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Reprint of: Dynamics of discrete screw dislocations on glide directions ☆

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ABSTRACT

We consider a simple discrete model for screw dislocations in crystals. Using a variational discrete scheme we study the motion of a configuration of dislocations toward low energy configurations. We deduce an effective fully overdamped dynamics that follows the maximal dissipation criterion introduced in Cermelli and Gurtin (1999) and predicts motion along the glide directions of the crystal.

1. Introduction

Dislocations are one-dimensional defects in the periodic structure of crystals, and their motion represents the microscopic mechanism of plastic flow in metals. In view of this fundamental role, dislocations have been extensively studied by theoretical, experimental and computational means. Classical models are mainly based on the so-called continuum theory of dislocations, in the context of linearized elasticity (see Hull and Bacon, 2001; Hirth and Lothe, 1982 for a comprehensive treatment). In recent years considerable efforts have been made in order to improve those models by including more information from the microscopic scale. Much insight has been gained on the microscopic structure of dislocations through fine numerical simulations (see e.g. Bulatov, 2002 and the references therein), and new phenomenological models accounting for microscopic effects have been proposed (e.g. Groma, 1997; Yefimov et al., 2004), while a variety of rigorous mathematical analyses has been done to bridge different scales (see Scardia et al., 2014; El Hajj et al., 2009; Conti et al., 2015 and the references therein; see also Mielke and Truskinovsky, 2012). A major issue behind those approaches is the formulation of a simple and efficient discrete model for dislocations that should be the starting point of a multi-scale analysis.

In this paper we consider a two dimensional model for screw dislocations that is inspired to the Frenkel–Kontorova model for dislocation dynamics (Frenkel and Kontorova, 1938). We consider an anti-plane discrete setting in which atoms

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can only move vertically and interact through a two-body periodic potential, a prototypical example being a piecewise quadratic function with wells at the integers. Such type of models have been proposed by many authors (e.g. Carpio and Bonilla, 2003; Salman and Truskinovsky, 2012; Flytzanis et al., 1977; Hudson and Ortner, 2014) and are based on the ideal mechanism of plastic slip governed by a Peierls potential (Hirth and Lothe, 1982). Periodic potentials show up naturally starting from three-dimensional particle interaction energies assuming crystallization and anti-plane deformations. We derive their specific form for some precise crystalline structures (as BCC, FCC and HCP lattices), starting from Lennard-Jones type energies and assuming nearest neighbor interactions. More general multi-body interaction energies could be considered, such as those used in the Embedded Atom Method (see Daw and Baskes, 1984; Ramasubramaniam et al., 2007 for a discussion on EAM in the context of dislocation dynamics). Our analysis can be performed also in these more general frameworks with minor changes, relying on the specific assumptions on the interaction potentials.

Our model follows the general approach developed in Ariza and Ortiz (2005). We adopt the formalism therein to introduce the notion of elastic and plastic strain defined on each bond of the lattice, and the notion of discrete dislocations associated to each cell of the lattice. One of the advantages of considering a genuine discrete model is that it does not need any artificial regularization of the core, which is otherwise common in linear continuum (or rather *semi-discrete*) theories.

According to the so-called low-energy dislocation structure assumption (LEDS, Kuhlmann-Wilsdorf, 1999), dislocations move following a steepest-descent criterion. Nevertheless, it is well known that at zero temperature discrete dislocations are pinned by the energy barriers due to the lattice structure. This has been proved analytically for the model under consideration in Hudson and Ortner (2014, 2015), Alicandro et al. (2014) and De Luca (2016). Clearly, the depinning mechanism is governed by fluctuations of the system that can tilt the potential allowing dislocations to overcome the energy barriers. Here we work in the simplified zero temperature context in which thermal effects are neglected and we describe the depinning and motion of dislocations toward states with lower energy, by considering a variational discrete (in time and space) scheme, already proposed in Ramasubramaniam et al. (2007) and Alicandro et al. (2014). Precisely, we introduce a parameter τ, that we refer to as *time step*, and at each time step we minimize the elastic energy stored in the crystal plus a term that accounts for the energy dissipated in moving dislocations from a site to another. The discrete parameter τ sets the size of the area that dislocations may explore in order to reach a local minimizer, mimicking thermal effects.

A rate-independent (1-homogeneous) dissipation in the presence of a time dependent load, in the spirit of Ramasubramaniam et al. (2007), would lead to a quasi-static evolution (see e.g. Mora et al., 2014 for a rate-independent evolution law for edge dislocations). Here we consider the case of a rate-dependent quadratic dissipation that leads to a fully overdamped dynamics, neglecting inertial effects as well as all the other external body forces (see Cermelli and Gurtin, 1999). Several different effects could be taken into account, leading to more complex continuum dynamics (see for instance Eshelby, 1953; Hirth and Lothe, 1982; Kresse and Truskinovsky, 2003).

We derive an effective dynamics, the so-called *discrete dislocation dynamics*, by means of a multi-scale analysis of the discrete elastic energy stored in the crystal (see also El Hajj et al., 2009). It turns out (Cermelli and Leoni, 2005; Alicandro et al., 2014; De Luca, 2016) that, in the limit as the lattice spacing tends to zero (or equivalently in the large-body limit) the elastic energy can be decomposed into a self-energy, which scales logarithmically in the core radius, plus an interaction energy $W(x_1, \ldots, x_M)$ depending on the dislocation positions x_i. The latter is determined by the behavior of the discrete periodic interaction potential at the bottom of the wells. In this respect, we validate the harmonic approximation of the far field as predicted by the continuum linear theory (see Scardia and Zeppieri, 2012; Müller et al., 2014).

We would like to remark that this analysis has many similarities with other theories in which the presence of topological defects plays an important role (Alicandro et al., 2011). This is the case of the Ginzburg–Landau model for vortices in superconductors (Bethuel et al., 1994; Sandier and Serfaty, 2007). Borrowing the terminology from that context, we refer to the interaction energy between dislocations $W(x_1, \ldots, x_M)$ as the *renormalized energy*. The gradient of the renormalized energy is nothing but the Peach–Koehler force j between dislocations; namely, $j_i = -\nabla_{x_i} W$ is the force acting on the dislocation at x_i. The corresponding overdamped dynamics is then driven by the Peach–Koehler force (see Forcadel et al., 2009).

A crucial issue in the time-discrete scheme is the specific choice of the dissipation potential. Choosing a quadratic isotropic dissipation, one recovers an implicit Euler scheme for the renormalized energy, and hence, in the limit of the time step to zero, the fully overdamped discrete dislocation dynamics $\dot{x}_i = j_i$ (see Alicandro et al., 2014).

Here we make a different choice. We consider a crystalline dissipation that accounts for the specific lattice structure and that is minimal exactly on the preferred glide directions (that in this model are considered as a given material property of the crystal). As a consequence of this choice, we derive an effective dynamics that forces the motion along the glide directions, and follows the *maximal energy dissipation criterion* postulated in Cermelli and Gurtin (1999). Indeed, dislocations move along the glide direction that maximizes the scalar product with the force $j = -\nabla W$. Clearly this direction could be not unique, so that dislocations can rapidly move from a glide direction to another. This effective dynamics may also predict cross-slip and fine cross-slip, according to Cermelli and Gurtin (1999) and the analysis and the simulations performed in the recent papers (Blass et al., 2015; Blass and Morandotti, 2014). In view of this lack of uniqueness of the velocity field of the dislocations, the effective dynamics turns out to be described by a differential inclusion rather than a differential equation (see Filippov, 1988).

Our discrete variational scheme provides a simple and natural model to describe the depinning and the dynamics of screw dislocations, taking into account the preferred glide directions. Moreover it provides an approximation of the effective dynamics proposed by Cermelli and Gurtin (1999), highlighting its gradient flow structure.