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Variational approach to formation of misoriented microstructures in plastic deformation

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The formation of misoriented microstructures in plastic deformation is explained within the framework of continuum mechanics as a result of the reduction of the energetically costly hardening in multislip by local lattice rotations.

1 Introduction

The formation of misorientations leads to the emergence of experimentally observed subgrains in creep as well as dislocation cells in severe plastic deformation [1]. The physical reason for the formation of the misorientations is well known. It is the reduction of the energetically costly hardening in multislip by locally decreasing the number of active slip systems by lattice rotations [2]. In contrast, a generally accepted mathematical framework for the modeling and simulation of the misorientation formation is still missing. Energetic consideration in the framework of continuum mechanics and crystal plasticity lead Kratochvíl and Sedláček [3, 4] to establishing a relation to the mathematical theory of incremental nonconvex energy minimization [5–7]. The idea is to minimize the work needed to accomplish an increment in the imposed deformation. The formation of misorientations leads to a local reduction in the number of active slip systems and so to a local decrease in the flow stress. The deformation with misorientations is 'energy saving' compared to the corresponding homogeneous deformation.

The standard (local) continuum mechanics approach based on the Biot's theory of incremental deformations [9] yields the misorientation formation. However, a vanishingly small cell size and an unrealistic orientation of the cell boundaries are predicted [4]. The recently proposed nonlocal model yields more realistic results [8]. Here we compare the two approaches.

2 Basic model of misorientation formation

The basic model of misorientation formation formulated as an incremental energy minimization problem has been presented by Sedláček and Kratochvíl in [4]. The model was developed in the framework of the rigid-plastic approximation to rate-independent plasticity. Plane strain and symmetric double slip were assumed.

The strain-hardening constitutive equations relate the increments in resolved shear stresses on the two slip systems considered, $\tau^{(i)}$, $i = 1, 2$, on a slip system to increments in plastic slip, $\gamma^{(1)}$ and $\gamma^{(2)}$,

$$\begin{aligned} \tau^{(1)} &= h_{11}\gamma^{(1)} + h_{12}\gamma^{(2)} , \\ \tau^{(2)} &= h_{12}\gamma^{(1)} + h_{11}\gamma^{(2)} , \end{aligned} \tag{1}$$

where h_{ij} are elements of the standard symmetric hardening matrix. The incompressibility of the rigid-plastic model is guaranteed by introducing the stream function $\psi(x, y)$ from which the displacements $u_x(x, y)$ and $u_y(x, y)$ are derived as

$$u_x = \partial_y \psi , \qquad u_y = -\partial_x \psi . \tag{2}$$

A kinematically admissible inhomogeneous deformation is described by the stream function in the form

$$\psi(x, y) = F(x + \xi y) , \tag{3}$$

with F being an arbitrary function of the argument $x + \xi y$. The stream function (3) represents simple shear parallel to planes $x + \xi y =$ const. Using the crystal plasticity framework and the principle of virtual displacements, the following variational functional has been derived,

$$\mathcal{J}(\xi) = \frac{1}{2} \int \left(4H_{xx}\xi^2 + H_{xy}(\xi^2 - 1)^2\right) (F'')^2 \,\mathrm{d}x \,\mathrm{d}y , \tag{4}$$

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that represents the work necessary for an increment of deformation. In eq. (4), H_{xx} and H_{xy} are coefficients depending on the elements of the hardening matrix, cf. eq. (1), and on the inclination ϕ of slip planes in the symmetric double slip model, $H_{ij} = H_{ij}(h_{11}, h_{12}, \phi)$. The detailed analysis of the functional (4) yields a misoriented pattern with infinitely thin lamellae oriented at $\xi \to \infty$, i.e. perpendicular to the tensile direction, as the most favorable pattern [4]. This unrealistic result is due to the lack of an internal length scale in the basic model of misorientation formation.

3 Nonlocal model of misorientation formation

An internal length scale can be introduced in the model by considering dislocation interactions. A suitable framework has been provided by Groma et al. [10] and implemented in the present model by Kratochvíl et al. [8]. It is assumed that the plastic deformation is carried by straight parallel edge dislocations on the two slip systems considered. The statistical treatment of the dislocation populations yields nonlocal strain-hardening constitutive equations that replace eqs. (1),

$$\begin{aligned} \tau^{(1)} &= \pm\Big(h_{11}\bar{\gamma}^{(1)} + h_{12}\bar{\gamma}^{(2)} + \tilde{h}_{11}(\boldsymbol{s}^{(1)}\cdot\mathrm{grad})^2\gamma^{(1)} + \tilde{h}_{12}(\boldsymbol{s}^{(1)}\cdot\mathrm{grad})(\boldsymbol{s}^{(2)}\cdot\mathrm{grad})\gamma^{(2)} + \tau_0\Big) \\ \tau^{(2)} &= \pm\Big(h_{12}\bar{\gamma}^{(1)} + h_{11}\bar{\gamma}^{(2)} + \tilde{h}_{12}(\boldsymbol{s}^{(2)}\cdot\mathrm{grad})(\boldsymbol{s}^{(1)}\cdot\mathrm{grad})\gamma^{(1)} + \tilde{h}_{11}(\boldsymbol{s}^{(2)}\cdot\mathrm{grad})^2\gamma^{(2)} + \tau_0\Big) \end{aligned} \tag{5}$$

The nonlocality is captured by the gradient terms in the slip directions $\boldsymbol{s}^{(i)}$, $i = 1, 2$, where $\tilde{h}_{ij}$ are nonlocal hardening coefficients. An energy functional can be constructed in a similar way as in the basic model. For simplicity, assuming a microstructure consisting of bands (lamellae) of misoriented crystal lattice, a reduced functional is considered here, yielding

$$\mathcal{I}(\xi, L) = \frac{\bar{\mu}_2 + \Delta\bar{\sigma}}{L^2}(\xi^4 + m_1\xi^2 + m_2) + \frac{4\hat{\mu}_2}{L^3}(\xi^4 + m\xi^2 + 1)\,. \tag{6}$$

For the precise meaning of the coefficients in eq. (6), the reader is referred to [8]. The microstructure forms if the inhomogeneous deformation is energetically more convenient than the corresponding homogeneous deformation, i.e. if $\mathcal{I} < 0$. Thus, regions of instability, that is regions in the parameter space where a microstructure forms, can be determined from the conditions that

$$\mathcal{I}(\xi, L) < 0\,, \qquad L > 0\,. \tag{7}$$

Important is also the explicit dependence of the functional (6) on the width of the misoriented lamellae L. Thus, the work necessary for an increment of deformation can be minimized relative to the orientation ξ and width L of the lamellae. An optimum microstructure is represented by a pair (ξ, L), such that

$$\frac{\partial\mathcal{I}}{\partial(\xi^2)} = 0\,, \qquad \frac{\partial\mathcal{I}}{\partial L} = 0\,. \tag{8}$$

A finite size, $L > 0$, and a realistic orientation, $\xi \neq \infty$, of the microstructure result [8].

4 Conclusions

The present model shows that the mathematical framework of nonconvex energy minimization is a suitable tool for analyzing the formation of misoriented microstructures in plastic deformation. The close correlations among dislocations, represented here by the plastic strain gradients, are an important ingredient of the model. The main obstacle to the quantification of the present model is the lack of information on the nonlocal hardening coefficients appearing in eqs. (5) and (6).

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