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# Predicting intragranular misorientation distributions in polycrystalline metals using the viscoplastic self-consistent formulation

Miroslav Zecevic [a, b], Wolfgang Pantleon [c], Ricardo A. Lebensohn [b], Rodney J. McCabe [b], Marko Knezevic [a, *]

[a] Department of Mechanical Engineering, University of New Hampshire, Durham, NH, 03824, USA
[b] Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM, 87544, USA
[c] Department of Mechanical Engineering, Technical University of Denmark, Produktionstorvet 425, 2800, Kgs. Lyngby, Denmark

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ABSTRACT

In a recent paper, we reported the methodology to calculate intragranular fluctuations in the instantaneous lattice rotation rates in polycrystalline materials within the mean-field viscoplastic self-consistent (VPSC) model. This paper is concerned with the time integration and subsequent use of these fluctuations to predict orientation-dependent misorientation distributions developing inside each grain representing the polycrystalline aggregate. To this end, we propose and assess two approaches to update the intragranular misorientation distribution within the VPSC framework. To illustrate both approaches, we calculate intragranular misorientations in face-centered cubic polycrystals deformed in tension and plane-strain compression. These predictions are tested by comparison with corresponding experiments for polycrystalline copper and aluminum, respectively, and with full-field calculations. It is observed that at sufficiently high strains some grains develop large misorientations that may lead to grain fragmentation and/or act as driving forces for recrystallization. The proposed VPSC-based prediction of intragranular misorientations enables modeling of grain fragmentation, as well as a more accurate modeling of texture using a computationally efficient mean-field approach, as opposed to computationally more expensive full-field approaches.



## 1. Introduction

During forming operations, polycrystalline metals are subjected to shape changes and plastic deformation that result in highly heterogeneous micromechanical fields (stress and strain fields) in the material [1]. It is well known that dislocation glide accommodates most of the imposed plastic deformation at the level of single grains. Crystallographic slip is potentially associated with local lattice rotations, which in turn induce anisotropy in the mechanical response by texture evolution and microstructure formation. Additionally, intra- and intergranular heterogeneities develop in the material, playing an important role in determining the deformation and hardening behavior, as well as the subsequent grain fragmentation and recrystallization of the deformed microstructure.

Intragranular orientation spreads have been related to the formation of transition bands, which are favorable places for recrystallization nucleation [2,3]. In addition, recrystallization nuclei forming near grain boundaries may have quite different crystallographic orientation compared to the average grain orientation due to large orientation variations developed across the grains [3,4]. Therefore, accurate predictions of intragranular orientation distributions are crucial to model recrystallization processes. Furthermore, such misorientation predictions can improve the modeling of deformation textures and provide a physical basis for grain fragmentation.

Plastic deformation of polycrystalline metals is usually modeled using either full-field or mean-field approaches. Full-field models, for example, can be based on the crystal plasticity finite element (CPFE) method [5–9] or on the spectral fast Fourier transform

* Corresponding author. University of New Hampshire, Department of Mechanical Engineering, 33 Academic Way, Kingsbury Hall, W119, Durham, NH, 03824, USA.
*E-mail address:* marko.knezevic@unh.edu (M. Knezevic).

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(FFT)-based approach of Moulinec and Suquet [10], extended to polycrystals by Lebensohn [11]. These models are able to predict local micromechanical fields, including intragranular orientation gradients, resulting from grain-to-grain interactions, at the expense of a relatively high computational cost. Among mean-field models, self-consistent schemes, originally conceived for linear problems [12] and later extended to non-linear material's behavior [13–16], are widely used for simulating plastic deformation of polycrystalline materials considering grain interaction in an average sense. These non-linear homogenization-based models are computationally efficient, but most of them use information on first moments of the intragranular fields only, for the definition of a material with linearized behavior on which the self-consistency is actually imposed. In the last two decades, improved homogenization techniques have been developed that also take into account second moments of the micromechanical fields to define an optimized linearization [17,18]. However, until very recently this available information on second moments of the intragranular fields had not been used in calculations of intragranular misorientation spreads.

There have been numerous phenomenological attempts to predict the development of intragranular orientation spreads without the use of computationally expensive full-field approaches. Berveiller et al. [19] divided grains into homogeneous regions where plastic deformation occurred by single or multiple slip. They showed that these regions developed quite different orientations upon plastic deformation, indicating the formation of an orientation spread. Bolmaro et al. [20] represented each grain within the viscoplastic self-consistent (VPSC) model by two fragments to which random neighbors were assigned. Co-rotation of grain fragments and their respective neighbors was assumed, resulting in the development of local misorientation between fragments. This model was later used to initialize the local states to drive a recrystallization model [21]. The idea of co-rotation in VPSC was further extended by Ref. [22], representing each grain by six fragments, each one co-rotating with its own neighbor. In a similar approach developed by Toth et al. [23], a Taylor-type polycrystal model was used, in which each grain was divided into two regions, one at the center of the grain and another close to grain boundaries. In the latter, rotation was impeded by "friction" with the surrounding medium. Due to the difference in rotation between the two regions, lattice curvature was predicted and in turn used in a fragmentation model. Raabe [24] estimated the intragranular misorientation by assuming one part of the grain was next to a hard grain and thus deformed according to the Taylor model, while another part had a soft neighbor and consequently deformed according to the Sachs model. In Ref. [2] rotation rate fields were analyzed to determine the divergent and convergent orientations under different applied strains. A similar idea was developed by Raabe et al. [25] where the divergence of the rotation rate field was used to determine which orientations would be prone to develop strong orientation differences. Lee and Duggan [26] used an intragranular deformation banding model within the Taylor framework to simulate rolling textures of copper. A similar model was later used by Leffers [27] for simulating microstructure development in rolled aluminum. Butler and McDowell [28] introduced additional plastic rotations within the Taylor model to account for accumulation of geometrically necessary dislocations related to grain subdivision. In recent work Guo and Seefeldt [29] have used VPSC to model formation of reorientation bands and resulting grain fragmentation, caused by slip bands in neighboring grains. Slip rate within slip band for slip system $s$ was assumed to be proportional to mean slip rate value within grain and the coefficient of proportionality was assumed to be a fitting parameter. A majority of the described approaches have been introduced to improve texture predictions and to allow incorporation of the effect of grain fragmentation. Detailed analysis of the orientation spreads for a large number of grains and comparison with experimental measurements were generally missing in the aforementioned approaches.

In this work, the widely-used VPSC model [15] is extended to calculate intragranular misorientation spreads. The VPSC model is able to provide intragranular second moments of stress and strain rate fields [30,31]. In turn, this information can be used to calculate second moments of the rotation rates within individual grains [32]. In this paper, the latter information is further utilized to calculate corresponding intragranular misorientation spreads. In doing so, we formulate two algorithms to predict accumulation of intragranular misorientations based on time integration of first and second moments of the rotation rate fields. The two approaches are applied to uniaxial tension of copper and plane-strain compression of aluminum. The predictions are compared with experimental measurements and also with predictions using the full-field viscoplastic FFT-based (VPFFT) model. Considering the approximations involved in the formulation of the proposed mean-field model, reasonable agreement with experiments and the VPFFT model predictions is demonstrated for both approaches.

## 2. Modeling framework

In what follows we provide a short summary of the VPSC model, including the expressions to calculate second moments of the micromechanical fields in the grains. In our notation, tensors are denoted by bold letters while scalars and tensor components are indicated in italics and not bold. The contracted product and the tensor product between two tensors are denoted by ":" and "⊗", respectively. The constitutive relationship between the viscoplastic strain rate, $\dot{\boldsymbol{\varepsilon}}$, and the deviatoric stress, $\boldsymbol{\sigma}$, at material point $\mathbf{x}$ is given by the rate-sensitivity equation:

$$\dot{\boldsymbol{\varepsilon}}(\mathbf{x}) = \sum_s \dot{\gamma}^s(\mathbf{x})\mathbf{m}^s(\mathbf{x}) = \dot{\gamma}_0 \sum_s \left(\frac{\boldsymbol{\sigma}(\mathbf{x}) : \mathbf{m}^s(\mathbf{x})}{\tau_c^s(\mathbf{x})}\right)^n \operatorname{sign}(\boldsymbol{\sigma}(\mathbf{x}) : \mathbf{m}^s(\mathbf{x}))\mathbf{m}^s(\mathbf{x}). \quad (1)$$

The constitutive parameters $\tau_c^s$, $\dot{\gamma}_0$, and $n$ are the critical resolved shear stress of slip system $s$, a reference shear rate, and the inverse of the rate sensitivity; $\dot{\gamma}^s$ is the shear rate and $\mathbf{m}^s$ is the symmetric part of the Schmid tensor, given by:

$$\mathbf{m}^s(\mathbf{x}) = \frac{1}{2}\left(\mathbf{b}^s(\mathbf{x}) \otimes \mathbf{n}^s(\mathbf{x}) + \mathbf{n}^s(\mathbf{x}) \otimes \mathbf{b}^s(\mathbf{x})\right), \quad (2)$$

with $\mathbf{n}^s$ and $\mathbf{b}^s$ denoting, respectively, the slip plane normal and the Burgers vector of slip system $s$.

The plastic *spin*, $\dot{\boldsymbol{\omega}}^p$, at material point $\mathbf{x}$ is given by:

$$\dot{\boldsymbol{\omega}}^p(\mathbf{x}) = \sum_s \dot{\gamma}^s(\mathbf{x})\boldsymbol{\alpha}^s(\mathbf{x}), \quad (3)$$

where $\boldsymbol{\alpha}^s(\mathbf{x}) = \frac{1}{2}(\mathbf{b}^s(\mathbf{x}) \otimes \mathbf{n}^s(\mathbf{x}) - \mathbf{n}^s(\mathbf{x}) \otimes \mathbf{b}^s(\mathbf{x}))$ is the antisymmetric part of the Schmid tensor of slip system $s$. By performing linearization of the nonlinear constitutive relationships, we obtain the following expressions:

$$\dot{\boldsymbol{\varepsilon}}(\mathbf{x}) = \mathbf{M}^{(r)} : \boldsymbol{\sigma}(\mathbf{x}) + \dot{\boldsymbol{\varepsilon}}^{0(r)}, \quad (4)$$

$$\dot{\gamma}^s(\mathbf{x}) = \eta^{s(r)}\tau^s(\mathbf{x}) + \dot{g}^{0s(r)}, \quad (5)$$

where $\tau^s(\mathbf{x}) = \mathbf{m}^s(\mathbf{x}) : \boldsymbol{\sigma}(\mathbf{x})$ is the resolved shear stress on slip