APPLICATIONS OF PARAMETRIC DISLOCATION DYNAMICS TO THE DESIGN OF NANO-STRUCTURED MATERIALS

Nasr M. Ghoniem

Mechanical & Aerospace Engineering Department
University of California, Los Angeles
Los Angeles, CA. 90095-1597

ABSTRACT We review recent developments in computational microscopic plasticity, which are based on simulation of the dynamics of large dislocation ensembles and their interactions within small volumes, characteristic of nano- and microstructures. The fundamental principles behind computer simulations will first be presented, followed by analysis of the state-of-the art approaches. A new formulation based on differential geometry is then discussed and shown to facilitate studies of dislocation generation, pileups, grain-boundary interactions, dipole dynamics, junction nucleation and destruction, and interaction with defect clusters. Emphasis is placed on computational issues of space and time resolution. A number of applications in the design of thin films, quantum dots, confined layer slip, single crystal deformation, and plastic instabilities of irradiated materials will be addressed.

INTRODUCTION: 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. Engineering ultra-strong, yet ductile nano-layered composites where multiple performance requirements are sought is now under intense investigation. Continuum methods for prediction of the mechanical properties of sub-micron structures fail to describe their plastic deformation and subsequent failure. In this paper, we review recent developments in computational microscopic plasticity (Kubin et al. 1992, Rhee et al. 1998, Ghoniem et al. 2000,2001a&b), which are based on computer simulations of the dynamics of large dislocation ensembles and their interactions within small volumes characteristic of nano- and microstructures. Such models a fundamental approach to accurately predict the strength and plastic deformation at nano- to micro- length scales. Development of the proposed computer models will allow future material designers to literally "engineer" nano- and micro-layered composites for optimized performance by large-scale computer simulations. The eventual aim of these approaches is to develop large-scale computational modeling capabilities for future engineering and design of optimized nano- and micro-scale multi-layer structures.

The fundamental principles behind computer simulations will first be presented, followed by an analysis of the state-of-the art in the various approaches in this area. The elastic field of complex 3-D dislocation ensembles is described by differential geometric representations, which allow computer simulations of microscopic plastic deformation

without additional ad hoc approximations for short-range dislocation reactions. Simple vector forms of differential geometry are shown to be independent of the coordinate system, and to facilitate studies of dislocation generation, pileup formation, grain-boundary interaction, finite-length dipole nucleation and break-up, junction nucleation and destruction, interaction with defect clusters, and self-consistent boundary conditions. A number of applications will also be considered to show their utility in the design of thin films, quantum dots, confined layer slip in nano-composites, single crystal deformation, and plastic instabilities of irradiated materials.

RESTULTS AND DISCUSSION: In Parametric Dislocation Dynamics (PDD), closed dislocation loops are described as an assembly of segments, each represented by a parametric space curve, as shown in Fig. 1. Their equations of motion are derived from an energy variational principle, thus allowing large-scale computer simulations of plastic deformation (Ghoniem 2000, 2001a&b). The limits of temporal and spatial resolution of strong dislocation interactions have been recently established. The method is be highly accurate, with unconditional spatial convergence that is limited to distances on the order of interatomic dimensions. The stability of dislocation line shape evolution requires very short time steps for explicit integration schemes, or can be unconditionally stable for implicit time integration schemes. Limitations of the method in resolving strong dislocation interactions have been established for a number of mechanisms: dislocation generation, annihilation, dipole and junction formation, pileup evolution, and interaction with atomic clusters.

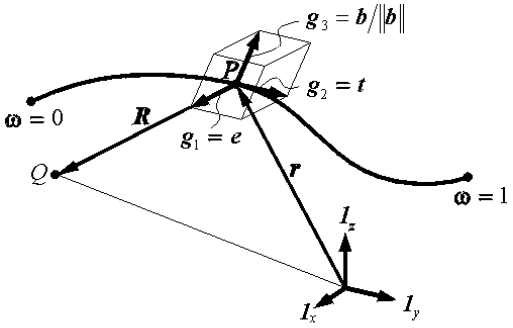

Fig.1 Parametric representation of a curved dislocation segment.

Two representative results of recent computer simulations are shown in Figs. 2 & 3 below. The initial dislocation microstructure is represented by complete dislocation loops with sessile and glissile segments, and a uniaxial stress is applied on a representative volume. Glissile dislocation segments expand on their respective glide plane, and interact amongst themselves forming junctions, dipoles and partially expanded Frank-Read sources, as can be seen in Fig. 2. A special form of a periodic boundary condition is used to provide analytical continuation of loop segments that expand outside the volume by injecting tem back into the simulation space. At constant applied strain rate, the initial hardening portions of the stress-strain curve are obtained.

Irradiated materials undergo plastic instabilities that are controlled by the interaction of small defect clusters with grown-in dislocations (Ghoniem et al. 2001a). Dislocations get locked-in in a similar way to the role of impurities in the Cottrell atmosphere mechanism. This mechanism is revealed by Monte Carlo computer simulations of the evolution of

defect cluster atmospheres and rafts in the vicinity of grown-in dislocations, and is shown in Fig. 3 after 50 ns at room temperature in irradiated Fe. Small prismatic dislocation loops glide one-dimensionally along highly packed crystallographic directions, with occasional rotation of their Burgers vector. Cluster-cluster-dislocation interaction is found to be essential for the formation of dislocation decorations, cluster rafts and pinned clusters, as can be seen in Fig. 3. Additional applications of PDD to the design of multi-layered nano-systems, and to the evolution of quantum dots will also be discussed.

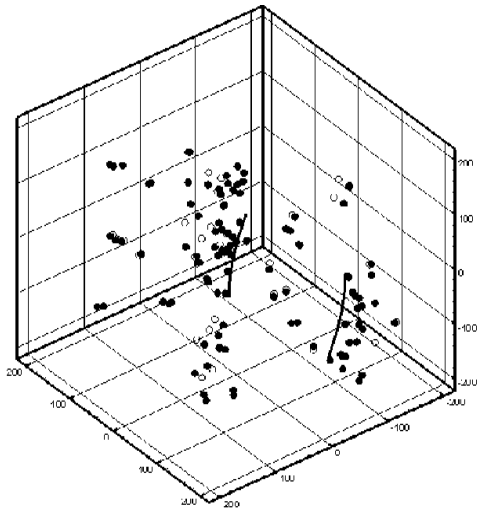

Fig.3 Formation of pinned defect clusters and dislocation loop rafts near grown-in dislocations in irradiated materials.

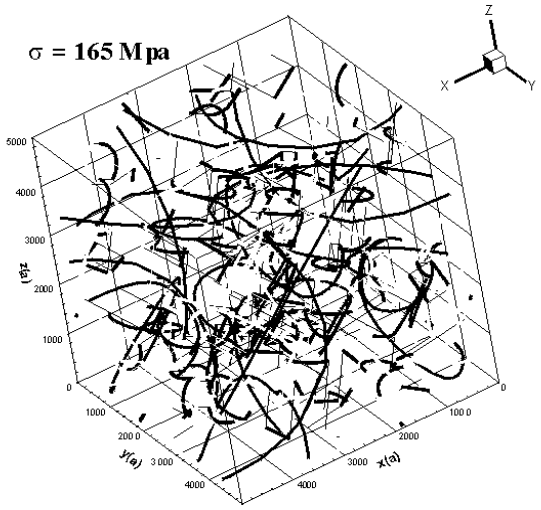

Fig.2 Effects of applied stress on the dislocation microstructure.

ACKKNOWLEDGEMENT: Support of this research by the US Department of Energy (OFES), through Grants DE-FG03-98ER54500 and DE-FG03-00ER54594, and the National Science Foundation Grant with UCLA is greatly appreciated.

REFERENCES:

Ghoniem, N.M., Tong, S.H., and Sun, L.Z., 2000 "Parametric Dislocation Dynamics: A Thermodynamcis-based Approach to Investigations of Mesoscopic Plastic Deformation", *Phys. Rev.* B, **B1(1):**913-927.

Ghoniem, N.M., Tong, S.H., Singh, B.N., and Sun, L.Z., 2001a, "On Dislocation Interaction with Radiation-induced Defect Clusters and Plastic Flow Localization in FCC Metals", *Phil. Mag.*, A, **81(1)**, 2743-2764.

Ghoniem, N.M., Huang, J., and Wang, Z., 2001b, "Affine Covariant-contravariant Vector Forms for the Elastic Field of Parametric Dislocations in Isotropic Crystals", *Phil. Mag. Lett*., in press.

Kubin, L.P., Canova, G., Condat, M., Devincre, B., Pontikis, V., and Brechet, Y., 1992," Dislocation microstructures and plastic flow: a 3D simulation," *Sol. State Phenomena*, **23/24**, 445.

Rhee M., Zbib H. M. and Hirth J. P., 1998, "Models for Long/Short Range Interactions in 3D Dislocation Simulation", *Modeling & Simulations in Maters. Sci. Eng*. **6**, 467-492.