PAMM · Proc. Appl. Math. Mech. 11, 449 – 450 (2011) / DOI 10.1002/pamm.201110216

Dislocation Transport in Single Crystals and Dislocation-based Micromechanical Hardening

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The higher-dimensional kinematical dislocation continuum theory of Hochrainer (2006) and a homogenized version thereof by Hochrainer, Zaiser and Gumbsch (2010) are reviewed. A three-dimensional Finite Element solution of the homogenized theory is presented, interpreted physically and compared to the results of the Geometrically Necessary Dislocations theory.

Introduction

We start from the additive decomposition of the displacement gradient

$$\boldsymbol{H} = \text{grad}\,(\boldsymbol{u}) = \boldsymbol{H}^e + \boldsymbol{H}^p \tag{1}$$

into an elastic part $\boldsymbol{H}^e$, and the plastic distortion $\boldsymbol{H}^p$, which is assumed for small deformations. In the case of single slip characterized by the slip direction $\boldsymbol{d}$, the associated slip plane normal $\boldsymbol{n}$ and the plastic slip γ, the plastic distorsion is given by $\boldsymbol{H}^p = \gamma \boldsymbol{d} \otimes \boldsymbol{n}$, where, for convenience, we choose $\boldsymbol{d} = \boldsymbol{e}_1$ and $\boldsymbol{n} = \boldsymbol{e}_3$.
According to Nye (1953), the total Burgers vector $\boldsymbol{b}_t$ associated to a given area A can be related to the dislocation density tensor, defined as $\boldsymbol{\alpha} := \text{curl}\,(\boldsymbol{H}^p)$ by using Stokes' theorem

$$\boldsymbol{b}_t = \int_{\partial A} \boldsymbol{H}^p \cdot \,\mathrm{d}\boldsymbol{x} = \int_A \text{curl}^\mathsf{T}\,(\boldsymbol{H}^p)\;\,\mathrm{d}\boldsymbol{a} = \int_A \boldsymbol{\alpha}^\mathsf{T}\;\mathrm{d}\boldsymbol{a} \qquad \text{with curl}(\boldsymbol{H}^p) := \epsilon_{ijk}\partial_i H^p_{lj} \boldsymbol{e}_k \otimes \boldsymbol{e}_l \tag{2}$$

For the case of single slip, i.e. $\boldsymbol{H}^p = \gamma \boldsymbol{e}_1 \otimes \boldsymbol{e}_3$, the dislocation density tensor reduces to $\boldsymbol{\alpha}^\mathsf{T} = \text{curl}^\mathsf{T}\,(\boldsymbol{H}^p) = \boldsymbol{b} \otimes \boldsymbol{\kappa}$, where the Burgers vector $\boldsymbol{b}$ and the dislocation density vector $\boldsymbol{\kappa} := 1/\|\boldsymbol{b}\|\,(\partial_2 \gamma \boldsymbol{e}_1 - \partial_1 \gamma \boldsymbol{e}_2)$ have been introduced.
For the special case that nearby dislocations are parallel and of the same sign, $\boldsymbol{\kappa}$ can be expressed equivalently in terms of the total dislocation density (the total line length per unit volume) and the line direction of the dislocations $\boldsymbol{e}_l$ as $\boldsymbol{\kappa} = \rho_t \boldsymbol{e}_l$. Accordingly, the dislocation density can be deduced from $\boldsymbol{\alpha}$ or $\boldsymbol{\kappa}$. For this special case the evolution equation of $\boldsymbol{\alpha}$ is given by (Mura, 1963)

$$\dot{\boldsymbol{\alpha}} = -\text{curl}\,(\boldsymbol{\nu} \times \boldsymbol{\alpha})\,, \tag{3}$$

where $\boldsymbol{\nu}$ is the dislocation velocity.
While the density of Geometrically Necessary Dislocations (GNDs) is taken into account by $\boldsymbol{\alpha}$, Statistically Stored Dislocations (SSDs) are not represented in the aforementioned formulae. Hence, $\boldsymbol{\alpha}$ allows only for modeling an hardening due to an arrangement of dislocations with equal signs. Many models (e.g. Becker and Miehe, 2004; Evers et al., 2004) propose a supplementary modeling of the density of SSDs (Fig. 1) based on classical local dislocation density models (e.g. Essmann and Mughrabi, 1979). Due to their locality, these SSD-models can generally not reproduce a spatial transport of dislocations.

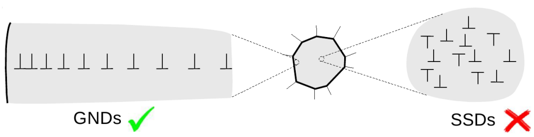

Fig. 1 Schematical representation of a dislocation pile-up and a typical SSD-configuration; while the first mechanism is well-represented through $\boldsymbol{\alpha}$, the SSDs are "invisible" using this dislocation desity measure.

The higher-dimensional dislocation density tensor

Hochrainer (2006) generalized the results (2) and (3) based on a higher-dimensional representation of discrete dislocations. This concept is discussed here in the case of plane dislocations which are virtually lifted according to their line orientation φ (the angle between the line tangent vector $\boldsymbol{e}_l$ and $\boldsymbol{e}_1$, Fig. 2). It can be verified that the slope of the lifted line is equal to the curvature k of the dislocations. Hochrainer (2006) introduced the higher-dimensional dislocation density tensor $\boldsymbol{\alpha}^{II}$ associated to the space $\{x, y, \varphi\}$ as a direct generalization of the dislocation density tensor $\boldsymbol{\alpha}$. For the special case where nearby lifted curves are parallel (i.e. they share the same curvature) it is obvious that equation (3) can be generalized the higher-dimensional case yielding the formally equivalent evolution equation for $\boldsymbol{\alpha}^{II}$ (it should be noted that this generalization is also possible in other cases, see Hochrainer (2006), p. 69).

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Hochrainer (2006) showed, that the higher-dimensional dislocation density tensor $\boldsymbol{\alpha}^{II}$ is completely defined by the density $\rho(\boldsymbol{x}, \varphi, t)$ and the curvature $k(\boldsymbol{x}, \varphi, t)$ based on a higher-dimensional generalization (see Fig. 2) of $\boldsymbol{\alpha}^{\mathsf{T}} = \boldsymbol{b} \otimes \boldsymbol{\kappa}$ (underscores denote matrices, single and double underscores correspond to vectors and matrices, respectively)

$$\underline{\underline{\boldsymbol{\alpha}}}^{II^{\mathsf{T}}}(\boldsymbol{x}, \varphi, t) \;:=\; \underline{\boldsymbol{b}}\,\underline{\boldsymbol{\kappa}}^{II^{\mathsf{T}}}(\boldsymbol{x}, \varphi, t)\,, \tag{4}$$

with $\underline{\boldsymbol{\kappa}}^{II} = \rho\,(\boldsymbol{x}, \varphi, t)\,\underline{\boldsymbol{e}}_L$, $\underline{\boldsymbol{e}}_L\,(\boldsymbol{x}, \varphi, t) = [\cos(\varphi), \sin(\varphi), k\,(\boldsymbol{x}, \varphi, t)]^{\mathsf{T}}$.
For a given dislocation velocity $\nu(\boldsymbol{x}, \varphi, t)$ and introducing the angular velocity $\vartheta := -\boldsymbol{e}_l \cdot \mathrm{grad}\,(\nu) - k\,\partial_\varphi \nu$, the higher-dimensional evolution equations

$$\partial_t \rho \;=\; -\mathrm{div}\,(\rho \boldsymbol{\nu}) - \partial_\varphi\,(\rho \vartheta) + \rho k \nu, \tag{5}$$

$$\partial_t k \;=\; -k^2 \nu + \boldsymbol{e}_l \cdot \mathrm{grad}\,(\vartheta) + k \partial_\varphi \vartheta - \boldsymbol{\nu} \cdot \mathrm{grad}\,(k) - \vartheta\,\partial_\varphi k \tag{6}$$

for the dislocation density and curvature can be derived from the evolution equation of $\boldsymbol{\alpha}^{II}$ (Hochrainer, 2006).

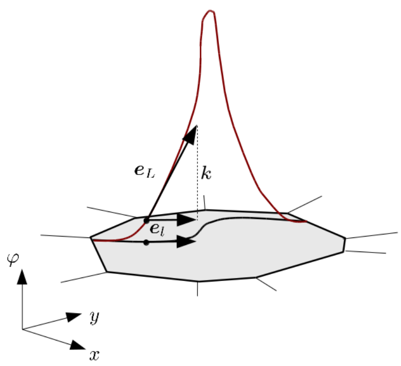

Fig. 2 A plane dislocation (black) and its higher-dimensional counterpart (red)

The simplified theory

Hochrainer, Zaiser and Gumbsch (2010) introduced the homogenized quantities $\rho_t\,(\boldsymbol{x}, t) := \int_0^{2\pi} \rho\,\mathrm{d}\varphi$ and $\overline{\rho k}(\boldsymbol{x}, t) := \int_0^{2\pi} \rho k\,\mathrm{d}\varphi$ and derived the associated evolution equation for ρ_t for an isotropic dislocation velocity

$$\partial_t \rho_t = -\mathrm{div}\left(\nu \boldsymbol{\kappa}^{\perp}\right) + \overline{\rho k}\nu, \text{ where } \boldsymbol{\kappa}^{\perp} := \kappa_2 \boldsymbol{e}_1 - \kappa_1 \boldsymbol{e}_2, \quad \partial_t \overline{\rho k} = -\mathrm{div}\left(\frac{\overline{\rho k}}{\rho_t} \nu \boldsymbol{\kappa}^{\perp}\right) - \frac{1}{2}\mathrm{div}\,(\rho_t \mathrm{grad}\,(\nu))\,. \tag{7}$$

The second evolution equation for $\overline{\rho k}$ is derived based on additional assumptions (see Hochrainer, Zaiser and Gumbsch, 2010). This model was numerically implemented and validated by discrete dislocation simulations by Sandfeld et al. (2011).
Fig. 3 shows new FE-simulation results of the simplified theory and a comparison to the GND theory for a cuboid single crystal ($3 \times 3 \times 1.5\,\mu$m). The plastic slip γ and the dislocation density ρ_t are kinematically coupled by Orowan's equation $\dot{\gamma} = \rho_t b \nu$. The plastic slip at the boundary is zero (micro-hard boundary conditions). We start from initial conditions $\rho_t(\boldsymbol{x}, t = 0) = 450\,\mu\mathrm{m}^{-2}$ and $k(\boldsymbol{x}, t = 0) = 16.7\,\mu\mathrm{m}^{-1}$ which corresponds to small (related to the size of the specimen) homogeneously distributed smeared dislocation loops.
The simulation results can be interpreted as follows: due to the micro-hard boundaries the dislocation velocity and the related plastic slip rate reach their maximum in the bulk.
The growth of the initially small smeared dislocation loops leads to an increase of the dislocation denstity ρ_t mainly in the bulk (Fig. 3, left). The GND-density at that time is small, thus the total dislocation density ρ_t is almost completely statistically stored. The initially small smeared bulk-dislocation loops keep growing and travel through the single crystal to the boundary where they build pile-ups, i.e. they transform from basically statistically stored to predominantly Geometrically Necessary Dislocation density. Comparing the final state, where ρ_t is dominated by GNDs, to the GND density computed from the gradient of the plastic slip (Fig. 3, right) the results are in good quantitative agreement. It can be concluded that in the final state the fraction of the SSDs is small compared to the GNDs.

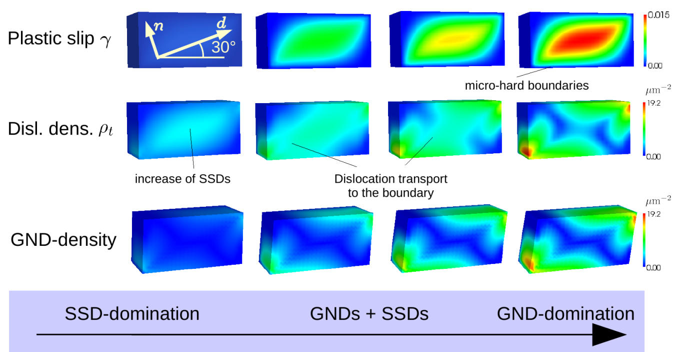

Fig. 3 FE-Simulation of the simplified kinematical theory and comparison with GND-theory. Only the backmost half of the single crystal is represented to visualize the fields in the single crystal.

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