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Building compact dislocation cores in an elasto-plastic model of dislocation fields

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An elasto-plastic theory of dislocation fields, where dislocation motion is accounted for by a dissipative dislocation density transport framework, is used to model in a continuous way planar dislocation core structures at nanoscale. A one-dimensional model for mixed edge/screw dislocations is developed. In order to avert endless relaxation of arbitrary initial dislocation core profiles and obtain convergence toward a compact equilibrium core structure, a Peierls-Nabarro-type misfit surface energy is introduced in the free energy density, leading to a restoring term in the driving force for dislocation motion. When using the Peierls sinusoidal potential for the restoring stress, arbitrary initial dislocation core profiles converge by relaxation towards the Peierls-Nabarro analytical solution, which corresponds to a minimum energy configuration. The model is extended by using generalized planar stacking fault energies. Basal and prismatic planar energies are obtained in titanium and zirconium from ab-initio and molecular statics simulations. Dissociation of basal edge and screw dislocations into partial mixed dislocations is predicted, whereas dissociated dislocations with partial Burgers vectors collinear to the Burgers vectors of the full dislocations are found in prismatic planes. Motion, deformation and anelastic relaxation mechanisms of dislocation cores under applied stresses are predicted by the model, as well as dislocation loop nucleation. In particular, deformation of the dislocation core under high stresses reduces the velocity of the dislocation and produces kinematic hardening at the core level.

1. Introduction

The celebrated Peierls-Nabarro model (Peierls, 1940; Nabarro, 1947) raised the fundamental question of the equilibrium configuration of a dislocation core in a crystal lattice from a continuum mechanics standpoint. Originally developed for planar dislocation cores, the Peierls-Nabarro model represents the core of a dislocation as a continuous dislocation density distribution, whose integration over the core area yields the Burgers vector. An equilibrium spatial distribution of the dislocation densities and the associated elastic displacement discontinuity, the so-called misfit, are found when the internal shear stress due to the dislocation core is counter-balanced by a lattice restoring stress. The latter originates from a non-convex periodic lattice misfit energy reflecting the resistance of the crystal to shear. Motivated by the success of this model, recent refined

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models have proposed to replace the Peierls sinusoidal misfit potential by generalized stacking fault energies obtained from atomistic calculations, which renders the model more realistic (Joós et al., 1994; Hartford et al., 1998; Lu et al., 2000; Schoeck, 2012; Wang et al., 2014). Instead of using a one-dimensional potential, these models rather introduce a two-dimensional energy that provides the shear resistance in all directions of a given glide plane. A striking feature of such models is their capability to predict the dissociation of dislocations into partials. Recent phase field-type models were also shown to be able to capture the evolution of dislocation cores in different slip planes in three dimensional settings (Denoual, 2004; Shen and Wang, 2004; Hunter and Beyerlein, 2014), the non-planar structure of dislocation cores in BCC metals (Denoual, 2007) and dislocation kinks (Wei and Xiang, 2009). The effects of solutes on dislocation motion, dislocation/grain boundary interactions, dislocation cross slip and twinning were also investigated by using such Peierls-Nabarro based frameworks (Hu et al., 2004; Zeng et al., 2016; Lu et al., 2004; Pi et al., 2016).

In the present paper, we propose to model planar dislocation cores within a recent elasto-plastic theory of dislocation fields (Acharya, 2001). In this theory, the net Burgers vector of dislocation ensembles is captured through Nye's polar dislocation density tensor (Nye, 1953). The latter is a continuous rendition, with divergence-free character, of the discontinuity of the elastic/plastic displacement induced by the dislocation ensemble. When this ensemble reduces to a single dislocation, the dislocation density field smoothly describes the dislocation core in the manner of the Peierls-Nabarro model, which allows regularizing its singular description. The elasto-static part of the theory naturally retrieves the elastic fields of a single dislocation, which it regularizes in the core region (Roy and Acharya, 2005). Beyond this static description, the theory also provides for the spatiotemporal evolution of a dislocation density field within a rigorous dissipative transport framework (Acharya, 2003). Dislocation motion is ruled by the dislocation transport equation (Mura, 1963), which expresses the conservation of the flux of the divergence-free dislocation density tensor, *i.e.* the Burgers vector, across elementary surfaces. When the dislocation ensemble reduces to a single dislocation, the dislocation velocity field describes the (possibly heterogeneous) motion of the differential dislocation elements. Hence, Peach-Koehler-type forces drive the motion of dislocation densities for the production of plastic deformation, including by possible deformation of the core. The elasto-plastic theory of dislocation fields is thus well adapted for the elasto-plastic investigation of the structure and dynamics of dislocation cores. It was also recently shown, by using a crossover method that derives kinematic fields from atomic structures (Tucker and Foiles, 2015), that such a framework can be applied to grain boundary core structures (Sun et al., 2016).

The objective of the present paper is to evidence the ability of the mechanical theory of dislocation fields to predict realistic compact dislocation cores and their dynamics under loading. More precisely, the predictive capabilities brought about by the introduction of a non convex periodic misfit surface energy in the free energy density are discussed, and it is shown how restoring stresses arising from this surface energy may yield compact equilibrium core structures, by self-relaxation of arbitrary initial core configurations. In Section 2, the elasto-plastic theory of dislocation fields (Acharya, 2001, 2003) is briefly recalled. A one-dimensional model is derived in Section 3 for mixed edge/screw dislocation cores. It is shown that, in the absence of a restoring force, endless relaxation of dislocation cores occurs. In Section 4, we show how to introduce a Peierls-type misfit energy in the formulation and how to derive from the latter the restoring force counterbalancing the above relaxation. Note that such a procedure was independently and recently proposed by (Zhang et al., 2015). The present formulation is validated by comparison with the Peierls-Nabarro analytical solution for a sinusoidal restoring force. Following recent papers (e.g. Shen and Wang, 2004; Wei and Xiang, 2009), the model is further developed in Section 5, in order to use generalized planar stacking fault energies as an input for the misfit energy and to describe dissociation of dislocations into partials. This extended model is applied to edge and screw dislocations in basal and prismatic planes in titanium and zirconium, by using stacking fault energies as obtained from atomistic calculations. In Section 6, the model is finally used to investigate the motion and deformation of dislocation cores under applied stresses, and the nucleation of dislocation loops under localized shear stress. Conclusions follow. In the Appendix, we provide details about the numerical calculations of generalized stacking faults energies in Zr and Ti, as well as useful mathematical notations.

2. Elasto-plastic model of dislocation fields

2.1. Incompatibility

In a small strain setting, the total distortion $\mathbf{U}$ of a continuum body elasto-plastically deformed is decomposed into elastic $\mathbf{U}^e$ and plastic $\mathbf{U}^p$ parts, such that $\mathbf{U} = \mathbf{U}^e + \mathbf{U}^p$. Because the total material displacement vector field $\mathbf{u}$ is continuously differentiable, the total distortion tensor can be defined as the gradient of that vector field. As such, it is curl-free. The following relations then hold:

$$\mathbf{U} = \mathbf{grad}\,\mathbf{u}, \tag{1}$$

$$\mathbf{curl}\,\mathbf{U} = \mathbf{0}. \tag{2}$$

In the presence of a dislocation or a polarised ensemble of dislocations, the occurrence of a non-zero net Burgers vector $\mathbf{b}$ induces a discontinuity of the elastic and plastic displacement vector fields. Hence, in addition to compatible curl-free parts $\mathbf{U}^{e\parallel}$ and $\mathbf{U}^{p\parallel}$, the elastic and plastic distortion tensors additionally contain incompatible parts $\mathbf{U}^{e\perp}$ and $\mathbf{U}^{p\perp}$ that are not gradients. Their non-zero curl defines Nye's polar dislocation density tensor α (Nye, 1953), such that (Kröner, 1980)