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Internal stresses in a homogenized representation of dislocation microstructures

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ABSTRACT

To develop a continuum theory based on the evolution of dislocation microstructures, two challenges have to be resolved: the correct representation of the kinematics of dislocation motion in terms of dislocation density and the formulation of a mobility law reflecting an effective description of the physical behavior of the discrete many-body problem.

Kröner's classical continuum theory has inspired different approaches to model plasticity based on the motion of dislocations. Amongst them, the Continuum Dislocation Dynamics (CDD) theory was formulated as a generalization of the classical theory. The CDD theory allows for a continuous representation of the evolution of dislocation microstructures and is found to be kinematically complete.

Here, a numerical formulation of the CDD theory is presented and constitutive laws for the incorporation of dislocation interactions are derived based on the representation of the dislocation microstructure in two dimensions. An error measure is introduced to analyze the constitutive law and the results are compared to discrete dislocation dynamics simulations. Important aspects for the implementation of a 3D theory are discussed.

1. Introduction

Phenomenological approaches to model material behavior based on experimental observations have proven to be a profound basis for continuum plasticity formulations. However, these models reach their limits when small scales are considered where inhomogeneous plastic deformation and size effects are observed experimentally (Arzt, 1998).

The understanding of the motion of dislocations as the basic physical mechanism that causes plastic deformation allows to derive physically motivated theories of plasticity. One can model such phenomena by discrete dislocation dynamics (DDD) simulations which predict the evolution of dislocation systems based on their mutual interactions (Ghoniem and Sun, 1999; Lemarchand et al., 2001; Weygand et al., 2002) and simple mobility laws (Bitzek and Gumbsch, 2005; Srivastava et al., 2013). Taking these results to a larger scale requires the introduction of meaningful averaging. In the 1950s, Kröner made a first attempt to formulate a classical continuum theory based on the evolution of dislocation densities (Kröner, 1958). A drawback of this classical theory is the loss of important microstructural information due to the fact that oppositely oriented line segments (statistically stored dislocations – SSD) contained within one averaging volume cancel out. To account for the SSDs, efforts have been made to couple strain gradient dependent theories with phenomenologically derived evolution

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equations of SSD densities (Ashby, 1970; Fleck and Hutchinson, 1993; Gurtin, 2002).

For the derivation of a physically motivated continuum theory of dislocation motion, it is necessary to represent the entire microstructure in a dislocation density formulation. For 2D systems, such theories have been developed based on the statistical nature of dislocation interactions (Groma, 1997; Groma et al., 2003) and first attempts have been made to derive a higher dimensional theory for curved dislocation lines in 3D (El-Azab, 2000). However, the theory is unable to account for the connectivity of dislocation lines and hence does not capture the whole picture of dislocation dynamics. This gap was closed by the Continuum Dislocation Dynamics (CDD) theory, where a higher-dimensional theory has been introduced in such a way that kinematic completeness can be achieved (Hochrainer et al., 2007; Sandfeld et al., 2011; Hochrainer et al., 2014). In this context, open questions are left for the numerical implementation of a fully continuous theory and the kinetic closure of the theory. In particular, the question arises of how a constitutive law for the dislocation velocity can be formulated in a dislocation density field theory (Sandfeld et al., 2013; Schulz et al., 2014; Xiang, 2009; Dickel et al., 2014; Chapman et al., 2015). The development of such a constitutive formulation requires a precise understanding of the dislocation stress fields and interactions in a homogenized numerical framework.

In this paper, we present a dislocation based continuum model (Hochrainer et al., 2014) for the description of the dislocation dynamics and discuss different representations of the dislocation microstructure. A thorough derivation of the stresses describing the interactions of dislocation densities is proposed. In Section 2, the considered density field theory of dislocation dynamics is reviewed and a flux based implementation is introduced for the evolution of the considered density fields using a finite volume method (FVM). In Section 3, the constitutive laws for the dislocation velocity are derived. Based on the representation of the dislocation microstructure, expressions for the internal stress are derived and applied to the density field model. The derivations are validated in Section 4 using suitable benchmark problems. The results are compared to ensemble averages computed from discrete dislocation dynamics (DDD) simulations in a 2D continuous representation and discussed with a particular focus on the aspect of coarse graining. Additionally, an error measure for the validation of the constitutive law is discussed. Conclusions are drawn for the validity of the presented method and consequences for a general implementation in a 3D Continuum Theory are discussed.

2. A density field theory of dislocation dynamics

A dislocation based continuum theory must contain a description of the kinematics of dislocation motion in an averaged sense and must be able to capture the behavior of discrete dislocations in a homogenized representation.

2.1. Continuum dislocation dynamics

For the correct averaging of dislocations, Hochrainer et al. (2007, 2014) have generalized the classical continuum theory of Kröner (1958) by introducing a mathematical description of dislocation densities which allows for the mapping onto a higher dimensional configuration space $\mathbf{Q}:=\mathbb{R}^2 \times [0, 2\pi)$ including dislocation line orientation. From the higher dimensional representation (Hochrainer et al., 2007), a simplified form is derived by a Fourier series expansion of the dislocation density ρ and the curvature density q (Hochrainer et al., 2014). The representation of the simplified system of evolution equations depends on the chosen closure approximations. The total dislocation density ρ_t, the geometrically necessary dislocation density tensor $\boldsymbol{\kappa} = (\kappa_1, \kappa_2, 0)$ and the curvature density q_t ($q_t = \rho_t \bar{k}$ with $\bar{k}$ being the mean curvature) represent the first coefficients of the expansion of the higher dimensional dislocation density and the higher dimensional curvature density (Hochrainer et al., 2014). v denotes the dislocation velocity and for simplicity is assumed to be isotropic. This leads to the following set of coupled evolution equations

$$\partial_t \rho_t = -\nabla\cdot(v\boldsymbol{\kappa}^{\perp}) + vq_t \tag{1}$$

$$\partial_t \boldsymbol{\kappa} = \nabla \times (\rho_t v \mathbf{n}) \tag{2}$$

$$\partial_t q_t = -v\nabla\cdot\left(\frac{q_t}{\rho_t}\boldsymbol{\kappa}^{\perp}\right) - \frac{1}{2}\Big((\rho_t + |\boldsymbol{\kappa}|)\nabla^2_{\mathbf{l},\mathbf{l}} v + (\rho_t - |\boldsymbol{\kappa}|)\nabla^2_{\mathbf{l}^{\perp},\mathbf{l}^{\perp}} v\Big) \tag{3}$$

where the slip plane normal is denoted by $\mathbf{n}$ and the orthogonal density tensor is defined as $\boldsymbol{\kappa}^{\perp} = (\kappa_2, -\kappa_1, 0)$. $\mathbb{R}^2$ is spanned by the orthonormal basis vectors $\mathbf{l} = \boldsymbol{\kappa}/|\boldsymbol{\kappa}|$ and $\mathbf{l}^{\perp} = \boldsymbol{\kappa}^{\perp}/|\boldsymbol{\kappa}|$. The closure of the set of Eqs. (1)–(3) is achieved by formulating a constitutive law for the dislocation velocity v based on the assumption that the dislocation velocity can be deduced from the momentary state of the dislocation microstructure. The accumulated plastic slip $\gamma^{(s)}$ in slip system s is computed from the generalized Orowan equation

$$\partial_t \gamma^{(s)} = |\boldsymbol{b}^{(s)}| v^{(s)} \rho_t^{(s)}, \tag{4}$$

where $v^{(s)}$ is the mean velocity in the slip system. The contributions from all slip systems are summed up to calculate the total plastic distortion