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Distribution of dislocations in twisted bars

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ABSTRACT

An asymptotically exact continuum dislocation theory of single crystal bars under torsion is proposed. The dislocation distribution minimizing energy of the bar with zero torque is shown to be uniform. If the applied torque is non-zero, the minimizer exhibits a dislocation-free zone at the outer ring of the bar's cross-section. The non-uniform distribution of dislocations in equilibrium as well as the twist angle per unit length are found in terms of the given torque. With the energy dissipation being taken into account, there exists an elastic core region, while dislocations are concentrated in a ring between two dislocation-free zones. This leads to the change of the stress distribution increasing the critical threshold of the torque.

1. Introduction

Dislocations appear to reduce energy of crystals. For large dislocation densities (which are typically in the range $10^8 \div 10^{15}$ dislocations per square meter) it makes sense to use the continuum dislocation theory (CDT) to predict the distribution of dislocations in equilibrium. Although the framework of CDT has been laid down long time ago by Nye (1953), Bilby et al. (1955) and Kröner (1958), the applicability of the theory became feasible only in recent years thanks to the progress in averaging ensembles of large numbers of dislocations (Berdichevsky, 2006b, 2016; Zaiser, 2015). The fundamental results obtained in Berdichevsky (2006b, 2016) showed clearly that the constitutive equations and the whole structure of CDT depend crucially on two key functions: free energy density and dissipation (see the development of CDT and its applications to various problems of crystal plasticity in Baitsch et al. (2015), Berdichevsky (2006a), Berdichevsky and Le (2007), Kochmann and Le (2008, 2009), Koster et al. (2015), Le (2016a, 2016b), Le and Günther (2014), Le and Nguyen (2013) and Le and Sembiring (2008a, 2008b, 2009)). Among alternative approaches let us mention here the (phenomenological) strain gradient plasticity suggested in Engels et al. (2012), Mayeur and McDowell (2014) and Öztop et al. (2013) as well as the continuum dislocation dynamics (CDD) initiated by Hochrainer et al. (2007) and developed further in Hochrainer et al. (2014), Li et al. (2014), Sandfeld et al. (2011, 2015), Wulfinghoff and Böhlke (2015), Zhu et al. (2014) and Zhu and Xiang (2015). The latter approach has the potential of predicting also the time evolution of the dislocation network to equilibrium. However, it remains still unclear how to relate CDD to thermodynamics of dislocation networks and variational principles of CDT for distribution of dislocations in equilibrium.

In view of the variety of dislocation based gradient plasticity theories the necessity of having exact solutions of benchmark problems, on which different models can be tested and compared, becomes obvious. One of the first investigated problem was the torsion of a single crystal bar. Fleck et al. (1994) used strain gradient plasticity theory to compute the torque–twist curve

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and compared it with the experimental data showing clearly the size effect. Based on an alternative strain gradient plasticity theory, Aifantis (1999) studied the same problem and found the size sensitivity of both yield stress and hardening rate. Horstemeyer et al. (2002) provided the experimentally measured torque–twist curve for a rod made of single crystal copper. Later on, Kaluza and Le (2011) used CDT with the logarithmic energy of dislocation network proposed in Berdichevsky (2006a) to find not only the torque–twist curve, but also the distribution of dislocations in a twisted bar. The comparison between the theoretical prediction for the torque–twist curve obtained in Kaluza and Le (2011) and experimental measurements provided in Horstemeyer et al. (2002) showed good agreement for small up to moderate twists. More recently, Weinberger (2011) computed the energy and distribution of screw dislocations in a free unloaded bar within the linear elasticity and provided the molecular dynamics simulations (Weinberger and Cai, 2010) and dislocation dynamics simulations (Akarapu et al., 2010; Espinosa et al., 2006) for the twisted bar. His results confirmed the qualitative agreement with our prediction in Kaluza and Le (2011) for the twisted bar but displayed at the same time some quantitative differences in the torque–twist curve and the distribution of dislocations in equilibrium.

Motivated by the above investigations as well as several existing discrepancies between theories and simulations, this paper studies the torsion of a single crystal bar with a constant circular cross-section using the asymptotically exact CDT proposed recently in Berdichevsky (2016). Our aim is to find the dislocation distribution in equilibrium as function of the given torque and compare with the similar results obtained by numerical simulations in Weinberger (2011). To simplify the analysis we assume that the crystal is elastically isotropic and all dislocations are screw. Besides, the side boundary of the bar is traction free and may therefore attract dislocations. We adopt the free energy formulation found by Berdichevsky (2016) that is proved to be asymptotically exact in the continuum limit. If the dissipation can be neglected, the displacement and the plastic distortion should be found by the energy minimization. First, we show that the dislocation distribution minimizing energy of the bar with zero torque is uniform. This agrees well with the result obtained by Weinberger (2011). Next, for the bar loaded by a nonzero torque we find an energetic threshold for the dislocation nucleation. If the twist exceeds this threshold, excess dislocations appear to minimize the energy. It turns out that there is a dislocation-free zone at the outer ring of the bar's cross-section. The non-uniform distribution of dislocations in equilibrium as well as the twist angle is found in terms of the given torque. In case the dissipation due to the resistance to dislocation motion is taken into account, the energy minimization should be replaced by a variational equation. The solution is shown to have an elastic core region in the middle of the cross section. Dislocations are concentrated in a ring between two dislocation-free zones. This leads to the change of the stress distribution increasing the dissipative threshold of the torque. We show that the dislocation-free zones as well as the threshold in twist angle depend on the radius of the bar's cross-section exhibiting the size effect. We compare the torque–twist curve with the experimental curve obtained in Horstemeyer et al. (2002) that shows a good agreement in the range of small plastic twist angles.

The paper is organized as follows. In Section 2 the setting of the problem is outlined and the energy minimizing dislocation distribution in a bar with zero torque is found. Section 3 studies the plastic torsion of the bar at zero dissipation through energy minimization. In Section 4, the plastic torsion of the bar at non-zero resistance to dislocation motion is analyzed and the comparison with experimental results is provided. Finally, Section 5 concludes the present paper.

2. Asymptotically exact energy of the bar

Consider a single crystal bar of length L loaded in torsion by given torques $\pm T$ acting at its ends. Let C be the cross section of the bar by planes $z = \text{const}$. For simplicity, we consider C to be a circle of radius R (see Fig. 1). The side boundary of the bar $\partial C \times [0, L]$ is free from tractions. The length of the bar is assumed to be much larger than the radius ($L \gg R$) to neglect the end effects. If the torque T is sufficiently small, it is natural to assume that the bar deforms elastically so that the twist is proportional to the torque, provided the bar is initially dislocation-free. If T exceeds some critical value, then screw dislocations may appear. We assume that the active slip planes are perpendicular to the vectors $\mathbf{e}_\theta$ in the cylindrical coordinate system, while the slip directions as well as the dislocation lines are parallel to the z-axis. Mention that this assumption is not likely to be realistic for single crystals. However, since the Burgers vector is parallel to a screw dislocation, any crystallographic plane containing the dislocation is a possible slip plane. Thus, the screw dislocations in single cubic primitive crystals with the

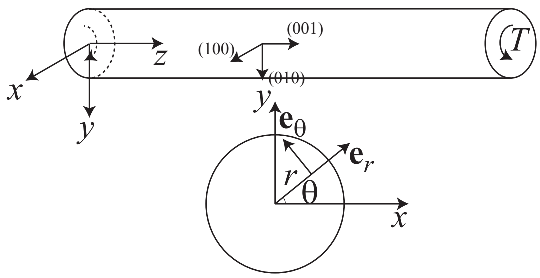

Fig. 1. A single crystal bar loaded in torsion and its cross section.