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Singularity-free dislocation dynamics with strain gradient elasticity

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ABSTRACT

The singular nature of the elastic fields produced by dislocations presents conceptual challenges and computational difficulties in the implementation of discrete dislocation-based models of plasticity. In the context of classical elasticity, attempts to regularize the elastic fields of discrete dislocations encounter intrinsic difficulties. On the other hand, in gradient elasticity, the issue of singularity can be removed at the outset and smooth elastic fields of dislocations are available. In this work we consider theoretical and numerical aspects of the non-singular theory of discrete dislocation loops in gradient elasticity of Helmholtz type, with interest in its applications to three dimensional dislocation dynamics (DD) simulations. The gradient solution is developed and compared to its singular and non-singular counterparts in classical elasticity using the unified framework of eigenstrain theory. The fundamental equations of curved dislocation theory are given as non-singular line integrals suitable for numerical implementation using fast one-dimensional quadrature. These include expressions for the interaction energy between two dislocation loops and the line integral form of the generalized solid angle associated with dislocations having a spread core. The single characteristic length scale of Helmholtz elasticity is determined from independent molecular statics (MS) calculations. The gradient solution is implemented numerically within our variational formulation of DD, with several examples illustrating the viability of the non-singular solution. The displacement field around a dislocation loop is shown to be smooth, and the loop self-energy non-divergent, as expected from atomic configurations of crystalline materials. The loop nucleation energy barrier and its dependence on the applied shear stress are computed and shown to be in good agreement with atomistic calculations. DD simulations of Lomer–Cottrell junctions in Al show that the strength of the junction and its configuration are easily obtained, without ad-hoc regularization of the singular fields. Numerical convergence studies related to the implementation of the non-singular theory in DD are presented.
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1. Introduction

Most mechanical properties of crystalline materials are controlled by the behavior and evolution of complex dislocation ensembles. This observation stands behind a long-standing goal to develop plasticity theory on a physical, rather than

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empirical, basis. However, the difficulty associated with averaging individual dislocation properties across many length and time scales, from atomistic to continuum, arguably makes dislocation mechanics "the most difficult remaining problem of classical physics" (Cottrell, 2002). One has therefore to resort to models limited to a specific length and time scale of observation. In this multi-scale approach, the meso-scale range (1–100 μm) is occupied by the elastic theory of discrete dislocations (Friedel, 1967; Nabarro, 1987; Hirth and Lothe, 1992). The theory has proven not only extremely effective in explaining the elastic properties of crystal dislocations, but also well suited for numerical implementation. The computational side of the theory focused on the quasi-static evolution of a given dislocation configuration is known as the Discrete Dislocation Dynamics (DD) method (Lepinoux and Kubin, 1987; Ghoniem and Amodeo, 1988; Gulluoglu et al., 1989; Kubin et al., 1992; Schwarz, 1997; Zbib et al., 1998; Ghoniem et al., 2000; Weygand, 2002; Bulatov et al., 2004). The objective of the DD method is the prediction of the mechanical response of a mesoscopic material volume containing a large number of dislocations, in response to intrinsic (dislocation configuration, material properties, grain size, etc.) and extrinsic (applied load, strain rate, temperature, etc.) factors, without resorting to ad-hoc assumptions.

Despite its successes, the classical theory of dislocations and the computational methods that descend from it face intrinsic limitations on their numerical accuracy, as well as on their ability to access resolution at the atomic length scale. Such difficulties stem from the representation of crystal dislocations by means of Volterra dislocations, a special type of elastic distortion of multiply connected solids introduced well before crystal dislocations were discovered (Volterra, 1907). A well known collateral effect of this idealization is the emergence of singularities in the elastic fields of Volterra dislocations, which limit the validity of the solution to a somewhat arbitrary region outside the dislocation core. Consequently, several fundamental physical quantities become ill-determined (e.g. self energy/stress of dislocation loops and interaction energy/stress of intersecting dislocations). In order to overcome the difficulties associated with the unphysical singular character of Volterra dislocations, various methods of regularization of the elastic solution have been proposed. In the context of standard elasticity, a first class of methods comprises efforts based on the use of cut-off radii (Brown, 1964; Gavazza and Barnett, 1976), which avoid dealing with the singularity but introduce parameters of arguable physical interpretation. In contrast, a second category of methods removes the singularity adopting the concept of distributed dislocation core (de Wit, 1960). This concept, originally introduced by the celebrated Peierls (1940)–Nabarro (1947) model of lattice resistance, can be recognized in the standard core of Lothe (1992) and the isotropic core of Cai et al. (2006). Only the latter, however, is applicable to the study of curved dislocation loops in three dimensions.

An alternative approach to overcome the issue of singularity is to consider discrete dislocations in the broader field of generalized elasticity. This is a natural choice in light of the relationship between higher order stress measures (absent in classical elasticity) and the long-range effects of interatomic forces, which has been suggested by several authors (Kröner, 1963; Toupin and Gazis, 1965; Mindlin, 1972). Generalized elastic theories of discrete dislocations have been developed in three different frameworks: micropolar (Cosserat) elasticity, non-local elasticity, and gradient elasticity. In micropolar elasticity, Kessel (1970) found solutions for screw and edge dislocations and Minagawa (1979) for dislocation loops. However, these solutions not only present the classical singularities but also add new singularities related to the presence of modified Bessel functions. Similar results are also found in Nowacki (1986) and references therein. Straight screw and edge dislocations in non-local elasticity with exponential non-local kernel were considered by Eringen (1977b) and Eringen (1977a), respectively. The solution yields regularized stress but the strain and displacement fields remain classical (singular). Similar results using a non-local kernel of Helmholtz type were found by Eringen (1983) for screw dislocations and by Eringen (1984) for dislocation loops (see also Eringen, 2002). However the Green's function of the Helmholtz bi-Laplace equation used by Eringen lacks a term which prevents the regularization of the Peach–Koehler stress (see Lazar, 2014, for details). The first effort towards a non-singular dislocation theory in the framework of gradient elasticity was carried out by Lardner (1971), who considered straight screw and edge dislocations in the framework of Mindlin's gradient elasticity (Mindlin, 1964). Considering neither plastic distortion nor dislocation density, Lardner constructed solutions to a compatible elastic boundary value problem, and consequently failed to remove the classical singularities. More than two decades later, Gutkin and Aifantis (1996, 1997) studied straight screw and edge dislocations in a model characterized by the presence of gradient terms in Hooke's law. The model predicts non-singular strains and gives rise to a smooth displacement field in proximity of the dislocation core. However, the framework of Gutkin and Aifantis (1996, 1997) lacks double stresses and, consequently, the Cauchy stress remains singular. In a refined version of the theory, Gutkin and Aifantis (1999) were able to also regularize the stress field using a more sophisticated Hooke's law. Subsequent work has further developed the non-singular theory of straight dislocations in a special version of gradient elasticity containing only one characteristic parameter, which we shall refer to as gradient elasticity of Helmholtz type (Lazar and Maugin, 2005; Lazar et al., 2005; Lazar and Maugin, 2006). Only recently has the theory been extended to curved dislocation loops in three dimensions (Lazar, 2012, 2013). These recent developments in the gradient theory of elasticity endow DD with a level of maturity that is necessary for computer simulations of 3-D dislocation ensembles with near atomic resolution.

In this work we explore the use of the non-singular gradient theory of discrete dislocations (Lazar, 2012, 2013) in three-dimensional DD simulations, and show that it provides a simple and valuable alternative to the classical theory as the foundation for numerical implementation. The first objective of the paper is to highlight differences and advantages of the gradient formulation compared to its singular and non-singular counterparts in standard elasticity. Section 2 is dedicated to this topic. As part of the discussion, we derive a closed-form expression for the interaction energy between two dislocation loops in gradient elasticity of Helmholtz type. This expression will be used to determine the non-singular self-energy of a dislocation loop. We also address the theoretical issue of converting the generalized solid angle associated with the displacement field of dislocations having distributed