

PARAMETRIC DISLOCATION DYNAMICS: A THERMODYNAMICS-BASED APPROACH TO INVESTIGATIONS OF MESOSCOPIC PLASTIC DEFORMATION

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Extended Abstract

A thermodynamics-based variational method is developed and used to establish the equations of motion of three-dimensional (3-D) interacting dislocation loops. A fast sum method for the elastic field of dislocation ensembles is utilized to determine forces acting on generalized coordinates of arbitrarily curved loop segments. Each dislocation segment is represented as a parametric space curve of specified smooth shape functions and *Degrees of Freedom* (DF) associated with beginning and end nodes. Kinetic equations for the generalized coordinates describing dislocation motion are derived for computer simulation of mesoscopic plastic deformation of materials. For general climb/glide 3-D motion of a curved dislocation segment, we show that $N_{DF}(j)=3n$, where $n=1$ for linear; $n=2$ for cubic; and $n=3$ for quintic parametric splines, respectively. It is also shown that the position P , tangent T , and normal N vectors at segment nodes are sufficient to describe general 3-D motion. For constrained glide motion, however, we also show that only two degrees of freedom are adequate for determination of dislocation loop profiles, including crystal structure constraints. A number of examples are given to illustrate the following features of the method: (1) adaptive node generation on interacting segments, (2) variable time-step determination for integration of the equations of motion, (3) dislocation generation by the Frank-Read mechanism in fcc, bcc and sc crystals, (4) loop-loop deformation and interaction, (5) formation of dislocation junctions, and (6) dislocation microstructure evolution.

A fundamental description of plastic deformation is now actively pursued, where dislocations play a key role as basic elements of material plasticity. Although continuum plasticity models are extensively used in engineering practice, their validity is limited to the underlying data base. The reliability of continuum plasticity descriptions is dependent on the accuracy of the experimental data. Under complex loading situations, however, the database is often hard to establish. Moreover, the lack of a characteristic length scale in continuum plasticity makes it difficult to predict the occurrence of critical localized deformation zones. Although homogenization methods have played a significant role in determining the elastic properties of new materials from their constituents (e.g. composite materials), the same methods have failed to describe plasticity. It is widely appreciated that plastic strain is fundamentally heterogeneous, displaying high strains concentrated in small material volumes, with virtually undeformed regions in-between. Experimental observations consistently show that plastic deformation is internally heterogeneous at a number of length-scales. Depending on the deformation mode, heterogeneous dislocation structures appear with definitive wavelengths. It is common to observe Persistent Slip Bands (PSB's), shear bands, dislocation pile ups, dislocation cells and sub grains. However, a satisfactory description of realistic dislocation patterning and strain localization has been rather elusive. A relatively recent approach to investigating the fundamental aspects of plastic deformation is based on direct numerical simulation of the interaction and motion of dislocations. This approach, which is commonly known as Dislocation Dynamics (DD), was first introduced for 2-D straight, infinitely long dislocation distributions, and then later for complex 3-D microstructure. Dislocation loops in DD computer simulations are treated as dynamical systems, which can be described by the time dependence of specified coordinates. In this work, we describe the equations of motion for generalized coordinates in much the same way as in Lagrangian mechanics. Regardless of the dislocation loop shape

complexity, we will develop an integral equation of motion for each curved segment within the loop, such that only relationships between global thermodynamic variables are obeyed. For concreteness, we focus the current approach on dislocation line representation by parametric dislocation segments, similar to the Finite Element Method (FEM). Thus, the equations of motion for the transport of atoms within the dislocation core should be consistent with the thermodynamics of irreversibility. A challenging prospect in such a description is the enormous topological complexity of materials containing dislocations. Dislocation lines assume complex shapes, particularly during heavy deformation and at high temperatures where they execute truly 3-D motion as a result of combined glide and climb forces. These dislocations can be highly curved because of their strong mutual interactions, externally applied stress fields, as well as other thermodynamic forces. It is apparent that whenever large curvature variations are expected, the accuracy of computing the dynamic shape of dislocation loops becomes critical. Many applications of the present method are feasible, especially in areas where continuum descriptions of plastic deformation fall short. One such application is the simulation of the onset of plastic instabilities and the formation of dislocation channels in irradiated materials. It is concluded that the present method offers a number of potential advantages:

A natural description of dislocation loop geometry that is not determined by an underlying computational mesh, and which is able to conform to physical constraints imposed by the crystal structure.

Avoidance of numerical divergence problems for very short straight segments, and the loss of accuracy on long segments.

High resolution of short-range reactions in-between curved dislocation segments.
Flexibility in mixing segment types during the same computation, thus leading to a reduction in the overall computational burden.

Compatibility with the standard Finite Element Method, which may lead to direct coupling with the computational methods of continuum mechanics.