FAST SUM METHOD FOR THE ELASTIC FIELD OF 3-D DISLOCATION ENSEMBLES – N. M. Ghoniem and L. Sun (University of California at Los Angeles)

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Extended Abstract

Because the internal geometry of deforming crystals is very complex, a physically based description of plastic deformation can be very challenging. The topological complexity is manifest in the existence of dislocation structures within otherwise perfect atomic arrangements. Dislocation loops delineate regions where large atomic displacements are encountered. As a result, long-range elastic fields are set up in response to such large, localized atomic displacements. As the external load is maintained, the material deforms plastically by generating more dislocations. Thus, macroscopically observed plastic deformation is a consequence of dislocation generation and motion. A closer examination of atomic positions associated with dislocations shows that large displacements are confined only to a small region around the dislocation line (i.e. *the dislocation core*). The majority of the displacement field can be conveniently described as elastic deformation. Even though one utilizes the concept of dislocation distributions to account for large displacements close to dislocation lines, a physically based plasticity theory can paradoxically be based on the theory of elasticity!

Recently, a surge in interest towards understanding the physical nature of plastic deformation has developed. This interest is motivated by the extensive experimental evidence, which shows that the distribution of plastic strain in materials is fundamentally heterogeneous. Because of the complexity of dislocation arrangements in materials during plastic deformation, an approach, which is based on direct numerical simulations for the motion and interactions between dislocations is now being vigorously pursued. The study of dislocation configurations at short-range can be quite complex, because of large deformations and reconfiguration of dislocation lines during their interaction. Thus, adaptive gridding methods and more refined treatments of self-forces have been found to be necessary. In some special cases, however, simpler topological configurations are encountered. For example, long straight dislocation segments are experimentally observed in materials with high Peierel's potential barriers (e.g. covalent materials), or when large mobility differences between screw and edge components exist (e.g. some BCC crystals at low temperature). Under conditions conducive to glide of small prismatic loops on glide cylinders or the uniform expansion of nearly circular loops, changes in the loop *shape* is nearly minimal during its motion. It is therefore advantageous to reduce the number of interacting segments within a given computer simulation, or to develop more efficient approaches to computations of the long range field.

In this work, we aim at enhancing the current computational efforts on 3-D Dislocation Dynamics (DD). We present here a new numerical method for determination of a key ingredient in DD computer simulations; that is the elastic field of topologically complex dislocation ensembles. The main impetus for the present work is the need to describe the complex 3-D topology of dislocation loops in the most flexible way. A wide spectrum of dislocation line deformations, ranging from highly curved to rigid body translations arises within the same computational simulation. Existing methods are based on differential equations of motion for *straight* segments, where the elastic field variables affecting segment motion are computed at its center. When each segment moves under the influence of the stress field, the *connectivity* of the segments must be re-established, resulting in a number of possible complications. Thus, the motivation behind the current work can be stated as follows:

To reduce the computational burden by providing a high degree of flexibility in the selection of both length and shape of a dislocation segment.
To avoid numerical problems arising from singularities at intersecting straight segments.
To calculate the self-force on dislocation segments with a high degree of accuracy.
To provide a flexible tool which sheds more light on the physics of close-range interactions involving in-plane high curvature variations.
To effectively deal with the physics of climb and cross-slip, which require out-of-plane dislocation line curvature.

The fast sum method, which is based on a combination of dislocation loop geometry parameterization, and numerical quadrature integration along parameterized curves, is shown to be computationally feasible and highly accurate. All calculations involve simple algebraic operations, which can be systematically carried out by straightforward computer programming. Although we used FORTRAN-90 to implement the results of calculations, even spreadsheets on personal computers can be effectively utilized. The method is as efficient as analytical solutions, especially because of the index structure associated with tensor notation (i.e. the use of DO loops). However, because analytical solutions are available only for a limited number of special cases, the present approach can be used for calculations involving complex loop geometry. The present method is primarily intended for applications in Dislocation Dynamics computer simulations, where the need for accuracy is critical in close-range dislocation encounters. Moreover, one may consider the present method as an extension of the FEM technique in continuum mechanics. A variety of parameterized elements can thus be chosen (in much the same way as in the FEM approach) to handle special dislocation deformation problems. The method may also be exploited in crack problems, where dislocation distributions can be used to represent complex crack surfaces.

To handle the effects of free crystal surfaces on the redistribution of the elastic field inside the crystal, and hence on computed Peach-Kohler forces, the superposition method of Cleveringa et. al. is extended to 3-D applications. While only 2-D problems have been solved so far by their method, we show that 3-D problems can also be successfully implemented. However, the simple problem shown here required almost 10,000 elements, with an associated large number of degrees of freedom. Other methods (e.g. the Boundary Integral (BI) method) may be more appropriate for 3-D computer simulations, since the stress field should be updated very frequently during Dislocation Dynamics computer simulations.