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A link between microstructure evolution and macroscopic response in elasto-plasticity: Formulation and numerical approximation of the higher-dimensional continuum dislocation dynamics theory

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Micro-plasticity theories and models are suitable to explain and predict mechanical response of devices on length scales where the influence of the carrier of plastic deformation – the dislocations – cannot be neglected or completely averaged out. To consider these effects without resolving each single dislocation a large variety of continuum descriptions has been developed, amongst which the higher-dimensional continuum dislocation dynamics (hdCDD) theory by Hochrainer et al. (Phil. Mag. 87, pp. 1261–1282) takes a different, statistical approach and contains information that are usually only contained in discrete dislocation models. We present a concise formulation of hdCDD in a general single-crystal plasticity context together with a discontinuous Galerkin scheme for the numerical implementation which we evaluate by numerical examples: a thin film under tensile and shear loads. We study the influence of different realistic boundary conditions and demonstrate that dislocation fluxes and their lines' curvature are key features in small-scale plasticity.

1. Introduction

Plastic deformation of metals has been utilized by man since the copper age and the knowledge of how to process metals (by e.g. forging) has constantly grown. However, the physical mechanisms underlying the empirical procedures could not be understood until the crystalline structure of metals was investigated by Rutherford at the beginning of the 20th century. Subsequent attempts to explain the discrepancy between the theoretically predicted shear strength of a metal and the experimentally observed yield stresses lead to the concept of the 'dislocation' – a linear crystal defect – which was proposed in the 1930s independently by Orowan (1934), Polanyi (1934) and Taylor (1934a). Two decades later Kondo (1952), Nye (1953), Bilby et al. (1955) and Kröner (1958) independently introduced equivalent measures for the average plastic deformation state of a crystal in the form of a second-rank dislocation density tensor. This 'Kröner-Nye tensor' is introduced to link

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the microscopically discontinuous to a macroscopically continuous deformation state and is the fundamental quantity in Kröner's continuum theory of dislocations. It has been used widely until today (see e.g. the related works in Acharya and Fressengeas (2012); Taupin et al. (2013); Le and Günther (2014)). This tensor, however, only captures inhomogeneous plastic deformation states associated with so-called geometrically necessary dislocations (GNDs) and does not account for the accumulation of so-called statistically stored dislocations (SSDs) in homogeneous plasticity. This limits the applicability of the classical dislocation density measure within continuum theories of plasticity.

Phenomenological continuum models for plasticity which are not based on dislocation mechanics have been successful in a wide range of engineering applications. They operate on length scales where the properties of materials and systems are scale invariant. The scale-invariance, however, breaks down at dimensions below a few micro-meters, which is also a scale of growing technological interest. These microstructural effects become more and more pronounced in small systems and lead to so-called 'size effects' (e.g. Ashby, 1970; Arzt, 1998; Stolken and Evans, 1998; Greer and De Hosson, 2011). Phenomenological continuum theories incorporate internal length scales by introducing strain gradient terms – sometimes based on the consideration of GND densities – into their constitutive equations (e.g. Fleck et al., 1994; Nix and Gao, 1998; Gurtin, 2002; Gao and Huang, 2003; Zhang et al., 2014) but are not able to consider fluxes of dislocations or the conversion of SSDs into GNDs and vice versa. Refined continuum formulations (with or without strain gradients) include additional information in a mechanism-based approach (Engels et al., 2012; Li et al., 2014) or take multi-scale approaches by directly including information from lower scale models (Wallin et al., 2008; Xiong et al., 2012).

Discrete dislocation dynamics (DDD) models (e.g. Kubin and Canova, 1992; Devincre and Kubin, 1997; Fivel et al., 1997; Ghoniem et al., 2000; Weygand et al., 2002; Bulatov and Cai, 2002; Arsenlis et al., 2007; Zhou et al., 2010; Po et al., 2014) contain very detailed information about the dislocation microstructure and the interaction and evolution of dislocations and have been successful over the last two decades in predicting plasticity at the micro-meter scale. DDD simulations allow to investigate complex plastic deformation mechanisms but are, however, due to their high computational cost limited to small system sizes/small densities.

A different approach which is closely related to DDD and which generalizes the classical continuum theory of dislocations was undertaken by Groma et al. (Groma, 1997; Groma et al., 2003). They used methods from statistical physics to describe systems of positive and negative straight edge dislocations in analogy to densities of charged point particles. The resulting evolution equations are able to faithfully describe fluxes of signed edge dislocations and the conversion of SSDs into GNDs (and vice versa). This approach has been successfully used by a number of groups (e.g. Yefimov et al., 2004; Kratochvil et al., 2007; Hirschberger et al., 2011; Scardia et al., 2014). A generalization to systems of curved dislocation loops, however, is not straightforward. Pioneering steps into that direction have been undertaken by Kosevich (1979); El-Azab (2000); Sedláček et al. (2003). Furthermore, 'screw-edge' representations have been introduced as an approximation by Arsenlis et al. (2004); Zaiser and Hochrainer (2006); Reuber et al. (2014) and Leung et al. (2015); Xiang and co-workers developed a model for the evolution of curved systems of geometrically necessary dislocations (Xiang, 2009). Their model also includes line tension effects and was e.g. applied to model Frank-Read sources (Zhu et al., 2014). A new approach based on statistical averages of differential geometrical formulations of dislocation lines has been done by Hochrainer (Hochrainer, 2006; Hochrainer et al., 2007; Sandfeld et al., 2010) who generalized the statistical approach of Groma towards systems of dislocations with arbitrary line orientation and line curvature introducing the higher-dimensional *Continuum Dislocation Dynamics* (hdCDD) theory. The key idea of hdCDD is based on mapping spatial, parameterized dislocation lines into a higher-dimensional configuration space, which contains the local line orientation as additional information. This is particularly useful in situations with complex microstructure (Sandfeld et al., 2010, 2015). In order to avoid the high computational cost of the higher-dimensional configuration space, 'integrated' variants of hdCDD – denoted by CDD – have also been developed recently and their simplifying assumptions already have been benchmarked for a number of situation (Hochrainer et al., 2009; Sandfeld et al., 2011; Hochrainer et al., 2014; Zaiser and Sandfeld, 2014; Monavari et al., 2014). Furthermore, very recently one CDD variant has been coupled to a strain gradient plasticity model (Wulfinghoff and Böhlke, 2015) and was used to study size effects of a composite material. Until now hdCDD nonetheless serves as reference method for all CDD formulations, since it can be considered as an almost exact continuum representation of ensembles of curved dislocations and allows to access many relevant microstructural information.

In this article, we derive and formulate the governing equations for hdCDD in a general crystal plasticity context. We start by introducing the formulation for single-crystal plasticity and the elasto-plastic boundary value problem and connect this to the dislocation system in a staggered scheme. The evolution of the dislocation density and the dislocation curvature density is computed in representative slip planes depending on the dislocation velocity. This is approximated by a discontinuous Galerkin (DG) scheme introduced in Sect. 3 with a local Fourier ansatz suitable for the higher dimensional configuration space. Numerical examples in Sect. 4 – tension and shearing of a thin film – demonstrate the influence of passivated and non-passivated surfaces on the microstructure evolution. Furthermore we study the influence of the lines' curvature on the plastic deformation behavior and also on the stress-strain response of the specimen and compare with the formulation of Groma.

2. Crystal elasto-plasticity based on the hdCDD theory

In this section we introduce the elastic eigenstrain problem and its variational formulation (Sect. 2.1 and Sect. 2.2) and two different models for representing slip planes (Sect. 2.3) in a continuum framework. Then we outline the hdCDD theory extending the classical quantities from Kröner's continuum theory: the governing equations for the evolution of dislocation