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Continuum representation of systems of dislocation lines: A general method for deriving closed-form evolution equations

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ABSTRACT

Plasticity is governed by the evolution of, in general anisotropic, systems of dislocations. We seek to faithfully represent this evolution in terms of density-like variables which average over the discrete dislocation microstructure. Starting from T. Hochrainer's continuum theory of dislocations (CDD) (Hochrainer, 2015), we introduce a methodology based on the 'Maximum Information Entropy Principle' (MIEP) for deriving closed-form evolution equations for dislocation density measures of different order. These equations provide an optimum representation of the kinematic properties of systems of curved and connected dislocation lines with the information contained in a given set of density measures. The performance of the derived equations is benchmarked against other models proposed in the literature, using discrete dislocation dynamics simulations as a reference. As a benchmark problem we study dislocations moving in a highly heterogeneous, persistent-slip-band like geometry. We demonstrate that excellent agreement with discrete simulations can be obtained in terms of a very small number of averaged dislocation fields containing information about the edge and screw components of the total and excess (geometrically necessary) dislocation densities. From these the full dislocation orientation distribution which emerges as dislocations move through a channel-wall structure can be faithfully reconstructed.

1. Introduction

The development of physically based and predictive models for plasticity on the micro-meter scale has been a challenging task ever since the connection between dislocations and the macroscopic material response has been made in the 1930s. On the one hand, continuum approaches based on naive averaging for obtaining continuous densities without taking into account the curved and line-like nature of systems of dislocations must fail in many cases because important microstructural information is being lost; discrete approaches, on the other hand, contain full information about the microstructure. However, the number of dislocations or accumulated plastic strain can be high which can easily become a limiting factor even for today's discrete dislocation dynamics (DDD) models. Continuum models of dislocation systems which average over the discrete dislocation microstructure do not suffer from this restriction and hence might have advantages over discrete models, provided the motion of dislocations can be correctly captured in such a continuum (or dislocation-density based) framework.

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Historically, dislocation density-based plasticity models have evolved along several independent lines. The first line originates from the continuum theory of dislocations and internal stresses as developed by Kröner (1958) and Nye (1953). This theory is formulated in a geometrically rigorous manner and provides generic relationships between the dislocation microstructure, the plastic distortion and the associated internal stress fields. The fundamental object of the theory is the dislocation density tensor $\boldsymbol{\alpha}$ which is defined as the curl of the plastic distortion, $\boldsymbol{\alpha} = -\,\mathrm{curl}\,\boldsymbol{\beta}^{\mathrm{pl}}$. This theory was extended by Mura (1963) who formulated a kinematic equation of evolution for the dislocation density tensor, $\partial_t \boldsymbol{\alpha} = -\,\mathrm{curl}[\boldsymbol{v} \times \boldsymbol{\alpha}]$ where $\boldsymbol{v}$ is the dislocation velocity vector. In this form the theory provides a full description of dislocation microstructure evolution and of plastic deformation for situations where all dislocations are geometrically necessary dislocations (GND), i.e., where they can be envisaged as contour lines of the plastic shear strain on the respective slip systems (e.g. Sedláček et al., 2003; Xiang, 2009; Zhu and Xiang, 2015). In the general case where dislocations of multiple orientations and slip systems are present, such a field theory, in order to fully capture the evolution of the dislocation microstructure, requires a spatial resolution that is well below the spacing of the individual dislocation lines in order to make the dislocation velocity field $\boldsymbol{v}$ uniquely defined (see e.g. Xia and El-Azab, 2015; Zhang et al., 2015 for such implementations). A similar spatial resolution is also required for phase field approaches to dislocation microstructure evolution who directly simulate the evolution of the shear strain fields (Wang et al., 2001; Rodney et al., 2003). Such simulations, which evidently incur a high computational cost, may be envisaged as field-theoretical approaches to discrete dislocation dynamics simulation and will not be discussed in the following. Instead our focus of interest is on *average*, statistical descriptions of the dislocation microstructure which work in situations where dislocations of multiple orientations are present within the same volume element, such that a mapping on corresponding density-like variables provides an efficient compression of information. On such a coarse grained level, approaches which are directly based on spatial averaging of the classical dislocation density tensor $\boldsymbol{\alpha}$ can work only in exceptional circumstances: once the fine structure of the plastic strain field is smoothed over, the dislocation lines associated with the averaged out features are no longer represented by the dislocation density tensor. Unfortunately, this background of "statistically stored" dislocations still contributes both to plastic flow and to work hardening. We are thus faced with the fundamental problem how they can be incorporated into a density-based theory.

The second line of continuum models, which originates from the work of Johnston and Gilman (1959) and Kocks (1976), solved this problem by taking the radical approach of disposing with geometry altogether and considering only the "statistically stored" contribution to the dislocation density, which is characterized by a scalar density measure ρ of dimension $1/\mathrm{length}^2$. For this density measure, phenomenological evolution equations are formulated which relate the dislocation density to the strain, $\rho = \rho(\gamma)$, and these equations were combined with other phenomenological relations which relate the scalar density of dislocations to the flow stress (e.g., the Taylor relationship $\tau = aGb\rho^{1/2}$ where G is the shear modulus, b the Burgers vector modulus, and a a dimensionless constant) and to the plastic flow rate (e.g. the Orowan relation $\mathrm{d}\gamma/\mathrm{d}t = \rho b v$ where v is the scalar magnitude of the dislocation velocity). This modelling approach and its derivatives were successfully used to formulate phenomenological models of work hardening and plastic flow (e.g. Estrin and Mecking, 1984; Caceres and Blake, 2007; Bouaziz et al., 2013). Generally speaking, the approach works well as long as deformation is, on the scale of the description, homogeneous such that geometrically necessary dislocations – or, equivalently, strain gradients – need not to be taken into account.[1]

In recent years, several attempts have been made to unify both strands of continuum modeling and to arrive at models which can capture the combined evolution of "statistically stored" and "geometrically necessary" dislocation densities in a framework which can faithfully represent the underlying motion of the discrete dislocation lines. Pioneering work was done on two-dimensional (2D) systems of straight parallel dislocations by Groma (1997), Zaiser et al. (2001), Groma et al. (2003) who systematically formulated evolution equations for 2D dislocation densities as statistical averages over the dynamics of the corresponding discrete dislocation systems. Generalizing this approach to three-dimensional systems of curved dislocations has, however, proven to be quite challenging: straight parallel dislocations can be envisaged as points in the intersecting plane, and both the mathematical definition of densities of such objects and a consistent formulation of their kinematics are almost trivial tasks. Three-dimensionally moving dislocations, on the other hand, are curved lines which move perpendicular to their line direction while remaining topologically connected, and the definition of densities of such objects and corresponding formulation of their kinematics is far from straightforward. As a consequence, models have been (and up to date still are) developed that intentionally neglect some aspects: e.g. screw-edge representations (Arsenlis et al., 2004; Reuber et al., 2014; Leung et al., 2015) are a coarse way of approximating continuously curved dislocation loops, while other approaches rely on a geometrically consistent description of the evolution of the GND content as described by the Kröner–Nye density tensor but complement this with phenomenological ad hoc assumptions regarding the evolution of the statistically stored dislocation density and/or the contribution of such dislocations to the plastic strain rate (e.g. Acharya and Roy, 2006; Fressengeas et al., 2011).

We finally note another line of continuum dislocation theories which is based on the low-energy dislocation structure (LEDS) hypothesis proposed by Hansen and Kuhlmann-Wilsdorf (1986). The LEDS-hypothesis to a certain extent dismisses the role of the history (initial dislocation microstructure and deformation path) and indicates that among all admissible

[1] The limitations of the line of Gilman and Kocks can easily be seen: consider, for instance, the deformation of a polycrystal before grain boundaries yield plastically. Any approach which considers the dislocation density an increasing function of the strain will predict that dislocation densities are largest in the grain interior, where the strains have their maximum. However, it is obvious that in reality dislocation densities will be largest near the grain boundaries where dislocation motion is constrained and dislocations form pile ups which accommodate the associated strain gradients.

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