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Continuum dislocation theory accounting for redundant dislocations and Taylor hardening

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ABSTRACT

This paper develops the phenomenological continuum dislocation theory accounting for the density of redundant dislocations and Taylor hardening for single crystals. As illustration, the problem of anti-plane constrained shear of single crystal deforming in single slip is solved within the proposed theory. The distribution of excess dislocations in the final state of equilibrium as well as the stress-strain curve exhibiting the Bauschinger translational work hardening and the size effect are found. Comparison with the stress-strain curve obtained from the continuum dislocation theory without the density of redundant dislocations and Taylor hardening is provided.

1. Introduction

Macroscopically observable plastic deformations in single crystals and polycrystalline materials are caused by nucleation, multiplication and motion of dislocations. There are various reasonable experimental evidences supporting the so-called low energy dislocation structure hypothesis formulated first by Hansen and Kuhlmann-Wilsdorf (1986): dislocations appear in the crystal to reduce its energy (see also (Kuhlmann-Wilsdorf, 1989; Laird, Charsley, & Mughrabi, 1986)). This turns out to be the consequence of Gibbs variational principle applied to crystals with dislocations in case of vanishingly small Peierls stress (see Berdichevsky (2009)). Motion of dislocations yields the dissipation of energy which, in turn, results in a resistance to the dislocation motion. The general structure of continuum dislocation theory (CDT) must therefore reflect this physical reality: energy decrease by nucleation of dislocations and resistance to the motion of dislocations due to dissipation. Just in recent years various phenomenological models of crystals with continuously distributed dislocations which are able to predict the average dislocation density as well as the accompanying size effects have been proposed in Acharya and Bassani (2001); Berdichevsky (2006a,b); Berdichevsky and Le (2007); Gurtin (2002); Gurtin, Anand, and Lele (2007); Kaluza and Le (2011); Kochmann and Le (2008, 2009a,b); Le (2016a); Le and Nguyen (2012, 2013, 2010), Le and Piao (2016); Le and Sembiring (2008a,b, 2009), Le and Tran (2016) (see also the finite strain CDT proposed by Koster and Le (2015); Koster, Le, and Nguyen (2015); Le (2016b); Le and Günther (2014); Le and Stumpf (1996a,b,c), Ortiz and Repetto (1999); Ortiz, Repetto, and Stainier (2000)).

The continuum dislocation theory must in principle be obtained from averaging ensembles of large numbers of dislocations in crystals (see, e.g., (Berdichevsky, 2006b; Limkumnerd & Van der Giessen, 2008; Poh, Peerlings, Geers, & Swaddiwudhipong, 2013; Zaiser, 2015)). From the point of view of averaging procedure all dislocations in crystals belonging to

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one slip system can be fully characterized by two densities. In addition to the above mentioned average dislocation density (which we call density of excess dislocations), there exists another density of dislocations which does not show up in the non-uniform plastic slip but nevertheless may have significant influences on the nucleation of excess dislocations and the work hardening of crystals. For any closed circuit surrounding an area, which is regarded as infinitesimal compared with the characteristic size of the macroscopic body but may still contains a large number of dislocations, the resultant Burgers vector of these dislocations always vanishes, so the closure failure caused by the incompatible plastic slip is not affected by them. Ashby (1970) called them statistically stored dislocations, but we prefer the shorter and more precise name of redundant dislocations given earlier by Cottrell (1964). Let us also point out the important difference between the above classification and the classification of dislocations into mobile and immobile dislocations used in the discrete dislocation dynamics (see, e.g., (Han, Hartmaier, Gao, & Huang, 2006; Rhee, Zbib, Hirth, Huang, & De la Rubia, 1998; Zhou, Biner, & LeSar, 2010) and the references therein). The latter classification is not related to the averaging procedure but rather to the physical properties of dislocations (Cottrell, 1952). However, in one physical aspect one can see some similarity between the redundant and immobile dislocations. It turns out that, as a rule, the redundant dislocations in unloaded crystals at low temperatures exist in form of dislocation dipoles in two-dimensional case or pairs of small planar dislocation loops of opposite Burgers vectors whose sizes is comparable with the atomic distance in three-dimensional case. The simple reason for this is that the energy of a dislocation dipole (or a pair of small planar dislocation loops) is much smaller than that of dislocations apart, so the bounded state of dislocations renders low energy to the whole crystal in equilibrium. From the other side, due to their low energy, the dislocation dipoles (loops) can be created (as well as annihilated) by thermal fluctuations or, alternatively, by the mutual trapping in a random way. The redundant dislocations play two important roles in the plastic deformations of crystals: (i) together with the Frank-Read source (Hirth & Lothe, 1968) they provide additional sources for the nucleation of excess dislocations due to the fact that, when the applied shear stress becomes large enough, the dislocation dipoles dissolve to form the freely moving excess dislocations, (ii) the neutral dipoles (loops) of redundant dislocations act as obstacles that impede the motion of excess dislocations leading to the nonlinear work hardening.

In view of their roles in ductile crystals, the account of redundant dislocations in the CDT would make the material models more realistic. Since the statistical or spatial averaging procedures applied to ensembles of large numbers of dislocations are still in an embryonal stage (see the above cited references), various phenomenological approaches have been proposed in recent years. Arsenlis, Parks, Becker, and Bulatov (2004) developed a set of evolution equations for the densities of excess and redundant dislocations within the crystal plasticity. The density of redundant dislocations evolves through Burgers vector-conserving reactions, while that of excess dislocations evolves due to the divergence of dislocation fluxes. Except the missing thermal fluctuations in the nucleation of redundant dislocations, it was also unclear whether such an approach could be related to the energetics of crystals containing dislocations. Berdichevsky (2006a) was the first who included the density of redundant dislocations in the free energy density of the crystal. However, to the best of our knowledge, the more pronounced influence of the redundant dislocations on the yield stress and the dissipation within the CDT has not been considered up to now. The aim of this paper is to propose a phenomenological continuum dislocation theory, whose dissipation function depending on the densities of both excess and redundant dislocations in such a way that the obtained yield stress combines the constant contribution due to the Peierls barrier and the Taylor contribution that is proportional to the square root of the total density of dislocations (Taylor, 1934). Then we apply the proposed theory to the problem of anti-plane constrained shear. We solve this problem numerically and find the distribution of excess dislocations in the final state of equilibrium as well as the stress-strain curve. We show the size effect for the threshold stress, the nonlinear work hardening due to the combined excess and redundant dislocations, and the Bauschinger effect for the loading, elastic unloading, and loading in the opposite direction.

The paper is organized as follows. In Section 2 the kinematics of CDT accounting for densities of excess and redundant dislocations is laid down. Section 3 proposes the thermodynamic framework for this type of CDT. In Section 4 the problem of anti-plane constrained shear is analyzed. Section 5 presents the numerical solution of this problem and discusses the distribution of excess dislocations, the stress-strain curve, the Bauschinger translational work hardening and the size effect. Finally, Section 6 concludes the paper.

2. Kinematics

In the following we restrict ourselves to the small strain (or geometrically linear) continuum dislocation theory for single crystals. For simplicity we shall use some fixed rectangular cartesian coordinates and denote by $\mathbf{x}$ the position vector of a generic material point of the crystal. Kinematic quantities characterizing the observable deformation of this single crystal are the displacement field $\mathbf{u}(\mathbf{x})$ and the plastic distortion field $\boldsymbol{\beta}(\mathbf{x})$ that is incompatible. For single crystals having n active slip systems, the plastic distortion is given by

$$\boldsymbol{\beta}(\mathbf{x}) = \sum_{\alpha=1}^{n} \beta^{\alpha}(\mathbf{x})\mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha} \quad \left(\beta_{ij} = \sum_{\alpha=1}^{n} \beta^{\alpha} s_i^{\alpha} m_j^{\alpha} \right), \tag{1}$$

with β^{α} being the plastic slip, where the pair of constant and mutually orthogonal unit vectors $\mathbf{s}^{\alpha}$ and $\mathbf{m}^{\alpha}$ is used to denote the slip direction and the normal to the slip planes of the corresponding α-th slip system, respectively. Thus, there are altogether $3+n$ degrees of freedom at each point of this generalized continuum. Here and later, equivalent formulas for