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A PERSPECTIVE ON DISLOCATION DYNAMICS

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A fundamental description of plastic deformation has been recently pursued in many parts of the world as a result of dissatisfaction with the limitations of continuum plasticity theory. Although continuum models of plastic deformation are extensively used in engineering practice, their range of application is limited by the underlying database. The reliability of continuum plasticity descriptions is dependent on the accuracy and range of available 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 heterogenous, displaying high strains concentrated in small material volumes, with virtually undeformed regions in-between. Experimental observations consistently show that plastic deformation is heterogeneous at all length-scales. Depending on the deformation mode, heterogeneous dislocation structures appear with definitive wavelengths. A satisfactory description of realistic dislocation patterning and strain localization has been rather elusive. Attempts aimed at this question have been based on statistical mechanics, reaction-diffusion dynamics, or the theory of phase transitions. Much of the efforts have aimed at clarifying the fundamental origins of inhomogeneous plastic deformation. On the other hand, engineering descriptions of plasticity have relied on experimentally verified constitutive equations.

At the macroscopic level, shear bands are known to localize plastic strain, leading to material failure. At smaller length scales, dislocation distributions are mostly heterogeneous in deformed materials, leading to the formation of

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a number of strain patterns. Generally, dislocation patterns are thought to be associated with energy minimization of the deforming material, and manifest themselves as regions of high dislocation density separated by zones of virtually undeformed material. Dislocation-rich regions are zones of facilitated deformation, while dislocation poor regions are hard spots in the material, where plastic deformation does not occur. Dislocation structures, such as Persistent slip Bands (PSB's), planar arrays, dislocation cells, and subgrains, are experimentally observed in metals under both cyclic and steady deformation conditions. Persistent slip bands are formed under cyclic deformation conditions, and have been mostly observed in copper and copper alloys. They appear as sets of parallel walls composed of dislocation dipoles, separated by dislocation-free regions. The length dimension of the wall is orthogonal to the direction of dislocation glide.

Dislocation planar arrays are formed under monotonic stress deformation conditions, and are composed of parallel sets of dislocation dipoles. While PSB's are found to be aligned in planes with normal parallel to the direction of the critical resolved shear stress, planar arrays are aligned in the perpendicular direction. Dislocation cell structures, on the other hand, are honeycomb configurations in which the walls have high dislocation density, while the cell interiors have low dislocation density. Cells can be formed under both monotonic and cyclic deformation conditions. However, dislocation cells under cyclic deformation tend to appear after many cycles. Direct experimental observations of these structures have been reported for many materials.

Two of the most fascinating features of micro-scale plasticity are the spontaneous formation of dislocation patterns, and the highly intermittent and spatially localized nature of plastic flow. Dislocation patterns consist of alternating dislocation rich and dislocation poor regions usually in the μm range (e.g., dislocation cells, sub-grains, bundles, veins, walls, and channels). On the other hand, the local values of strain rates associated with intermittent dislocation avalanches are estimated to be on the order of 1–10 million times greater than externally imposed strain rates. Understanding the collective behavior of defects is important because it provides a fundamental understanding of failure phenomena (e.g., fatigue and fracture). It will also shed light on the physics of elf-organization and the behavior of critical-state systems (e.g., avalanches, percolation, etc.)

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!

Studies of the mechanical behavior of materials at a length scale larger than what can be handled by direct atomistic simulations, and smaller than what allows macroscopic continuum averaging represent particular difficulties. When the mechanical behavior is dominated by microstructure heterogeneity, the mechanics problem can be greatly simplified if all atomic degrees of freedom were adiabatically eliminated, and only those associated with defects are retained. Because the motion of all atoms in the material is not relevant, and only atoms around defects determine the mechanical properties, one can just follow material regions around defects. Since the density of defects is many orders of magnitude smaller than the atomic density, two useful results emerge. First, defect interactions can be accurately described by long-range elastic forces transmitted through the atomic lattice. Second, the number of degrees of freedom required to describe their topological evolution is many orders of magnitude smaller than those associated with atoms. These observations have been instrumental in the emergence of meso-mechanics on the basis of defect interactions by Eshelby, Kröner, Kossevich, Mura and others. Thanks to many computational advances during the past two decades, the field has steadily moved from conceptual theory to practical applications. While early research in defect mechanics focused on the nature of the elastic field arising from defects in materials, recent computational modelling has shifted the emphasis on defect ensemble evolution.

Although the theoretical foundations of dislocation theory are well-established, efficient computational methods are still in a state of development. Other than a few cases of perfect symmetry and special conditions, the elastic field of 3-D dislocations of arbitrary geometry is not analytically available. The field of dislocation ensembles is likewise analytically unattainable. 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. In DD simulations of plastic deformation, the computational effort per time-step is proportional to the square of the number of interacting segments, because

of the long-range stress field associated with dislocation lines. The computational requirements for 3-D simulations of plastic deformation of even single crystals are thus very challenging.

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 grid generation 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 Peierls 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. Also, helical loops of nearly constant radius are sometimes observed in quenched or irradiated materials under the influence of point defect fluxes. It is clear that, depending on the particular application and physical situation, one would be interested in a flexible method which can capture the essential physics at a reasonable computational cost. A consequence of the long-range nature of the dislocation elastic field is that the computational effort per time step is proportional to the square of the number of interacting segments. 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.

While continuum approaches to constitutive models are limited to the underlying experimental data-base, DD methods offer new directions for modeling microstructure evolution from fundamental principles. The limitation to the method presented here is mainly computational, and much effort is needed to overcome several difficulties. First, the length and time scales represented by the present method are still short of many experimental observations, and methods of rigorous extensions are still needed. Second, the boundary conditions of real crystals are more complicated, especially when external and internal surfaces are to be accounted for. Thus, the present approach does not take into account large lattice rotations, and finite deformation of the underlying crystal, which may be important for explanation of certain scale effects on plastic deformation. And finally, a much expanded effort is needed to bridge the gap between atomistic calculations of dislocation properties on the one hand, and continuum mechanics formulations on the other. Nevertheless, with all of these limitations, the DD approach is worth pursuing, because it opens up new possibilities for linking the fundamental nature of the microstructure with realistic material deformation conditions. It can thus provide an additional tool to both theoretical and experimental investigations of plasticity and failure of materials.

Two main approaches have been advanced to model the mechanical behavior in this *meso* length scale. The first is based on statistical mechanics methods. In these developments, evolution equations for statistical averages (and possibly for higher moments) are to be solved for a complete description of the deformation problem. The main challenge in this regard is that, unlike the situation encountered in the development of the kinetic theory of gases, the topology of interacting dislocations within the system must be included. The second approach, commonly known as Dislocation Dynamics (DD), was initially motivated by the need to understand the origins of heterogeneous plasticity and pattern formation. An early variant of this approach (the cellular automata) was first developed by Lepinoux and Kubin [1], and that was followed by the proposal of DD [2–4]. In these early efforts, dislocation ensembles were modelled as infinitely long and straight in an isotropic infinite elastic medium. The method was further expanded by a number of researchers, with applications demonstrating simplified features of deformation microstructure.

Since it was first introduced in the mid-eighties independently by Lepinoux and Kubin, and by Ghoniem and Amodeo, Dislocation Dynamics (DD) has now become an important computer simulation tool for the description of plastic deformation at the micro- and meso-scales (i.e., the size range of a fraction of a micron to tens of microns). The method is based on a hierarchy of approximations that enable the solution of relevant problems with today's computational resources.

In its early versions, the collective behavior of dislocation ensembles was determined by direct numerical simulations of the interactions between infinitely long, straight dislocations [5]. Recently, several research groups extended the DD methodology to the more physical, yet considerably more complex 3-D simulations. The method can be traced back to the concepts of internal stress fields and configurational forces. The more recent development of 3-D lattice dislocation dynamics by Kubin and co-workers has resulted in greater confidence in the ability of DD to simulate more complex deformation microstructure [6–8]. More rigorous formulations of 3-D DD have contributed to its rapid development and applications in many systems [9–15]. We can classify the computational methods of DD into the following categories:

1. The Parametric Method: The dislocation loop can be geometrically represented as a continuous (to second derivative) composite space curve. This has two advantages: (1) there is no abrupt variation or singularities associated with the self-force at the joining nodes in between segments, (2) very drastic variations in dislocation curvature can be easily handled without excessive re-meshing. Other approximation methods have been developed by a number of groups. These approaches differ mainly in the representation of dislocation loop geometry, the manner by which the elastic field and self energies are calculated, and some additional details

related to how boundary and interface conditions are handled. The suitability of each method is determined by the required level of accuracy and resolution in a given application. dislocation loops are divided into contiguous segments represented by parametric space curves.

2. The Lattice Method: Straight dislocation segments (either pure screw or edge in the earliest versions , or of a mixed character in more recent versions) are allowed to jump on specific lattice sites and orientations. The method is computationally fast, but gives coarse resolution of dislocation interactions.
3. The Force Method: Straight dislocation segments of mixed character in the are moved in a rigid body fashion along the normal to their midpoints, but they are not tied to an underlying spatial lattice or grid. The advantage of this method is that the explicit information on the elastic field is not necessary, since closed-form solutions for the interaction forces are directly used.
4. The Differential Stress Method: This is based on calculations of the stress field of a differential straight line element on the dislocation. Using numerical integration, Peach–Koehler forces on all other segments are determined. The Brown procedure [16] is then utilized to remove the singularities associated with the self force calculation.
5. The Phase Field Microelasticity Method: This method is based on the reciprocal space theory of the strain in an arbitrary elastically homogeneous system of misfitting coherent inclusions embedded into the parent phase . Thus, consideration of individual segments of all dislocation lines is not required. Instead, the temporal and spatial evolution of several density function profiles (fields) are obtained by solving continuum equations in Fourier space [17].

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