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A variational formulation of constrained dislocation dynamics coupled with heat and vacancy diffusion

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ABSTRACT

We present a formulation of the discrete Dislocation Dynamics (DD) method based on Onsager's variational principle. The motion of discrete dislocations is treated as a generalized irreversible flux associated with conjugate thermodynamic forces causing internal production of entropy. Intrinsic in the variational principle is the role of physical constraints that limit the choice of generalized fluxes. We leverage the concept of constrained maximization to introduce the requirement that dislocation climb must be sustained by the flux of vacancies into the dislocation core. The constrained variational approach results naturally in the coupling between plastic deformation induced by discrete dislocations, vacancy diffusion, and heat propagation in solid crystals. In particular, this coupling requires that dislocation velocity and chemical potential of vacancies at the dislocation core be found simultaneously. A new numerical formulation of DD that accounts for generalized constraints imposed on dislocations is presented, based on a network discretization of the dislocation configuration. Applications illustrate the significance of constrained motion of dislocations confined in channels and pillars, and the attainment of heterogeneous dislocation structures.

1. Introduction

In the field of computational plasticity of crystals, the discrete Dislocation Dynamics (DD) method is a technique that prospects the possibility of resolving individual dislocation interactions without resorting to all atomistic details. Thus, the scope of applications of the method extends between length scales proper of current atomistic models (i.e. tens of nms), and those typical of continuum models (i.e. larger than tens of mms). This "mesoscopic" range is sufficiently broad to capture the collective dynamics of defect ensembles that determines the mechanical behavior of crystals. Although the original goal of the early efforts in the development of the DD method was to shed light on the physical origins and the conditions for dislocation pattern evolution (Lepinoux and Kubin, 1987; Ghoniem and Amodeo, 1988; Gulluoglu et al., 1989; van der Giessen and Needleman, 1995), many other applications have shown the utility of this approach. During the past two decades, three dimensional DD codes have been developed (Kubin et al., 1992; Schwarz, 1997; Zbib et al., 1998; Ghoniem et al., 2000; Weygand et al., 2002; Bulatov et al., 2004) and used in massive dislocation dynamics simulations for investigating the fundamental mechanisms of dislocation plasticity. Such computer simulations are now directly and successfully compared to experiments on nano- and micro-scale materials, such as thin films (Pant et al., 2003; Miller et al., 2004), nano-indentation (Kreuzer and Pippan, 2004; Fivel et al., 1997), and the deformation of micro-pillars (Tang et al., 2007; El-Awady et al., 2008; Akarapu et al., 2010). Recent progress

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in experimental techniques at the nano- and micro-scale, coupled with the fundamental nature of DD simulations is converging to reveal the physical origins of plasticity.

Despite substantial differences between various implementations, the kernel of the DD method consists in evolving a given configuration of crystal dislocations according to the equation representing the balance of the net force per unit length of dislocation. This balance equation is interpreted as an "equation of motion" in the sense of a closure equation for the dislocation velocity. Several DD implementations seek a solution to the equation of motion based on the idea of Kukta (1998) of vanishing the total force in a weak sense, where a weighted residual is obtained multiplying the net force f_i by an arbitrary test velocity $\tilde{w}_i$, and integrating over the dislocation loop $\mathcal{L}$ itself:

$$\oint_{\mathcal{L}} f_i \tilde{w}_i \, d\ell = 0 \tag{1}$$

We shall call this the *virtual-power* formulation of the DD method. A variant of the virtual-power formulation based on thermodynamic arguments was also developed by Ghoniem et al. (2000).

In this paper, we develop an alternative to the virtual-power approach mentioned above. This alternative is a *variational* formulation of the DD method, where the equation governing the evolution of the dislocation microstructure, i.e. a generalization of (1), is derived as the necessary condition for some functional to attain an extremum. This approach epitomizes the viewpoint of irreversible thermodynamics, the branch of the thermodynamics of continua focused on the concept of internal production of entropy (De Groot and Mazur, 1984), a typically non-negligible quantity in plastically-deformed metals.[1] In particular, the perspective of this work can be regarded as an application of a more general variational statement of irreversible thermodynamics, first proposed by Onsager (1931) as an addendum to his famed proof of the universality of reciprocal relations. Onsager embraced (Rayleigh, 1873)'s concept of dissipation-potential and showed that, near thermodynamic equilibrium, irreversible processes are governed by a variational principle. Although his principle expresses the maximum of a functional with units of entropy, Onsager coined the name *principle of least dissipation of energy* in homage to a result obtained by Rayleigh (1913) in hydrodynamics. In referring to this principle, we shall follow the terminology of Ziegler (1963), who pointed out that the title of Onsager's principle "is not consistent with its actual content" and renamed it *principle of maximum rate of entropy production* (PMEP) or, in units of energy, *principle of maximum rate of dissipation work* (PMD). Ziegler actually extended Onsager's principle to non-linear problems, and extensively discussed its usefulness in deriving constitutive equations for continua (cf. Ziegler, 1958, 1963, 1983; Ziegler and Wehrli, 1987). The use of variational principles in conjunction with the continuum theory of dislocations is discussed in an inspiring paper by Berdichevsky (2006). Nevertheless, the application of similar variational principles of irreversible thermodynamics to discrete dislocation plasticity does not appear to have been attempted, and hence a fundamental variational foundation of discrete DD is still lacking.

There are two good reasons for seeking a variational formulation of the discrete DD method. The first is that it allows us to set up the problem in the familiar framework of continuum mechanics where, once kinematics and thermodynamic potentials are specified, constitutive equations governing the irreversible behavior of the system are obtained as an outcome of the variational procedure and without additional (and possibly arbitrary) assumptions. The second advantage of the variational approach is that it provides a natural framework to account for physical constraints that limit the motion of dislocations and result in coupling between different physical processes. A well-known example of this coupling is the mutual relation between non-conservative motion of dislocations (climb) and flux of point-defects (Nabarro, 1987, ch. 6). Although two- and three-dimensional DD models incorporating climb have been proposed (Roters et al., 1996; Davoudi et al., 2012; Keralavarma et al., 2012; Cai and Bulatov, 2004; Mordehai et al., 2008; Bako et al., 2011), the self-consistent implementation of climb in three-dimensional DD remains an open matter. The origin of the difficulty associated with climb can be traced back to the virtual-work formulation of DD, which offers no indication on how to couple the problem of dislocation motion and flux of point defects. On the other hand, this difficulty is removed in the current approach because physical constraints are accounted for at the outset and as an intrinsic requirement of the PMEP.

We also remark that, even when diffusion of point defects can be neglected (e.g. at low temperature and far from non-equilibrium concentrations), the climb constraint must still be considered. In this case, the proposed formulation of DD gracefully falls back to the discrete version of existing thermodynamic approaches to plastically incompressible plasticity (Collins and Houlsby, 1997, and references therein). On the other hand, the virtual-work formulation of DD encounters the conceptual difficulty that chemical forces become undetermined, therefore leaving room for a certain degree of arbitrariness in the numerical implementation.

The paper is organized as follows: in Section 2 we develop the irreversible thermodynamics of discrete dislocation motion constrained by the diffusion of point defects and heat. The variational procedure based on PMEP leads to a weak statement of the law governing the motion of discrete dislocations which includes the climb constraint. The numerical implementation of this weak statement is formulated in Section 3 for arbitrary networks of discrete dislocations subject to generalized constraints. The practical applicability of the proposed formulation of DD becomes clear when the latter is used to resolve the motion of complex topological dislocation structures. An application of the condition of plastic incompressibility to the motion of dislocation junctions in f.c.c. metals is reported in Section 4, together with other examples of confined evolution of dislocation networks. Conclusions are finally given in Section 5.

[1] When scaled by temperature, entropy production measures the amount of energy that internal irreversibilities dissipate into heat, which typically prevails over the amount of energy stored in crystal microstructures and revealed as latent heat. See Stroh (1953) for a summary of the large body of experimental evidence.