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Three-dimensional continuum dislocation theory

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The paper is dedicated to the 70th birthday of my teacher V. Berdichevsky.

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ABSTRACT

A three-dimensional continuum dislocation theory for single crystals containing curved dislocations is proposed. A set of governing equations and boundary conditions is derived for the true placement, plastic slips, and loop functions in equilibrium that minimize the free energy of crystal among all admissible functions, provided the resistance to dislocation motion is negligible. For the non-vanishing resistance to dislocation motion the governing equations are derived from the variational equation that includes the dissipation function. A simplified theory for small strains is also provided. An asymptotic solution is found for the two-dimensional problem of a single crystal beam deforming in single slip and simple shear.

1. Introduction

Dislocations appear in ductile crystals to reduce their energy. In view of a huge number of dislocations appearing in plastically deformed crystals (which typically lies in the range $10^8 \div 10^{15}$ dislocations per square meter) the necessity of developing a physically meaningful continuum dislocation theory (CDT) to describe the evolution of dislocation network and predict the formation of microstructure in terms of mechanical and thermal loading conditions becomes clear to all researchers in crystal plasticity. One of the main guiding principles in seeking such a continuum dislocation theory has first been proposed by Hansen and Kuhlmann-Wilsdorf (1986) in form of the so-called LEDS-hypothesis: the true dislocation structure in the final state of deformation minimizes the energy of crystal among all admissible dislocation configurations. 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). Because of numerous experimental evidences supporting this hypothesis (see, i.e., Hughes and Hansen, 1997; Kuhlmann-Wilsdorf, 1989, 2001; Laird et al., 1986), the latters use in constructing the continuum dislocation theory seems to be quite reasonable and appealing. For the practical realization one needs to (i) specify the whole set of unknown functions and state variables of the continuum dislocation theory, and (ii) lay down the free energy of crystals as their functional to be minimized. Berdichevsky and Sedov (1967) were the firsts to have proposed the variational formulation of CDT that extended Gibbs variational principle to crystals with continuously distributed dislocations (see also its further development in Berdichevsky (2006a)). The developed CDT has been successfully applied to various two-dimensional problems of dislocation pileups, bending, torsion, as well as formation of dislocation patterns in single crystals with straight dislocation lines (see Baitsch et al., 2015; Berdichevsky and Le, 2007; Kaluza and Le, 2011; Kochmann and Le, 2008a,b, 2009; Koster et al., 2015; Koster and Le, 2015; Le and Günther, 2015; Le and Nguyen, 2012, 2013; Le and Sembiring,

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2008a,b, 2009). Let us mention here the similar approaches suggested in Acharya and Bassani (2000), Acharya (2001), Engels et al. (2012), Gurtin (2002), Gurtin et al. (2007), Mayeur and McDowell (2014) and Öztop et al. (2013) which do not use the LEDS-hypothesis explicitly but employ instead the extended principle of virtual work for the gradient plasticity. However, as experiences and experiments show, dislocation lines are in general loops that, as a rule, can change their directions and curvatures depending on the material properties, loading condition, and crystal's geometry. Therefore the extension of CDT to networks of dislocations whose lines are curves in the slip planes is inevitable. To the best of author's knowledge, such three-dimensional continuum dislocation theory based on the LEDS-hypothesis for curved dislocations has not been developed until now. It became also clear to him that the latter's absence was due to the missing scalar dislocation densities for the network of curved dislocations.

The first attempt at constructing a continuum theory that can predict in principle not only the dislocation densities but also the direction and curvature of the dislocation lines has been made by Hochrainer et al. (2007) in form of the so-called continuum dislocation dynamics. Their theory starts with the definition of the dislocation density that contains also the information about the orientation and curvature of the dislocation lines. Then the set of kinematic equations is derived for the dislocation density and curvature that requires the knowledge about the dislocation velocity. The relation between the dislocation density and the macroscopic plastic slip rate via the dislocation velocity is postulated in form of Orowan's equation. The couple system of crystal plasticity and continuum dislocation dynamics becomes closed by the constitutive equation of a flow rule type (see Hochrainer et al., 2014; Sandfeld et al., 2011, 2015; Wulfinghoff and Böhlke, 2015). In addition to the heavy computational cost of such theory, the relation to thermodynamics of crystal plasticity and to the LEDS-hypothesis is completely lost: the equilibrium solution found in this theory may not minimize the energy of crystal among all admissible dislocation configurations. Let us mention also a continuum approach proposed by Xiang (2009), Zhu and Xiang (2010), Zhu et al. (2014) and Zhu and Xiang (2015) in which the three-dimensional dislocation network is characterized by two families of disregistry functions that may take only integer values. As will be seen later, a loop function introduced in the present paper to describe the kinematics of curved dislocations is quite similar to one of the disregistry functions employed in the above cited references. However, this similarity between two approaches is restricted only to the kinematics. As the governing equations for the displacements, plastic slip, and loop function and the basic principle to derive them are concerned, our approach differs strongly from that proposed in Zhu et al. (2014) and Zhu and Xiang (2015). The coupled system of equations in Zhu and Xiang (2015) is derived from the underlying discrete dislocation dynamics for the displacement and disregistry functions. This approach is subject to the same critics as that developed in Hochrainer et al. (2007).

The aim of this paper is to extend the nonlinear continuum dislocation theory (CDT) developed recently by Le and Günther (2014) to the case of crystals containing curved dislocations. Provided the dislocation network is regular in the sense that nearby dislocations have nearly the same direction and orientation, we introduce a loop function whose level curves coincide with the dislocation lines. Taking an infinitesimal area perpendicular to the dislocation line at some point of the crystal, we express the densities of edge and screw dislocations at that point through the resultant Burgers vectors of dislocations. Such scalar densities, found in this paper for the first time, contain not only the information about the number of dislocations, but also the information about the orientation and curvature of the dislocation lines. In case of dislocation motion we introduce the vector of normal velocity of dislocation line through the time derivative of the loop function. Following Kröner (1992) and Berdichevsky (2006b) we require that the free energy density of crystal depends only on the elastic deformation tensor and on the above scalar densities of dislocations. Then we formulate a new variational principle of CDT according to which the placement, the plastic slip, and the loop function in the final state of equilibrium minimize the free energy functional among all admissible functions. We derive from this variational principle a new set of equilibrium equations, boundary conditions, and constitutive equations for these unknown functions. In case the resistance to dislocation motion is significant, the variational principle must be replaced by the variational equation that takes the dissipation into account. This enables crystals with dislocations to stay in equilibrium not at the minimum of the free energy. Note, however, that the incremental minimization of the "relaxed" energy can be applied instead (Ortiz and Repetto, 1999; Carstensen et al., 2002). The constructed theory is generalized for single crystals having a finite number of active slip systems. We provide also the simplifications of the theory for small strains. As compared to the continuum dislocation dynamics proposed in Hochrainer et al. (2007) and Zhu and Xiang (2015) our theory is advantageous not only in the computational cost due to its simplicity, but also in its full consistency with the LEDS-hypothesis. In the problem of single crystal beam having only one active slip system and deforming in simple shear, the energy minimization problem reduces to the two-dimensional variational problem. We solve this problem analytically for the circular cross section and asymptotically for the rectangular cross section. We will show that this solution reduces to that found in Berdichevsky and Le (2007) for the beams with thin and long cross-sections.

The paper is organized as follows. After this introduction we present in Section 2 the three-dimensional kinematics for single crystals deforming in single slip. Section 3 formulates the variational principles of the three-dimensional CDT and derives its governing equations. Section 4 extends this nonlinear theory to the case of single crystals with n active slip system. Section 5 studies the three-dimensional small strain CDT. Section 6 is devoted to the analytical and asymptotic solutions of the two-dimensional energy minimization problem of a single crystal beam deforming in simple shear. Section 7 concludes the paper and discusses several open issues. Finally, in Appendix we give a detailed asymptotic analysis of the energy minimization problem posed in Section 6.