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Continuum dislocation dynamics: Towards a physical theory of crystal plasticity

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ABSTRACT

The plastic deformation of metals is the result of the motion and interaction of dislocations, line defects of the crystalline structure. Continuum models of plasticity, however, remain largely phenomenological to date, usually do not consider dislocation motion, and fail when materials behavior becomes size dependent. In this work we present a novel plasticity theory based on systematic physical averages of the kinematics and dynamics of dislocation systems. We demonstrate that this theory can predict microstructure evolution and size effects in accordance with experiments and discrete dislocation simulations. The theory is based on only four internal variables per slip system and features physical boundary conditions, dislocation pile ups, dislocation curvature, dislocation multiplication and dislocation loss. The presented theory therefore marks a major step towards a physically based theory of crystal plasticity.

1. Introduction

Since the bronze age men use the relative ease of plastically deforming metallic materials to produce tools and structures of ever growing variety in shape and function. The plastic properties of metals and of crystalline materials in general are largely controlled by the presence and characteristics of dislocations. Dislocations are line defects of the crystal lattice which may move when subjected to stresses, thereby introducing a permanent shear of the lattice without altering the lattice structure. Despite the enormous economic importance of metal plasticity and a significant amount of knowledge regarding the characteristics of individual dislocations and their interactions, no physical continuum theory of plasticity has yet emerged (Kröner, 2001). At first glance this appears astonishing since key issues in plasticity like the phenomenon of strain hardening can directly be related to the multiplication and interactions of dislocations and ‘physically informed’ models have been formulated which describe strain hardening in terms of the evolution of dislocation densities, see e.g. Kocks and Mecking (2003), Devincre et al. (2008). However, even the most sophisticated models rely on local laws which relate the evolution of dislocation density measures to the rate of plastic deformation. This engenders a conceptual paradox: even though plastic flow occurs by the motion of dislocations, dislocation transport is not captured by these models. This

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conceptual problem is inconsequential in traditional engineering applications concerned with large polycrystalline structures, where each volume element contains many grains and local constitutive laws are usually viable since grain boundaries constrain dislocation transport. In fact, the common approach in engineering plasticity has been to dispose altogether of dislocation considerations and to rely on phenomenological parameterization of local constitutive laws by fitting model parameters to the results of mechanical testing.

In small scale structures, however, local constitutive laws have been challenged since the 1990's by observations of size dependent plastic behavior, see e.g. Fleck et al. (1994), Arzt (1998), Volkert and Kraft (2001). These observations stimulated many efforts to make phenomenological plasticity models size dependent by introducing internal length scales, mostly by adding gradients of the plastic strain into traditional constitutive frameworks (Fleck and Hutchinson, 1993; Nix and Gao, 1998; Gurtin, 2002). However, recent small scale experiments display size effects also in deformation geometries where strain gradients are absent, as in the uniaxial compression of micro pillars (Uchic et al., 2004; Volkert and Lilleodden, 2006). While discrete dislocation simulations can correctly describe such size effects as well as those stemming from strain gradients (Zhou et al., 2010; Senger et al., 2008; von Blanckenhagen et al., 2004), current continuum theories cannot. This emphasizes the need for a physical theory of plasticity to overcome the shortcomings of phenomenological modelling by direct consideration of the kinematics of dislocation systems.

For the formulation of a statistical continuum theory of dislocations one important challenge already appears at the most fundamental level, namely at representing the dislocation arrangement and kinematics by continuous field variables. This difficulty stems from the nature of dislocations as curved and connected lines: as line segments of different orientation move into different directions, maintaining connectivity requires continuous changes in line length. The resulting kinematic problems have recently been overcome by Hochrainer et al. (2007) through the use of a higher dimensional configuration space containing variables that characterize the dislocation line direction. While this approach is satisfying from a theoretical point of view, numerical solution of the obtained equations is difficult and computationally expensive owing to the necessity of discretizing the continuous orientation space at each spatial point (Sandfeld et al., 2010). Low resolution of the orientation space, e.g. by considering only ‘screw’ orientations parallel and ‘edge’ orientations orthogonal to the Burgers vector, as in Arsenlis et al. (2004) or Zaiser and Hochrainer (2006), leads to point particle-like kinematics which have to be patched up with sophisticated rules to account for changes in line length and in dislocation character during dislocation motion. High resolution, on the other hand, results in simulations that are expensive both in terms of storage space and computation time. Here we show that these problems can be overcome in a systematic manner by considering multipole expansions of the orientation dependence of the density functions. In the simplest case, this yields a closed set of evolution equations for the total dislocation density, the dislocation curvature density and the components of the dislocation density tensor (Kröner–Nye tensor). These equations define a physical theory of plasticity that accounts for transport and storage of dislocations, dislocation multiplication and dislocation loss and that enables the formulation of physically based boundary conditions in terms of dislocation fluxes. In other words, the equations constitute the basis for a *continuum dislocation dynamics* (CDD) field theory.

2. Continuum dislocation dynamics (CDD)

In single crystals, plastic slip occurs in a discrete set of slip systems characterized by slip direction $\boldsymbol{m}$ and slip plane normal $\boldsymbol{n}$. The shear displacement produced by the dislocation as it moves in its slip plane is given by the Burgers vector $\boldsymbol{b} = b\boldsymbol{m}$. Locally, the direction of a dislocation line is characterized by its tangent $\boldsymbol{l}$. There are two classical dislocation density measures: the total dislocation density $\rho_{\rm t}$ (line length per unit volume) and the dislocation density tensor $\boldsymbol{\alpha}$. Besides its continuum definition as the curl of the plastic distortion tensor $\boldsymbol{\beta}^{\rm pl}$ (Kröner, 1958), $\boldsymbol{\alpha}$ can be obtained by averaging as follows: for dislocations of one slip system (sharing the same Burgers vector $\boldsymbol{b}$) one sums up the vectors $\boldsymbol{t}$ connecting the point of entry and exit of each dislocation crossing a volume element Ω with volume $|\Omega|$ to obtain the density vector $\boldsymbol{\kappa} = \sum \boldsymbol{t}/|\Omega|$. Combining this with the Burgers vector into a tensor gives the dislocation density tensor of the slip system, $\boldsymbol{\alpha} = \boldsymbol{\kappa} \otimes \boldsymbol{b}$. The overall dislocation density tensor derives by summing the tensors from the slip systems. As averaged objects, however, these dislocation density measures cannot be systematically evolved since essential kinematic information is missing.

A kinematically closed theory of plasticity can be built upon a higher dimensional analogue of the dislocation density tensor: the second order dislocation density tensor $\boldsymbol{\alpha}^{\rm II}$ (Hochrainer et al., 2007) (SODT). The basic idea is to assign to each point of the dislocation line the angle φ which the local tangent $\boldsymbol{l}$ forms with the Burgers vector $\boldsymbol{b}$ to define a ‘lifted’ curve in an extended configuration space that contains the angle as an independent parameter. The tangent vectors to these lifted curves contain both the local spatial line direction and the curvature given by the change of the angle φ along the curve. Averaging these second order tangent vectors in much the same way as described above with regard to the classical dislocation density tensor yields $\boldsymbol{\alpha}^{\rm II}$.

To formulate the new equations we introduce a coordinate system on a slip system such that the slip plane is the 1–2 plane and the Burgers vector points in 1-direction: $\boldsymbol{b} = (b, 0, 0)$. Points in the plane are denoted by p while a point in the higher dimensional configuration space is given by $P = (p, \varphi)$. The tensor $\boldsymbol{\alpha}^{\rm II}$ is uniquely defined by two density functions: the dislocation density $\rho(p, \varphi)$, which measures at p the area density of dislocations with line direction $\boldsymbol{l}(\varphi)$ threading a perpendicular area element, and the *curvature density* $q(p, \varphi)$, which characterizes the variation of direction along the dislocation lines and relates to the local dislocation line curvature $k(p, \varphi)$ by $q(p, \varphi) = \rho(p, \varphi)k(p, \varphi)$. The corresponding evolution equations are summarized in Appendix A1.