional to the film thickness. However, the energy of defects responsible for relaxation (misfit dislocations) has a non-zero lower limit and a weaker dependence on thickness. The critical thickness of a film is the thickness at which the fully strained layer becomes unstable, indicating strain relaxation by misfit dislocations lying at the interface [33]. Matthews et al. first proposed a simple analytical model to give a critical thickness at which the threading dislocation begins to move to create a misfit dislocation. Freund [33] gave a more rigorous derivation for the equilibrium critical thickness. These results overestimate the layer thickness at low strains. Based on our proposed 3D DD framework, we will be able to numerically calculate the energies of dislocations of realistic shapes,

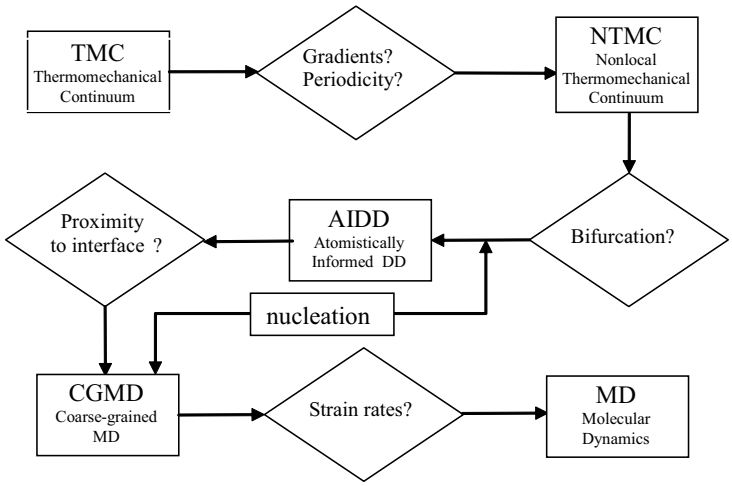

Figure 8: Model error estimators and adaptive model selection

accounting for their interaction with multiple interfaces, as we found to be the case for very thin nano-laminates [11]. This physically meaningful addition should render a monotonic dependence of the critical thickness on strain. In addition, crystal orientation and anisotropy will be considered during this simulation. As the growth surface is tilted away from (001), some of the misfit dislocations become more efficient at relieving strain whereas others become less efficient. This type of geometric anisotropy will affect the determination of critical thickness. Elastic anisotropy also changes the strain energy of the strained film. Simulation results will be compared with previous analytical predictions and available experimental data. Multiple free surface and interface effects will be embedded in the computer code. During each time step, and as a result of the strong inhomogeneity of the nano-layers, threading dislocation segments near the lower interface will tend to be near their equilibrium configuration, while the upper misfit dislocation segments will increase the self-energy from line tension as they curve to accommodate surface image forces. In addition, interface orientations (e.g. (100), (110) and (111)) will automatically be part of our 3-D numerical simulations, without the need for any simplifying assumptions.

We will investigate in this task the main deformation mechanisms, which determine the maximum level of attainable strength, and the distribution of plastic strain on slip planes of multi-layers. The main objectives here are:

1. To determine the dependence of the critical flow stress and subsequent plastic strain on: (a) layer-to-layer material design parameters (e.g. fcc/fcc, fcc/bcc, elastic modulus distributions, initial elastic mismatch, interface dislocation structure, Peierls stress jumps, slip geometry, etc.); (b) deformation mode (e.g. shear, tensile and indentation).

2. To validate developed computational models with available experimental information.

Another potential problem is the stress sate, which may develop as a result of differences in coefficients of thermal expansion, or lattice mismatch (transformation strains). We plan here to consider the effects of both thermal and transformation strains by implementing a realistic and accurate applied stress field into our adaptive hierarchical multiscale framework. We will determine the dependence of threading dislocation motion on thermal and biaxial transformation stress fields, since threading dislocations

could occupy both multi-layer and substrate areas, where the stresses show great heterogeneity.

(II)-Nano-twinned Cu as Free-standing Interconnects

Two of the most common and important modes of plastic deformation in fcc metals at low temperatures are slip and deformation twinning (DT). Slip is propagated through dislocations while deformation twinning occurs when a region of crystal is transformed by the external loading into its twin (mirror) counterpart. The likelihood of a material to twin, as opposed to slip, is referred to as its twinnability. Recently, pure copper samples with a high density of nanoscale growth twins showed a tensile strength about ten times higher than that of conventional coarse-grained copper, while retaining an electrical conductivity compatible to that of pure copper. Experimental observations have shown that a low intrinsic stacking fault energy (SFE) is correlated with a higher tendency to twin in fcc metals. It has also been suggested experimentally that the SFE of the metal will have to be less than some critical value for a metal to exhibit deformation twinning. Twins prefer to nucleate at grain boundaries (GBs) to reduce the grain boundary energies by means of the twinning-induced orientation change. The formation of twins depends strongly on the ratio of the twin boundary energy, γ_{TB}, to the GB energy, γ_{GB}, $\alpha = \gamma_{TB}/\gamma_{GB}$. Large twins densities may be obtained in metals with smaller α values. Another important micro structural parameter influence deformation twinning is the grain size in the metal. It has been reported that increasing the average grain size results in a lower twin nucleation stress for a given metal. Experimental results and isotropic elasticity estimates show that the dominant mechanism that controls the strength and hardness of multi-layer thin films is the influence of the dislocation image force associated with a mismatch in elastic properties between adjacent film layers [18]. For layered materials with a large mismatch in elastic properties, a significant hardness enhancement was observed.

Two models are often used to explain the observed behavior of hardness (or flow stress) in thin films. In the threading dislocation model [20,21], the flow stress is determined by the energy balance between the threading glide dislocation segment and the misfit dislocation left behind at the interface. This model results in a flow stress that scales approximately with the inverse of the film/layer thickness. In this model, interfaces are introduced as impenetrable planes for dislocations. The second model is an extension of the well-known Hall-Petch effect. Here, dislocations are assumed to form a pile-up at a boundary until a critical stress is reached. This results in a flow stress, which is inversely proportional to the square root of the layer thickness or grain size. Both models qualitatively explain the increase in the flow stress with decreasing film/layer thickness, but not the behavior as the layer thickness decreases below tens of nano-meters. As individual layers become very thin (i.e. in the tens of nanometers), only single dislocations can propagate and expand upon the application of an externally applied stress. However, because the layer thickness is very small, the curvature of the dislocation loop in segments subtended between layers would be extremely high, and thus self-forces in these regions are very substantial. The externally applied stress would have to overcome such large self-forces if these curved segments are to expand. The applied P-K force on those segments that are parallel to the interface does not have to overcome self-forces because the curvature of these segments is small. Rather, the image force from neighboring and other interfaces would have to be overcome by the applied P-K force. Since we regularized the solution by selecting a cut-off radius of one Burgers vector on either side of the interface, the dislocation will be repelled with a maximum image force on one side of the interface, and then attracted with a different maximum force once it crosses the interface. If the applied stress is high enough that the maximum P-K force on the straight dislocation segments close to the interface overcomes both repulsive and attractive forces, the dislocation will cross from one layer to the neighboring one, and Confined Layer Slip (CLS) is finally lost.

The main issues that we plan to address here are: 1. Nucleation of nano-twins; 2. Dislocation motion in nano-twinned Cu, 3. Dislocation interaction with twin interfaces; and 4. The effects of electron

conduction on dislocation motion and transmission across twinned interfaces. To understand these four areas, which control the mechanisms of twin formation and subsequent plastic deformation and strength, we plan to apply the proposed AHMF framework. We will also employ classical Molecular Dynamics (MD) simulations based on empirical potentials (such as the EAM-Mishin potential [34]) to determine the critical forces required to propagate dislocations across twin interfaces. Our recent results indicate that dislocations in nano-laminate Cu dissociate into partials as in bulk materials. However, the width of the stacking fault and the dislocation velocity are strong functions of the laminate width. While the leading partial can cross a nano-laminate interface, the trailing partial can be impeded for a long time, and the dislocation core can spread over many nano-laminates. We will investigate this interesting behavior of dislocations in nano-twins. The ability of dislocations to cross twin boundaries will ultimately determine the maximum attainable strength. To ascertain the importance of this point, we display in Figure 9 the experimental data of Lu et al. [1] that clearly show a square root dependence of the strength on the density of twins, which is reminiscent of the scaling laws of strength with dislocation density of conventional materials.

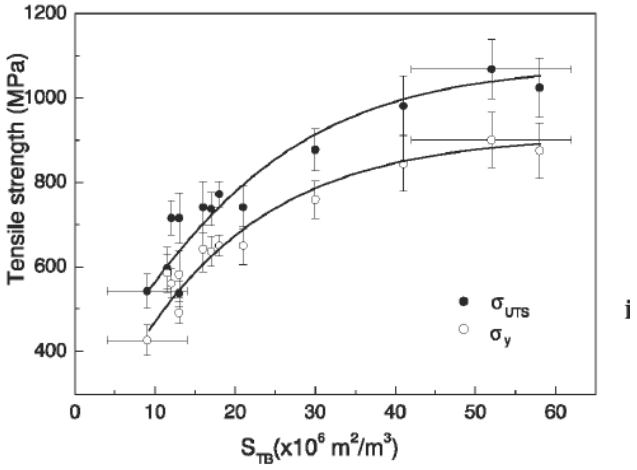

Figure 9: Experimental measurements for the dependence of the strength on the twin boundary area [1]

2.3 Educational Program

2.3.1 General

The analysis of ultra-strong materials for aerospace, interconnect and packaging components applications requires substantial, in-depth interdisciplinary training in the mathematics, science and computations. The current educational system does not provide the broad range of interdisciplinary knowledge. While PIs are in no position to change the educational system overnight we intend to develop two online interdisciplinary courses to be taught in the collaborating institutions. The first of these courses will focus on foundation in quantum and molecular science, statistical and continuum mechanics with strong emphasis on computational science. The second will focus on scale bridging science and applications to nano-structured materials. Our vision is that the educational segment of this proposal will significantly accelerate and enhance the understanding of multiscale processes and provide us with a means to actively engage students in the lifelong learning process. It is our intent that this effort will directly aid students in becoming successful applicants for faculty and industrial

positions, and thereby become tomorrow's leaders in our expanding and increasingly diverse technical community. The following educational efforts will be pursued.

2.3.2 Graduate courses

The development of graduate courses in multiscale science and engineering is critical to the training of the next generation of researchers. The two PIs developed an innovative symbiotic relation between research-level short courses and graduate courses, which has provided a mechanism for developing state-of-the-art materials. We will develop two courses in Multiscale Computational Methods for Nano-structured Materials with former focusing on fundamental and later on applications. Portions of this course were jointly taught by Professors Fish and Ghoniem in Brazil during summer 2004, and were sponsored by NSF. The two-course sequence will be further developed on-line for US graduate students to prepare them for global competition and research.

2.3.3 Student exchanges

In order to fully benefit from the multidisciplinary nature of the project, students need to learn from and be exposed to the complementary expertise of the two PIs. This will be accomplished by substantial (in length of time) and frequent exchanges of graduate students and postdoctoral researchers between UCLA and RPI.

2.3.4 Training undergraduate students

Undergraduate students will be intensively exposed to the project through Undergraduate Research Program (URP) involvement. URP positions will be especially targeted at students from under-represented groups. It is our sincere hope that exposing such students to an exciting area of research will attract them to graduate study in multiscale modeling and computations.

Tasks	Timeline		
	Year 1	Year 2	Year 3
1. TMC development and validation			
2. NTMC development and validation			
3. AIDD development and validation			
4. CGMD development and validation			
5. Model error estimators development			
6. Adaptive model selection strategy			
7. Application to Nano-Composites			
8. Application to nano-twinned materials			
9. Development of Multiscale Fundamental course			
10. Development of Multiscale Applications course			

Figure 10: Task time-line for the proposed research

2.4 Tasks and Time-line

Figure 10 summarizes various tasks and gives the time-line of various tasks. The general responsibility of Prof. Ghoniem will be on development of atomistically informed dislocation dynamics (AIDD) method, the two applications selected and development of multiscale applications course. Prof. Fish will lead the development of TMC, NTMC and CGMD methods and Multiscale Fundamentals course. Development of model error estimators and adaptive strategy will be equally shared by the two PIs. To accomplish the goals of the project close collaboration between the two PIs will be established. For instance, the TMC developed in Year 1 will be used to formulate the AIDD model in subsequent years; model error estimators developed in Year 2 will be needed to guide the construction of adaptive strategy in Year 3; the adaptive hierarchical multiscale framework in its beta version will be released sometimes in Year 2 and will be applied to analyze the two applications in Years 2 and 3.

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3 Biographical Sketches

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PROFESSIONAL PREPARATION

- B.S. University of Alexandria, Egypt, Dept. of Nuclear Engineering (1971)
- M.Eng. McMaster University, Canada, Dept. of Engineering Physics (1974)
- M.S. University of Wisconsin, USA, Dept. of Nuclear Engineering (1975)
- Ph.D. University of Wisconsin, USA, Dept. of Nuclear Engineering (1977)

APPOINTMENTS

- University of California Distinguished Professor, UCLA (2006-)
- Professor, Materials Science & Engr. Dept. (joint), UCLA (2002-)
- Professor & Vice Chair, Mechanical & Aerospace Engr. Dept., UCLA (86-)

HONORS & AWARDS

- Co-chair, World Congress of Computational Mechanics (1600 attendants) (2006)
- Member, International Advisory Committee, PERFECT Project sponsored by the EU (2005)
- General Chair, Second Multiscale Materials Modelling Conference (2004)
- Royal Society of London Visiting Professorship in Hong Kong (2000)
- Research fellowship of Japan Society for the Promotion of Science (JSPS) (1999)
- Lifetime Outstanding Achievement Award of ANS (1998)
- Fellow of the American Nuclear Society (1994)
- Who's Who in Frontier Science and Technology (1983)
- Outstanding Young Man of America Award (1978)
- First world patent on Low Activation Ferritic Steels, U.S. Patent No. 4,622,067 (1986)
- Co-founder (w/ Kubin- France) of Dislocation Dynamics for microplasticity . (1987)

SYNERGISTIC ACTIVITIES

- **Member:** The American Nuclear Society (ANS), the American Academy of Mechanics, the Materials Research Society (MRS); The American Society for Mechanical Engineers (ASME), and the American Physical Society (APS).
- **Associate Editor:** Defect and Diffusion Forum, Solid State Phenomena (Scitec Publishers);
- **Editorial Boards:** J. Nucl. Mater.; J. Comp. Methods in Eng. Sci. (CMES); International J. of Mate. and Mechanics in Design (Kluwer), J. of Comp. & Theoretical Nanoscience (ASP)
- **Guest Editor:** J. Comp. Aided Mater. Des. (JCAD); MRS Proc., Phil. Mag. , Vacuum, J. Nucl. Mater.

PUBLICATIONS: Over 230 articles (170 refereed journal articles) on the mechanics and physics of defects, computational materials science, radiation interaction with materials, instabilities and self-organization in non-equilibrium materials.

Five most related publications

1. Nasr M. Ghoniem, Editor, "Proceedings of the Second International Conference on Multiscale Materials Modeling," UCLA Publication, October 11-15, 2004, Los Angeles, California, 600 pages.

2. Xinwei Zhang, Shafigh Mehraeen, Jiun-Shyan Chen, and Nasr Ghoniem, "Multi-scale Formulation for Modeling Dislocation Induced Plastic Deformation in Polycrystalline Materials ", International Journal for Multi-scale Computational Engineering, In Press (2005)

3. N. M. Ghoniem, H. Huang, E. Busso, and N. Kioussis, "Multiscale Modeling of Nano- and Micro-Mechanics: an Overview," Phil. Mag. 83(31-34), 3475-3528 (2003).

4. N. M. Ghoniem, S. H. Tong, and L. Z. Sun, "Parametric Dislocation Dynamics: A Thermodynamics based Approach to Investigations of Mesoscopic Plastic Deformation," Phys. Rev. B 61(1), 913-927 (2000).

5. Nasr M. Ghoniem and Xueli Han, "Dislocation Motion in Anisotropic Multi-layer Materials," Phil Mag., 85(4): 2809-2830 (2005).

Five other significant publications

1. N. M. Ghoniem and K. Cho, "The Emerging Role of Multiscale Modeling in Nano- and Micromechanics of Materials," J. Comp. Meth. Engr. Science, CMES 3(2), 147-173 (2002).

2. R. Martinez and N. M. Ghoniem, "The Influence of Crystal Surfaces on Dislocation Interactions in Mesoscopic Plasticity: A Combined Dislocation Dynamics- Finite Element Approach," J. Comp. Meth. Engr. Science, CMES 3(2), 229-243 (2002).

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PROFESSIONAL EXPERIENCE

- 2005-present The Rosalind and John J. Redfern, Jr. '33 Chaired Professor in Engineering
- 1998-2005 Professor, Mechanical, Aerospace and Nuclear Engineering, and Civil and Environmental Engineering (joint), RPI.
- 2001 Visiting Chair Professor, Ecole Normale Superieure de Cachan, France.
- 1994 - 1998 Associate Professor, Mechanical, Aerospace and Nuclear Engineering, and Civil and Environmental Engineering (joint), RPI.
- 1989 - 1994 Assistant Professor, Civil and Environmental Engineering, RPI.
- 1984 - 1986 Research Engineer, Methods Development Group, Aircraft Industries, Israel.
- 1982 - 1984 Structural Engineer, Civil Engineering Consulting, Inc., Tel-Aviv, Israel

FIVE PUBLICATIONS RELATED TO THIS PROPOSAL (out of 120)

1. J. Fish and K. L. Shek, "Finite Deformation Plasticity of Composite Structures: Computational Models and Adaptive Strategies," Comp. Meth. Appl. Mech. Engng., Vol. 172, pp. 145-174, (1999).
2. J. Fish, W.Chen and G. Nagai, "Nonlocal dispersive model for wave propagation in heterogeneous media. Part I and Part II," International Journal for Numerical Methods in Engineering, Vol. 54, pp. 331-346, pp. 347-363 , (2002).
3. J. Fish and C. Schwob, "Towards Constitutive Model Based on Atomistics," International Journal of Multiscale Computational Engineering, Vol. 1 pp. 43-56, (2003).
4. J. Fish and Z. Yuan, "Multiscale Enrichment based on the Partition of Unity," International Journal for Numerical Methods in Engineering, Volume 62, Issue 10, pp. 1341-1359 (2005).
5. J.Fish, "Discrete to Continuum Multiscale Bridging ," to appear in Multiscaling in Molecular and Continuum Mechanics, Springer 2006.

SYNERGISTIC ACTIVITIES

- USACM Computational Structural Mechanics Award,

- 2005 Rensselaer School of Engineering Research Award,
- 2003 Fellow, International Association for Computational Mechanics,
- 2002 Fellow, US Association for Computational Mechanics,
- 2001 ASME, International Computers in Engineering Conf., Best Paper Award,
- 1995 USACM Travel Award,
- 1994. AIAA/SDM, Computational Mechanics, Best Paper,
- 1993. National Science Foundation Presidential Young Investigator Award,
- 1992. Summa Cum Laude, B.S
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EDITORSHIPS

- Editor-in-Chief, International Journal of Multiscale Computational Engineering, 2002-
- Editor, Bulletin of U.S. Association for Computational Mechanics, 1994-1997
- Associate Editor, Journal of Engineering Mechanics, 1999-2001
- Editorial Board Member, Journal of Computational Engineering Science, 2003-
- Editorial Board Member, International Journal for Numerical Methods in Engineering, 2001-
- Editorial Board Member, Computer Methods in Applied Mech. and Eng., 2005-

MEMBERSHIPS/AFFILIATIONS

- President, U.S. Association for Computational Mechanics, 2002-2004
- Chair, ASCE Computational Mechanics committee, 1999-2001.
- Member, National Research Council for the Air and Ground Vehicle Technology, 2000-2004
- Member of IUTAM Working Party on Computational Fluid and Solid Mechanics, 2004-
- External Reviewer, Sandia Computer Information Sciences Center, 2004
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4.1 Nasr M. Ghoniem -UCLA

Current Support:

- **Project Title:** *ITR/AP (MPS): Collaborative Research on Large-Scale Dislocation Dynamics Simulations for Computational Design of Semiconductor Thin Film Systems*
  Source of Funding: NSF; Amount: $327,895 ; Dates: 08/15/01 - 07/31/06; Location: UCLA; Faculty Time: 0.0 summer, 0.45 AY
- **Project Title:** *Modeling the Deformation of Nano-Layered Structures by Computer Simulation*; Source of Funding: AFOSR ; Amount: $359,999 ; Dates: 01/03/03 - 03/30/06 ; Location: UCLA ; Faculty Time: 0.5 summer, 0.2 AY
- **Project Title:** *Micro-engineered Surfaces for High Average Power Laser (HAPL) Chambers*; Source of Funding: Naval Research Laboratory ; Amount: $465,000 ; Dates: 05/22/03 - 05/21/06; Location: UCLA ; Faculty Time: 0.5 summer, 0.15 AY
- **Project Title:** *Multiscale Modeling of Deformation, Fracture and Failure of Fusion Materials and Structures*; Source of Funding: Department of Energy ; Amount: $1,897,999 ; Dates: 07/15/03 - 10/31/07 ; Location: UCLA ; Faculty Time: 1.0 summer, 0.15 AY
- **Project Title:** *Development of Robust IFE Laser Mirrors and Multi-Scale Modeling of Pulsed Radiation Effects*; Source of Funding: Department of Energy ; Amount: $420,000 ; Dates: 07/15/03 - 07/14/06 ; Location: UCLA ; Faculty Time: 0.0 summer, 0.15 AY
- **Project Title:** *NIRT: Nanostructured Materials for Interconnect and Packaging Technology*; Source of Funding: NSF; Amount: $1,300,00.00 ; Dates: 08/01/2005 07/31/2009 ; Location: UCLA; Faculty Time: 0.5 summer, 0.5 AY
- **Project Title:** *Multiscale Modeling of the Deformation of Advanced Ferritic Steels for Generation IV Nuclear Energy*; Source of Funding: Department of Energy ; Amount: $495,000.00 ; Dates: 03/15/06 - 3/141/09 ; Location: UCLA & CSUN ; Faculty Time: 0.5 summer, 0.15 AY

Pending Support:

- **Project Title:** *Multiscale Atomistic-Continuum Simulations of the Deformation of Ultra-Strong Nano-structured Materials* ; Source of Funding: NSF ; Amount: $395,000.00; Dates: 08/01/06 - 07/30/09 Location: UCLA & RPI; Faculty Time: 0.25 AY
- **Project Title:** *Survival and Reliability Assessment of Chamber Structural Materials for High Average Power Laser (HAPL) Systems*; Source of Funding: Naval Research Laboratory ; Amount: $533,000 ; Dates: 04/01/06 - 03/31/09; Location: UCLA ; Faculty Time: 0.5 summer, 0.15 AY

4.2 Jacob Fish - RPI

Current Support:

- **Project Title:** *Modeling and Simulation Framework at the Nanoscale Application, (NSF) Multiscale Systems Engineering for Nanocomposites* (NSF)

- **Project Title:** *Multiscale Model for Crash Prediction of Composite Structures (GM, Ford, Chrysler) Ceramic Matrix Composite Design Tool and Lifting Code* (Rolls-Royce)

- **Project Title:** *Adaptive Multiscale Computational Framework for Transient Problems (NSF) Multiscale Capabilities for Impact Simulation Metal-Polyurea Layered Plates* (ONR)

- **Project Title:** *Adaptive Multiscale Modeling and Simulation for Munitions Simulations* (AFRL)

- **Project Title:** *A Mathematical Analysis of Atomistic-to-Continuum Multiscale Approaches* (DOE)

Pending Support:

- **Project Title:** *Probabilistic Multiscale Analysis: Validated Predictive Models for Reliable Material Design*

- **Project Title:** *Multiscale Atomistic-Continuum Simulations of the Deformation of Ultra-Strong Nano-structured Materials* ; Source of Funding: NSF ; Amount: $395,000.00; Dates: 08/01/06 - 07/30/09 Location: UCLA & RPI; Faculty Time: 0.25 AY

5 Research Facilities

The project is mainly computational and its implementation will rely heavily on state-of-the art computing facilities. At UCLA, the ISIS computational facility will be utilized in performing Molecular Dynamics and Dislocation Dynamics, while the computational aspects of Multiscale Modeling will be developed at RPI.

5.1 The UCLA ISIS Computational Cluster

The ISIS Computational Cluster at the University of California at Los Angeles, under the direction of Professor Nasr Ghoniem of the Mechanical and Aerospace Engineering Department, and managed by Dr. Robert Amodeo, is a "Beowulf Cluster"consisting essentially of 90 computers and a fileserver. The cluster is housed in the Micro and Nano Mechanics Laboratory in the Math Sciences Building at UCLA.

The primary purpose of this cluster is to reduce the time it takes to run Monte Carlo, Molecular Dynamic, and Dislocation Dynamic codes which can rely heavily on many body interactive forces. Computations which may be on the O NxN can be reduced significantly, by distributing the process over 90 dual processor computers (180 "effective"nodes, 90 physical nodes). A secondary purpose of the cluster is to investigate the nature of parallel processing, in conjunction with the associated physics driving micro and nano-mechanical processes. The cluster is "operational"at this time, and is currently running PGI v4.0 Fortran Compilers, on SuSE Linux 8.0 OS. The cluster has passed fundamental benchmarks, and is currently being tested by users at UCLA and Los Alamos National Laboratory.

The system consists (shown in Figure 11) of one large scale fileserver, which runs the main computational operating system, and serves accounts. Data (source code, input files, output files) are located on this file server. The 90 nodes are used primarily for their processing units, and also have large disks for scratch storage. The visualization workstations have high memory video cards for displaying resulting data, and running structural visualization, animation, and design programs. The webserver is used exclusively to serve up data / information in various formats (database, flash and other animations, pictures, etc.) to the global community.

Figure 11: ISIS computational cluster

The characteristics of the ISIS Beowulf cluster are:

- Nodes

  - 90 Multiwave Dual AMD MP 1800 processor systems
  - each: Kingston 1.0 GB PC2100 DDR RAM
  - each: IBM 40 GB 7200 RPM Hard drive
- Fileserver
  - 1 Multiwave Dual AMD MP 1900 processor system
  - Kingston 1GB PC2100 DDR RAM
  - 4 IBM 35 GB SCSI Hard Drives in RAID 5
  - 2 IBM Ultra 120 GB IDE 7200 RPM Hard Drives
- Visualization Workstations
  - 2 Multiwave Dual AMD MP 1800 processor systems
  - each: Kingston 1.0 GB PC2100 DDR RAM
  - each: 1 IBM Ultra 120 GB IDE 7200 RPM Hard Drive
  - each: ATI RADEON 7200 64MP AGP Video Card
- Webserver
  - 1 Multiwave Dual AMD MP 1800 processor system
  - Kingston 1.0 GB PC2100 DDR RAM
  - IBM 40 GB 7200 RPM Hard drive
- Switch
  - D-Link DES-6000 128 port 10/100 and Fast Ethernet Switch
  - D-Link DES-6003 16 port modules, 5 total (80 ports)

Beowulf clusters traditionally use versions of the popular UNIX operating system Linux. In particular, SuSE Linux is a well known, and superior version of Linux which is currently being considered as a world-unified standardized version. The installation, GUI, hardware compatibility, and superior integration with the cluster development software made it the prime choice. The Portland Group software suite provides the versions of Fortran and C++ used in our system, in addition to Cluster Development Kit which combines or cluster debugger, cluster profiler, integrated mpich libraries and PBS (portable batch-queueing system).

- OS (for fileserver, nodes): SuSE Linux 8.0)
  - OS (for visual workstations): Windows 2000
  - OS (for webserver): Windows 2000 Server
- Compilers: Portland Group PGI Fortran 77, Fortran 90, C, and C++
- Portland Group CDK (Cluster Development Kit)
  - PBS (portable batch-queueing system)
  - PBS (portable batch-queueing system)

- MPI (message passing interface)
- MPICH libraries

The 90 tower units are mounted on 5 metal racks, which hold 15 units apiece; 5 units each on 3 plywood shelves (per rack). 4 of the racks hold 59 computers and the D-Link switch, and one rack holds 5 computers, the 2 visualization workstations and monitors, 2 web servers, 1 printer, and 2 scanners. The racks are bolted into the ground, and the units are secured onto the plywood rack shelves. The units are also secured against theft.

Executing Codes

Individual jobs are run from the user's home directory, which is a mapped share to the RAID 5 drives on the fileserver. The batch processing and message passing occurs (and is distributed over) the 90 nodes (or fraction thereof, depending upon access privileges). The output is designed to be transferred to the larger (non-redundant) drives, and from there will be transferred to the visualization workstations for processing.

Basically, the batch processing (PBS) is used to distribute individual jobs over the different nodes. Message passing (MPI) is used to run portions of code, especially CPU intensive portions, over different nodes. The latter is the prime element for parallel processing, and will be used extensively in the studies undertaken by the UCLA Materials Group.

For using PBS (portable batch-queueing system), jobs submitted are queued according to priority. At the current time, the small number of users does not warrant close monitoring of usage. However, in the future, as more outside agents begin to use the cluster, we will prioritize the usage of the cluster nodes, and delegate portions of it for different classes of users. Cooling

Large Scale A/C Unit

The room is approximately 25 'x50', and is cooled by a large scale Air Conditioning Unit which provides more than adequate 24 hour cooling to the 90 plus machines - it is specifically ducted to pass air over the cluster group (5 racks), and turbulently cool the remainder of the room. The temperature is set to 69 F. The types of codes which are ideal for the cluster are the following: Monte Carlo, Molecular Dynamics, and Dislocation Dynamics.

5.2 RPI Facilities

SCOREC Computation Facilities (RPI)

Data Server - Sun E3501 with two 400MHz UltraSPARC II Processors 2GB Memory, 510GB Disk Array and 1TB Tape Backup Robot.

Application Server - Sun E450 with two 300MHz UltraSPARC II Processors, 1GB Memory, 150GB Disk

Information Servers: - Sun Ultra-2 mail server (2 UltraSPARC-II 200MHz processors, 896MB memory, 22GB Disk); Sun Ultra-2 terminal server (2 UltraSPARC-I 170MHz processors, 1GB memory, 72GB Disk); 4 Sun SparcServer-10 information servers.

Parallel Computational Facilities

- Sun cluster with 48 UltraSPARC-IIe 400MHz processors, 30GB Memory (640MB/processor), 960GB of disk, and E220R front-node (UltraSPARC-II 360MHz processor). Cluster uses dedicated FastEthernet network for inter-processor communications

- SGI Onyx2 with R10000 Processors, 3.5GB Memory and18GB Disk
- Dell PowerEdge 6450 with 4 PentiumIII 700MHz, 3.5GB Memory, 50GB Disk

Visualization Facilities

- 1 Intel Dual 500 MHz PentiumIII Xeon Processors with 512MB Memory, 18GB Disk, and Intergraph's Wildcat OpenGL accelerator
- The SGI Onyx2 listed above includes an Infinite Reality Engine graphics subsystem with 1 Raster Manager
- 3 SUN Ultra60 Dual 360MHz UltraSPARC II Processors, 2GB of Memory, 9GB of Disk, and an Elite 3D-m6 Graphics Subsystem
- 3 SUN Ultra60 360MHz to 450MHz UltraSPARC-II Processor, 1GB of Memory, 9GB of Disk and an Elite 3D-m6 Graphics Subsystem
- 11 SUN Ultra10 360MHz UltraSPARC IIi Processor, 1GB of memory, 9 GB disk and an Elite 3D-m3 Graphics Subsystem
- Fakespace VersaBench - a large format adjustable display (4'x6') with stereo viewing, 3D head tracking, and a 3-D pointer.

Application & Development Workstations

- 1 Intel Dual 500 MHz PentiumIII Xeon Processors, 512MB memory
- 3 Intel 500 MHz PentiumIII's, 256MB memory with E&S 3D graphics
- 2 Intel 933 MHz PentiumIII workstations, 256MB memory
- 9 UltraSPARC IIi 360MHz to 440MHz Suns with Creator 3D graphics
- 2 SGI Indigo2 R10000 Systems - one with a Max Impact graphics subsystem
- 4 Sun SparcStations-10 Workstations
- 3 SGI Indigo2 Extreme Workstations
- 6 Sun Ray 1 terminals (being deployed)

Network Firewall - Cisco PIX 515, unlimited clients

Network Backbone:

- 1 Intel Gigabit Ethernet Gigaswitch
- 5 FastEthernet switches connected to the Intel Gigaswitch
- 2 Bay Networks Centillion 100 Ethernet switch The Data and Application Servers are directly connected to the Gigaswitch. All other computers are connected directly to a switched port.

Shared Parallel Computing Facilities

- 70 Proc. IBM SP (16 4-way & 3 2-way SMP),20GB Memory, 216 GB Disk (Campus)
- Intel Cluster with 32 Processors (4 Quad 500MHz Pentium III Xeon Processors and 8 Dual400MHz Pentium II Processors), 8GB Memory (256MB/processor) and 352 GB of total disk. The cluster uses a high speed Myrinet switch for communications between machines. (Joint with CS)

6 Results from Prior NSF support

6.1 Nasr Ghoniem - UCLA

ITR/AP (MPS): Collaborative Research on Large-Scale Dislocation Dynamics Simulations for Computational Design of Semiconductor Thin Film Systems, NSF-0113555, $ 284,595, 9/1/2001 - 07/31/2004, PI: N. Ghoniem, Co-PI: L. Sun.

The research achievements of this project are: (1) 'Parametric Dislocation Dynamics (PDD)' method for analyzing dynamics and interactions of dislocations in anisotropic crystals; (2) determination of equivalent 'averaged' isotropic elastic properties and the effects of elastic anisotropy in anisotropic crystals; (3) full three-dimensional simulations of complex dislocation loop ensembles in anisotropic crystals; (4) new solutions for the elastic fields of interfacial dislocation arrays in thin, multi-layered films; (5) simulations of the stress and surface deformation fields resulting from buried interfacial dislocation arrays in Si / SiGe systems; (6) simulation of atomic surface diffusion with the periodic stress field generated by dislocation arrays using the Kinetic Monte Carlo (KMC) method. Four journal papers have been published.

6.2 Jacob Fish - RPI

Adaptive Multiscale Computational Framework for Transient Problems- NSF 0408359. Pi: J. Fish.

Project supported one PhD student and resulted in two manuscripts. Developed failure and fragmentation models of composite materials and structures subjected to impact loading. This was accomplished using mathematical homogenization technique combined with model reduction methods aimed reducing the computational cost of solving the continuum unit cell problem. Verification studies of the model were conducted on structural components made of fibrous and woven composite microstructure.

NIRT: Modeling and Simulation Framework at the Nanoscale- NSF 0211474. co-PIs: J. Fish, C. Picu, K. Anderson and M. Shephard.

RPI team developed an adaptive multiscale modeling and simulation methodology aimed at designing and manufacturing of nanomaterials and nanodevices. The framework consists of space-time adaptive multiscale modeling methodology capable of coupling behaviors from the atomic to continuum scale for polymeric nanocomposites. Two publications resulted from this work.

Multiscale Systems Engineering for Nanocomposites- NSF 0303902. (12 co-PIs and investigators)

Dr.Fish developed the Generalized Mathematical Homogenization theory and validated it for polymer melts. The GMH developed provides coupled atomistic-continuum formulation. The fine scale problem derived can be interpreted as a molecular statics (at 0K) problem, where the coarse scale problem derived is a constitutive law-free continuum equation, which calculates the Cauchy stress directly from the atomistics. Two publications resulted from this work.