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Plastic flow and dislocation strengthening in a dislocation density based formulation of plasticity

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ABSTRACT

Modeling dislocation interaction on a mesoscopic scale is an important task for the description of flow stress and strain hardening in a continuum model. In dislocation based continuum theories, different flow stress formulations are commonly used in the literature. They are usually based on the average dislocation spacing related to the square root of dislocation density, but differ in their degree of homogenization of dislocation interactions, namely whether only total dislocation density is considered in a Taylor term or whether an interaction matrix is used. We analyze the impact of both terms in different crystal orientations as well as homogeneously and inhomogeneously distributed initial dislocation densities. In the dislocation based continuum formulation used here, both terms act as a short-range stress additionally to the "mean field" long-range stress field of elastic dislocation interaction. We demonstrate that the simplifying assumption of an average over all possible interaction types is a reasonable reduction of complexity in high symmetry systems with homogeneous density distribution. However, we also demonstrate that under specific boundary conditions and for inhomogeneities between slip systems a significantly different density evolution is obtained on slip systems with similar Schmid-factors, when considering different interaction strengths for different types of dislocation interaction. This is in agreement with findings in discrete dislocation dynamics simulations in the literature.

1. Introduction

In classical, macroscopic continuum models, flow stress and strain hardening are usually provided by phenomenological parameters based on experimental data. Thus, the material behavior is determined by parameters, which are only valid on the macroscopic scale. It is well known, that continuum models based on these macroscopic parameters are not able to account for microscopic effects such as size effects. Flow stress and strain hardening are input parameters to such models and cannot be considered as a predictive outcome. Physically, dislocation interaction processes and obstacle interactions can be made responsible for the macroscopically measurable flow stress and strain hardening.

Various formulations exist which enhance classical macroscopic approaches by microscopic considerations. One example are strain gradient plasticity models, e.g. [1–5], which apply a critical yield stress and a flow rule according to a work hardening rate. Although the formulations show good results in a certain regime, the models are based on a rather phenomenological top-down approach. Thus the interpretation of these models is often limited to the specific system they intend to represent.

In contrast to that, other approaches to continuum formulations are derived bottom-up by homogenizing discrete dislocation lines and their interactions [6–9]. These models formulate flow stress and strain hardening by physical considerations like the classical Taylor interaction stress [10], which relates a local interaction stress to the mean dislocation distance given as the inverse of the square root of the dislocation density ρ:

$$\tau_{\mathrm{fl},s} = \alpha\mu b\sqrt{\rho} \tag{1}$$

Here, μ is the shear modulus, b is the Burgers vector, and α is a constant factor of 0.35 ± 0.15 [11]. An extended Taylor relation has been developed by Franciosi et al. [12]

$$\tau_{\mathrm{fl},s}^{\mathrm{mat}} = \mu b\sqrt{\sum_j a_{sj}\rho_j} \tag{2}$$

accounting for an individual interaction stress on a slip system s based on the interaction strengths between different slip systems j by pairing coefficients a_{sj} and therefore distinguishing between different slip systems, that lead to different dislocation reactions. In contrast to the factor α in the Taylor term, which is dependent on the mode of deformation, see [13], the coefficients a_{sj} in the enhanced term have been

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determined as an interaction matrix by discrete dislocation dynamics (DDD) simulations [14–16].

Even though the classical Taylor interaction stress is still a commonly used formulation due to its simplicity using the total dislocation density and combining all possible interactions between slip systems into one coefficient, it has already been shown in 2d single slip, that such a formulation can oversimplify the local processes in a microstructure [17]. The formulation by Franciosi et al. has been applied and further extended e.g. by [18], who replace the self-hardening coefficients with more physical considerations. A mean free path model incorporating dislocation storage and recovery, as well as the influence of line-tension effects on the interaction constants has been presented in [19,20]. Further investigation of the flow stress and interaction of slip systems in continuum theories has been done by considering obstacle dislocations [21] and dipoles [22].

Although models incorporating the "Franciosi term" in crystal plasticity frameworks, as e.g. [18,19,23], have shown accurate results compared to experiments, both, the Taylor term and the Franciosi term, are still commonly used in their basic form in parallel in the literature. A thorough comparison of both formulations is still missing. However, in order to state the reduction of complexity in a continuum model as central objective, it is a necessity to know in which configurations a simplification is adequate without losing physicality.

Comparing the Taylor term and the Franciosi term, a difference in the microstructural behavior is expected if the system is dominated by a specific type of interaction. It has been shown with DDD-simulations, that the collinear reaction leads to a very strong interaction of the respective slip systems and essentially prevents the activation of two slip systems sharing the same Burgers vector [24,25]. Since the key parameter determining the interaction stress in the considered formulations is the dislocation density, a difference in interaction stress can occur, if the density is inhomogeneously distributed between the different slip systems.

In this paper, we compare both interaction stress formulations in their basic form. Incorporated in a dislocation density based continuum formulation, we use a set of simple example systems to analyze the dislocation density evolution and the impact of the interaction stress terms with respect to different initial density distributions and systems showing homogeneous as well as heterogeneous density evolutions due to their Schmid factors or microstructural constraints. Starting with most simple configurations leading to an inhomogeneous density distribution, we focus on the effect of collinear reactions in a system setup with just two active slip systems, as in [24]. Then, we extend the analysis to a full fcc single crystal with 12 slip systems. We show, that the classical Taylor interaction stress produces reasonable results when assuming a homogeneous density distribution under ideal loading conditions. Averaging all occurring interactions into a single factor can be adequate if the system behavior is not dominated by a specific interaction or stabilized in high symmetry configurations. However, using the Franciosi relation, even small variations of the resolved shear stress or initial density lead to a distinctive density evolution on slip systems originating from the collinear interaction coefficient. Such a behavior is in agreement with DDD-simulations [24] and has been proposed as a possible explanation for the strong orientation dependency of certain load orientations [20,24]. For a continuum theory, trying to mimic such a configuration using the classical Taylor relation, leads to an oversimplification of the complex interactions involved. In contrast, the stronger influence of specific interaction mechanisms in the Franciosi relation allow for a deformation behavior, which can be significantly different to the Schmid law.

2. Method

2.1. Dislocation based continuum model

We consider a dislocation based continuum formulation of crystal plasticity based on the classical decomposition of the distortion tensor into an elastic and a plastic part

$$\mathrm{D}\mathbf{u} = \boldsymbol{\beta}^{\mathrm{pl}} + \boldsymbol{\beta}^{\mathrm{el}}. \tag{3}$$

The plastic slip γ_s is the result of dislocation motion on N slip systems defined by the index s, the orthonormal basis $\{\mathbf{d}_s,\mathbf{l}_s,\mathbf{m}_s\}$ and the Burger's vector $\mathbf{b}_s = b_s\mathbf{d}_s$. Therefore, the plastic distortion $\boldsymbol{\beta}^{\mathrm{pl}}$ consists of the sum of the plastic slip over all slip systems

$$\boldsymbol{\beta}^{\mathrm{pl}} = \sum_{s=1}^{N} \gamma_s \mathbf{d}_s \otimes \mathbf{m}_s. \tag{4}$$

The evolution of the plastic slip is given by the Orowan equation

$$\partial_t\gamma_s = \partial_t v_s b_s \rho_s \tag{5}$$

where ρ_s is the dislocation density and v_s the velocity on the individual slip system. Regarding the density evolution, we use the Continuum Dislocation Dynamics (CDD) equations introduced by [6]

$$\begin{aligned}
\partial_t\rho_s &= -\nabla\cdot(v_s\boldsymbol{\kappa}_s^{\perp}) + v_s q_s \qquad \text{with} \qquad \boldsymbol{\kappa}_s^{\perp} = \boldsymbol{\kappa}_s \times \mathbf{m}_s\\
\partial_t\boldsymbol{\kappa}_s &= \nabla \times (\rho_s v_s \mathbf{m}_s)\\
\partial_t q_s &= -\nabla\cdot\left(\frac{q_s}{\rho_s}\boldsymbol{\kappa}_s^{\perp} v_s + \frac{1}{2|\boldsymbol{\kappa}_s|^2}\left((\rho_s + |\boldsymbol{\kappa}_s|)\boldsymbol{\kappa}_s \otimes \boldsymbol{\kappa}_s - (\rho_s - |\boldsymbol{\kappa}_s|)\boldsymbol{\kappa}_s^{\perp} \otimes \boldsymbol{\kappa}_s^{\perp}\right)\nabla v_s\right),
\end{aligned} \tag{6}$$

where $\boldsymbol{\kappa}_s$ denotes the vector of the geometrically necessary dislocations (GND-density) and q_s the curvature density. We assume a linear dependency on the resolved shear stress on each slip system τ_s, thus the equations can be closed by the velocity law

$$v_s = \frac{b_s}{B}\tau_s \qquad \text{with} \qquad \tau_s = \tau_{\mathrm{ext},s} + \tau_{\mathrm{int},s} \tag{7}$$

where B denotes a friction stress of 5×10^{-5} Pa s. $\tau_{\mathrm{ext},s}$ includes stresses induced by external loading resolved on the slip system, whereas $\tau_{\mathrm{int},s}$ accounts for internal stresses induced by dislocations. Regarding $\tau_{\mathrm{int},s}$, we distinguish between long- and short-range stresses in the continuum model. In order to represent long-range stress fields, we consider a mean field approach as given in [26] resulting in the "mean field stress" $\tau_{\mathrm{mf},s}$. Since the mean field stress is proportional to $\int \kappa$, it accounts for the contribution of the slip on a specific slip system to the long-range stress field on all slip systems. However, the mean field stress disappears in configurations of statistically stored dislocations and neglects interactions of dislocation densities inside an averaging volume. Thus, it delivers no information about the strength of the physical interaction and reactions between different slip systems.

To solve this problem, additional stress formulations are used to describe the interaction between slip systems within one averaging volume. We consider the "Taylor term" according to Eq. (1), which relates the interaction stress to the square root of the total density averaged over all slip systems within one averaging element. Thus, the interaction stress is the same on all slip systems and all possible interaction types are concentrated into the parameter α. In this study, we choose $\alpha = 0.35$, unless otherwise stated. In addition, the "Franciosi term" according to Eq. (2) is incorporated into the formulation, which summarizes the interaction strengths of each individual slip system pairing, a_{sj}, multiplied by the density of the respective slip system ρ_j. Thereby, the different interaction mechanisms are considered separately, which in general leads to different interaction stresses on different slip systems. Regarding the interaction strengths a_{sj}, we consider the interaction matrix according to [14]. For the self-interaction and coplanar cases, i.e. $j = s$ and $j = s \pm 1$, we chose the Lomer coefficient given as 0.122 [20].

The Taylor term as well as the Franciosi term act on the velocity of each slip system. Therefore the velocity law can be derived as

$$v_s = \begin{cases} \frac{b_s}{B}(|\tau_s| - \tau_{\mathrm{fl}})\,\mathrm{sign}\tau_s & \text{if } |\tau_s| > \tau_{\mathrm{fl}}\\ 0 & \text{if } |\tau_s| \leqslant \tau_{\mathrm{fl}} \end{cases} \tag{8}$$