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Modeling the evolution of dislocation populations under non-proportional loading

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ABSTRACT

The two-phase composite approach of Estrin et al. (1998) describes an evolving dislocation cell structure with dislocation populations for cell walls and the interior. Mckenzie et al. (2007) enhanced the model to capture the effects of hydrostatic pressure and temperature during severe plastic deformation. The main goal of the present study is to extend this microstructural model to non-proportional deformation in order to develop a framework suitable for the simulation of dislocation density evolution upon load path changes. Thereby, the two-phase composite approach is examined carefully. Both physical and numerical drawbacks are revealed and possible solutions are presented. Here, a special aim is to ensure that values of the dislocation densities remain within a physically reasonable range. Moreover, some improvements concerning reliable parameter identification are suggested as well. The material parameters are identified for an aluminum alloy using TEM cell size measurements. The extension to non-proportional deformation aims to predict the experimentally observed dissolution of cells and reduction of total dislocation density shortly after load path change. In order to capture these effects, some tensor-valued state variables are introduced which couple the refined micro model with the macroscopic viscoplasticity framework proposed by Shutov and Kreißig (2008a). As a result, a new system of constitutive equations is obtained. In order to demonstrate the framework's capability to respond to load path changes, load cases as typical for Equal Channel Angular Pressing (ECAP) are considered. The obtained evolution of dislocation populations differs significantly depending on which ECAP route is applied.

1. Introduction

An adequate description of evolving dislocation structures is of great importance for physically based modeling of many metallic materials. There are sophisticated multi-scale approaches to model dislocation dynamics in a discrete or continuous manner (e.g., Devincre et al., 2001; Groh et al., 2009; Cai et al., 2006; Le and Sembiring, 2008). Within such approaches, precious insights into the collective behavior of dislocations can be obtained (for an overwiew, cf. Bulatov and Cai, 2006). However, the scale bridging to engineering plasticity applications where large deformations and long time frames occur is still an open problem.

The number of degrees of freedom can be drastically decreased by introducing dislocation densities as state variables into continuum scale models. Corresponding evolution equations can be deduced from microstructural considerations. Depending on the number of introduced dislocation populations these approaches are called one-parameter-model (only total

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dislocation density) or multi-parameter-models, respectively (cf. Goerdeler and Gottstein, 2001; Ding and Guo, 2001). Within the last decade, this approach has been used by many researchers to include an evolving dislocation structure in continuum-scale modeling of metal plasticity. In particular, such information can be incorporated within models of crystal plasticity (cf. and references therein Gérard et al. (2013) or even purely phenomenological modeling (cf. Shutov and Ihlemann, 2012). There are numerous theoretical and experimental indications that dislocations within crystals constitute self-organizing systems (Amodeo and Ghoniem, 1990b; Yamaki et al., 2006; Gregor, 1998). As a characteristic feature, they tend to distribute inhomogeneously and thus form spatial patterns. Among others, the three-dimensional cell structure (Langlois and Berveiller, 2003) is typical for a class of metals and alloys. After the dislocation structure has emerged, further monotonic deformation results in the shrinkage of the structural characteristics: dislocation spacing, wall thickness and cell size. In the case of non-monotonic deformation the behavior seems to be different. Experimental findings (Hasegawa et al., 1975, 1986) suggest that load path changes can lead to the dissolution or disruption of cells. As the evolving cell structure governs the macroscopic behavior, such non-proportional loading can result in a very complex material response (Benallal et al., 1989). Its reproduction by pure phenomenological models is a challenging task (e.g., Benallal and Marquis, 1987; Freund et al., 2012). Thus, microstructural considerations should be used to enable a more adequate description of the material behavior under load path changes.

It is well known (Tóth et al., 2010) that dislocation cells can serve as precursor of forthcoming subgrains even leading to nanocrystalline microstructures under severe plastic deformation (SPD). In particular, Equal Channel Angular Pressing (ECAP) is a promising SPD technique which allows development of an ultrafine-grained microstructure (Segal, 1995). The characteristic feature of ECAP is that a billet is pressed repeatedly through an angular channel without net change in the billet's shape. Depending on how the billet is rotated after each pass different routes are realized, which involve distinct load path changes.

In the current study, a framework suitable for the simulation of dislocation density evolution upon such load path changes is presented. It is based on the two-phase composite model of Estrin et al. (1998) and kept as simple as possible in order to enable the simulation of SPD processes within a reasonable simulation time. The paper is organized as follows: The two-phase composite approach of Estrin et al. (1998) is outlined and carefully analyzed in Section 2. Both physical and numerical drawbacks are identified and possible solutions are presented, thus leading to a refined model. The problem of a reliable parameter identification is discussed in Section 3. There, material parameters of the refined model are identified for the aluminum alloy AA 6016. In Section 4 the model is extended to non-proportional deformation in such a way that the evolution of dislocation densities becomes sensitive to load path changes. Towards that end, the refined micro model is coupled with the macroscopic viscoplasticity model of Shutov and Kreißig (2008a), which is also outlined briefly. Finally, a new system of constitutive equations is obtained including the micro model of Mckenzie et al. (2007) as a special case. In Section 5, the evolution of dislocation populations during Equal Channel Angular Pressing is considered. Finally, simulation results for routes A, C, B_c, and E are discussed.[1]

Let us briefly introduce the notations used in this paper. A second rank tensor is denoted by a small or capital letter with two underscores, e.g., $\underline{\underline{U}}$. The coefficients with respect to a certain Cartesian coordinate system $\underline{e}_a$ are $U_{ab} = \underline{e}_a \cdot \underline{\underline{U}} \cdot \underline{e}_b$. The trace of a tensor is denoted by the operator 'tr'. Using 'tr', the double contraction of two second-rank tensors is defined by $\underline{\underline{U}} \cdot\cdot \underline{\underline{V}} = tr(\underline{\underline{U}} \cdot \underline{\underline{V}})$. For the scalar product another double contraction in the form $\underline{\underline{U}} : \underline{\underline{V}} = tr(\underline{\underline{U}} \cdot \underline{\underline{V}}^{\mathrm{T}})$ is used. Arranging second-rank tensor coefficients in a quadratic matrix is denoted by $[U_{ab}]$ or just $[U]$. Bold symbols indicate real-valued matrices regardless of where the coefficients arise from, e.g., $\mathbf{x} = [1, 2, 3, 4]^{\mathrm{T}}$ is a 4-tuple or column matrix.

2. Two-phase composite model

The fundamental assumption of the dislocation density based two-phase composite model of Estrin et al. (1998) and Mckenzie et al. (2007) is that a dislocation cell structure has already formed. Among the variety of reported dislocation configurations (Amodeo and Ghoniem, 1990a), cells are characterized by regions of lower dislocation density (the cell interior) surrounded by high dislocation density walls. The latter represent a topologically continuous skeleton (Mckenzie et al., 2007). Hence, the polycrystal can be thought of as a solid consisting of grains which again consist of dislocation cells. Because of the large difference in dislocation density, cell walls and the interior show different mechanical behavior. Thus, the solid can effectively be treated as a two-phase composite (Mughrabi, 1987). Whereas the effect of grain orientations can be incorporated by using crystal plasticity (e.g., Yalcinkaya et al., 2009), further modeling is necessary to take into account the two phases due to dislocation cells.

2.1. Outline of the existing model

The "unit cell" of the dislocation arrangement is a single cube with an edge length of d and a wall thickness of $w/2$.[2] The cell wall volume V_{w} over the total volume V_{t} yields the volume fraction f of cell walls:

[1] A detailed explanation for routes A, C, B_c, and E is given in Section 5.1.

[2] In some studies, spherical dislocation cells are assumed in order to simplify the stress computation (Sauzay, 2008; Brahme et al., 2011).