Acta Materialia 104 (2016) 228–236

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Average intragranular misorientation trends in polycrystalline materials predicted by a viscoplastic self-consistent approach

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ARTICLE INFO

Article history:
Received 15 October 2015
Accepted 23 October 2015
Available online 15 December 2015

Keywords:
Polycrystal plasticity modeling
Micromechanics
Misorientation
Texture
Recrystallization

ABSTRACT

This work presents estimations of average intragranular fluctuations of lattice rotation rates in polycrystalline materials, obtained by means of the viscoplastic self-consistent (VPSC) model. These fluctuations give a tensorial measure of the trend of misorientation developing inside each single crystal grain representing a polycrystalline aggregate. We first report details of the algorithm implemented in the VPSC code to estimate these fluctuations, which are then validated by comparison with corresponding full-field calculations. Next, we present predictions of average intragranular fluctuations of lattice rotation rates for cubic aggregates, which are rationalized by comparison with experimental evidence on annealing textures of fcc and bcc polycrystals deformed in tension and compression, respectively, as well as with measured intragranular misorientation distributions in a Cu polycrystal deformed in tension. The orientation-dependent and micromechanically-based estimations of intragranular misorientations that can be derived from the present implementation are necessary to formulate sound sub-models for the prediction of quantitatively accurate deformation textures, grain fragmentation, and recrystallization textures using the VPSC approach.

1. Introduction

The 1-site viscoplastic (VP) self-consistent (SC) theory [1,2] is a continuum-level, microstructure-sensitive polycrystal plasticity formulation that has been widely adopted by the Mechanics of Materials community for computing the mechanical behavior, texture and microstructure evolution of polycrystalline materials. The VPSC code [3] is nowadays extensively used to simulate plasticity of polycrystalline aggregates based on the knowledge of deformation mechanisms at the single crystal level and validated by experiments on metals, minerals and polymers. Beyond numerous applications involving single material point calculations for simple geometries and boundary conditions, VPSC has recently been adapted to account for microstructural effects in multiscale calculations either by coupling it directly with Finite Elements (FE) (e.g. Ref. [4]) or by using VPSC-based fitting of anisotropic yield functions for subsequent use in the FE analysis (e.g. Ref. [5]). These new developments greatly expanded the scope of applications of the model.

VPSC balances efficiency—the number of degrees of freedom of the model, given by the number of mechanical phases, i.e. single crystal orientations or "grains" representing the polycrystal, typically does not exceed a few thousand; representativity—the predicted mechanical response is statistically representative of a large volumetric average over the aggregate; and ability to capture the underlying physical mechanisms of plastic deformation—geometry, activation and hardening of slip and twinning, texture and grain morphology-induced anisotropy, etc. For these reasons, VPSC is usually the best compromise compared with the more efficient but simplistic iso-strain Taylor formulation, and the fully space-resolved but more computational intensive full-field crystal plasticity (CP) formulations like CP-FEM (e.g. Ref. [6]) or FFT-based formulations (e.g. VPFFT [7,8]). There are, however, known limitations of the standard VPSC formulation, some of which have been mitigated at the expense of more sophisticated theoretical approaches and numerical implementations.

One of these limitations is related to the necessary approximation involved in applying the SC formulation to non-linear material behavior. The SC theory was originally formulated for linear elastic materials [9]. For non-linear aggregates deforming in the viscoplastic regime, several differing SC approximations are used to

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http://dx.doi.org/10.1016/j.actamat.2015.10.035
1359-6454/Published by Elsevier Ltd on behalf of Acta Materialia Inc.

linearize the non-linear mechanical behavior at the single crystal level. First-order SC formulations (known as secant [10], tangent [2], and affine [11] approximations) are based on linearization schemes that make use of relations between average field quantities only, disregarding higher-order statistical information of the micromechanical fields inside the mechanical phases. This assumption has been proven to be questionable [12–14], especially when strong directionality and large variations in local properties are expected, like in the cases of low rate-sensitivity materials, aggregates made of highly anisotropic grains, and multiphase polycrystals. In these cases, strong deformation gradients are likely to develop inside grains and the use of first moments of the micromechanical field distributions to linearize the behavior at single crystal level is insufficient. To overcome this limitation, a more accurate non-linear homogenization method, Ponte Castañeda's second-order approach [15,16], based on a linearization scheme that incorporates information on the second moments (average fluctuations) of the field distributions in each mechanical phase, has been added to VPSC [14]. A key aspect of this extension has been the implementation of an algorithm to calculate second moments of the stress field distribution inside each representative grain drawing upon [17–19], which is now available in the VPSC code [3].

Another limitation of the standard VPSC formulation is related to the fact that only the average values (first moments) of the micromechanical fields inside the mechanical phases are used to update the microstructure. In particular, the average lattice rotation calculated for each grain is applied to update its average orientation after each deformation increment, and the evolution of deformation texture is based on these average orientation updates. This approximation, which neglects the progressive build-up of intragranular orientation dispersion, has two deleterious effects on the quality of the predicted texture and microstructure evolution. First, the predicted deformation textures are systematically sharper than the experimental textures (e.g. Refs. [7,20]). This becomes a concern especially when the VPSC model is intended to quantitatively describe texture-induced anisotropy, e.g. in coupled FE-VPSC multiscale calculations. Second, since intragranular misorientation is not accounted for, phenomena like grain size reduction by grain fragmentation, and other important mechanisms affecting microstructure evolution that are driven in part by local lattice misorientation like recovery and recrystallization cannot be predicted based on strictly micromechanical considerations. Different ad-hoc, highly empirical models have been proposed to supplement VPSC calculations to predict smoother textures (e.g. Ref. [21]), grain fragmentation (e.g. Ref. [22]) and recovery and recrystallization (e.g. Ref. [23]).

In this work we demonstrate how the numerically tractable problem of estimating average fluctuations of the stress field distribution inside each mechanical phase, already implemented in the VPSC code as part of the second-order linearization procedure, can be used to calculate the corresponding second moments of the lattice rotation rate field in each grain.

In this initial contribution, we report the algorithm to calculate these average lattice rotation rate fluctuations in detail, and present results on axisymmetric deformation of cubic polycrystals. These are compared with experimental annealing textures of fcc and bcc polycrystals deformed in tension and compression, respectively, as well as with measured intragranular misorientation distributions in Cu polycrystals deformed in tension. In a future contribution [24], estimations of intragranular misorientations derived from these average fluctuations in lattice rotation rate will be applied to formulate sound models for the prediction of quantitatively accurate deformation textures, grain fragmentation, and recrystallization textures.

2. Model

In what follows, the inner products and the outer product between two tensors are denoted by ":" (twice contracted), "::" (four times contracted), and "⊗", respectively. The viscoplastic constitutive behavior at each material point **x** deforming by slip is described by means of the following non-linear equation:

$$\dot{\varepsilon}(\mathbf{x}) = \sum_k m^k(\mathbf{x})\dot{\gamma}^k(\mathbf{x}) = \dot{\gamma}_o \sum_k m^k(\mathbf{x}) \left(\frac{m^k(\mathbf{x}) : \sigma(\mathbf{x})}{\tau_o^k(\mathbf{x})}\right)^n \mathrm{sgn}\left(m^k(\mathbf{x}) : \sigma(\mathbf{x})\right) \quad (1)$$

where τ_o^k is the threshold resolved shear stress of slip system (k) (adopted to have a value 1 in arbitrary stress units, in all calculations that follow), $m_{ij}^k = \frac{1}{2}(n_i^k b_j^k + n_j^k b_i^k)$ is the symmetric Schmid tensor associated with slip system (k), where n^k and b^k are the normal and Burgers vector direction of such slip system, and $\dot{\varepsilon}$ and σ are the deviatoric strain rate and stress. The local shear rate on slip system (k), $\dot{\gamma}^k$, is given by:

$$\dot{\gamma}^k(\mathbf{x}) = \dot{\gamma}_o \left(\frac{\tau^k(\mathbf{x})}{\tau_o^k(\mathbf{x})}\right)^n \mathrm{sgn}\left(\tau^k(\mathbf{x})\right) = \dot{\gamma}_o \left(\frac{m^k(\mathbf{x}) : \sigma(\mathbf{x})}{\tau_o^k(\mathbf{x})}\right)^n \mathrm{sgn}\left(m^k(\mathbf{x}) : \sigma(\mathbf{x})\right) \quad (2)$$

where τ^k is the resolved shear stress on slip system (k), $\dot{\gamma}_o$ is a normalization factor (adopted to be 1 s^{-1} in all calculations that follow), and the stress exponent n is the inverse of the rate-sensitivity. If the shear rates are known, the lattice rotation rate or plastic spin associated with slip activity at single crystal material point **x** is given by:

$$-\dot{\omega}^p(\mathbf{x}) = -\sum_k \alpha^k(\mathbf{x})\dot{\gamma}^k(\mathbf{x}) \quad (3)$$

where $\alpha_{ij}^k = \frac{1}{2}(n_i^k b_j^k - n_j^k b_i^k)$ is the antisymmetric Schmid tensor.

Let us assume linear relations as approximations of the actual non-linear relations, Eqs. (1) and (2), in the mechanical phase (r):

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

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

where the moduli $M^{(r)}$ and $\dot{\varepsilon}^{o(r)}$ are the compliance and back-extrapolated strain rate (strain rate under zero stress) of grain (r), respectively, and $\eta^{k(r)}$ and $\dot{g}^{ok(r)}$ are the slip-level compliance and back-extrapolated shear rate, respectively. Depending on the linearization assumption, the above moduli can be chosen differently. For example, under the affine linearization the moduli are given by:

$$M^{(r)} = n\dot{\gamma}_o \sum_k \frac{m^{k(r)} \otimes m^{k(r)}}{\tau_o^{k(r)}} \left(\frac{m^{k(r)} : \sigma^{(r)}}{\tau_o^{k(r)}}\right)^{n-1} \quad (6)$$

$$\dot{\varepsilon}^{o(r)} = (1-n)\ \dot{\gamma}_o \sum_k \left(\frac{m^{k(r)} : \sigma^{(r)}}{\tau_o^{k(r)}}\right)^n \mathrm{sgn}\left(m^{k(r)} : \sigma^{(r)}\right) \quad (7)$$

$$\eta^{k(r)} = n\frac{\dot{\gamma}_o}{\tau_o^{k(r)}} \left(\frac{\tau^{k(r)}}{\tau_o^{k(r)}}\right)^{n-1} \quad (8)$$