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Short communication

Formation of grains and dislocation structure of geometrically necessary boundaries

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ABSTRACT

A continuum dislocation model of formation of grains whose boundaries have a non-vanishing thickness is proposed. For a single crystal deforming in simple shear the lamellar structure of grains with thin layers containing dislocations as the geometrically necessary boundaries turn out to be energetically preferable. The thickness and the energy of this type of grain boundary are computed as functions of the misorientation angle.

1. Introduction

One of the main guiding principles in seeking an appropriate theory of formation of grains in metals and alloys during and after cold working processes producing severe plastic deformations has first been proposed by Hansen and Kuhlmann-Wilsdorf [1] in the form of the so-called LEDS-hypothesis: the dislocation structures in the final state of deformation minimize the energy of crystals (see also [2–4]). The main reason why the formation of grains becomes energetically preferable at severe plastic deformations lies in the non-convexity of the energy of crystal in this range [5–8]. Within the conventional crystal plasticity considered in [5–7] the minimization of such non-convex energy leads immediately to the infinitely fine lamellar structure with grain boundaries as sharp interfaces. However, as mentioned by Kuhlmann-Wilsdorf and Hansen [4], typical grain boundaries, termed geometrically necessary boundaries, have as a rule a non-vanishing thickness and may contain a large number of dislocations and thus contradict the conventional crystal plasticity. The question then arises in this connection: what kind of continuum model may resolve this conflict? The present paper proposes a dislocation model of formation of grains within the continuum dislocation theory [9,10] which predicts the existence of such geometrically necessary boundaries. By including the energy of dislocation network containing the gradient of the plastic slip into the energy functional we regularize the non-convex energy minimization problem. It should be mentioned that the idea of adding the gradient term as the interfacial energy into the non-convex energy functional was proposed already in the 50s by Cahn and Hilliard [11] (see also the review of the recent phase-field approach in [12]). However, to the best of our knowledge, such gradient term having the clear meaning of the energy of dislocation network regularizing the non-convex energy in the context of crystal plasticity is proposed in this paper for the first time. We illustrate the application of the theory on the example of single crystal having one slip system and deforming in simple shear. We show that the geometrically necessary boundaries, in which the transition from one grain to the next occurs smoothly, have a small but finite thickness and contain a large number of dislocations. Although the resultant Burgers vector of dislocations in such grain boundary is non-zero, they do not produce long range stresses, and the lamellar structure of grains is in fact the low energy dislocations structure. We also compute the thickness of geometrically necessary boundaries and their energies as functions of the misorientation angles. Based on these results we estimate also the number of grains in terms of the specimen sizes. We show that the proposed theory agrees well with the experimental observations during ECAP experiment [13].

2. Continuum theory of formation of grains

We consider for simplicity an initially dislocation-free single crystal having only one active slip system. In this case the

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kinematic quantities characterizing its observable deformations are the placement field $\mathbf{y}(\mathbf{x})$ and the plastic slip field $\beta(\mathbf{x})$. The incompatible plastic deformation is given by

$$\mathbf{F}^p(\mathbf{x}) = \mathbf{I} + \beta(\mathbf{x})\mathbf{s} \otimes \mathbf{m},$$

with the pair of constant and mutually orthogonal unit lattice vectors $\mathbf{s}$ and $\mathbf{m}$ denoting the slip direction and the normal to the slip planes respectively. Using the multiplicative resolution of the total compatible deformation gradient $\mathbf{F} = \partial\mathbf{y}/\partial\mathbf{x}$ into the plastic and elastic parts [10], we find the incompatible elastic deformation in the form

$$\mathbf{F}^e = \mathbf{F}\cdot\mathbf{F}^{p-1} = \frac{\partial\mathbf{y}}{\partial\mathbf{x}}\cdot(\mathbf{I} - \beta\mathbf{s} \otimes \mathbf{m}).$$

The tensor of dislocation density measuring the incompatibility of $\mathbf{F}^p$ reads (see [5,10])

$$\mathbf{T} = -\mathbf{F}^p \times \nabla = \mathbf{s} \otimes (\nabla\beta \times \mathbf{m}).$$

If, in addition, all dislocation lines are straight lines parallel to the unit vector $\mathbf{l}$, then the scalar dislocation density (or the number of excess dislocations per unit area perpendicular to $\mathbf{l}$) can be determined as

$$\rho = \frac{|\mathbf{T}\cdot\mathbf{l}|}{b} = \frac{1}{b}|(\nabla\beta \times \mathbf{m})\cdot\mathbf{l}|,$$

with b being the magnitude of Burgers vector.

For crystals having as a rule small elastic strains we propose the free energy per unit volume of the undeformed configuration in the form

$$\psi(\mathbf{E}^e, \rho) = \frac{1}{2}\lambda(\mathrm{tr}\,\mathbf{E}^e)^2 + \mu\,\mathrm{tr}(\mathbf{E}^e\cdot\mathbf{E}^e) + \frac{1}{2}\mu k\frac{\rho^2}{\rho_s^2}. \tag{1}$$

Here $\mathbf{E}^e = \frac{1}{2}(\mathbf{F}^{eT}\cdot\mathbf{F}^e - \mathbf{I})$ corresponds to the elastic strain tensor, λ and μ are the Lamé constants, k a material constant, and ρ_s can be interpreted as the saturated dislocation density. The first two terms in (1) represent energy of crystal due to the macroscopic elastic deformation. The last term describes energy of the dislocation network for moderate dislocation densities. Note that for small or extremely large dislocation densities close to the saturated density the logarithmic energy proposed in [14] is more appropriate. We deform this crystal occupying in the initial configuration some region $\mathcal{V}$ of three-dimensional space by placing it in a displacement-controlled device such that, at the boundary $\partial\mathcal{V}$, the conditions

$$\mathbf{y}(\mathbf{x}) = \bar{\mathbf{F}}\cdot\mathbf{x}, \quad \beta(\mathbf{x}) = 0 \quad \text{for } \mathbf{x} \in \partial\mathcal{V} \tag{2}$$

are specified, with $\bar{\mathbf{F}}$ being a given overall deformation. If the deformation process is isothermal, no body force acts on this crystal, and the resistance to the dislocation motion can be neglected, then the following variational principle turns out to be valid: the true placement vector $\check{\mathbf{y}}(\mathbf{x})$ and the true plastic slip $\check{\beta}(\mathbf{x})$ in the *final* equilibrium state of deformation minimize the energy functional

$$I[\mathbf{y}(\mathbf{x}), \beta(\mathbf{x})] = \int_{\mathcal{V}} w(\mathbf{F}, \beta, \nabla\beta)\,dx \tag{3}$$

among all *continuously differentiable* fields $\mathbf{y}(\mathbf{x})$ and $\beta(\mathbf{x})$ satisfying constraints (2), where $w(\mathbf{F}, \beta, \nabla\beta) = \psi(\mathbf{E}^e, \rho)$. We will see that, due to the non-convexity of the free energy density (1) and the presence of $\nabla\beta$ in the energy functional via the energy of the dislocation network, the formation of grains with regular grain boundaries having a finite thickness is energetically preferable.

3. Energy minimizer in plane strain simple shear

Consider now the special case of plane strain simple shear of the specimen in the form of a cuboid of height H, width L, and depth D such that $y_3 = x_3$, while $y_1(\mathbf{x})$, $y_2(\mathbf{x})$ and $\beta(\mathbf{x})$ depend only on two cartesian coordinates x_1 and x_2 and satisfy at the side boundary the conditions

$$y_1 = x_1 + \gamma x_2, \quad y_2 = x_2, \quad \beta = 0,$$

with γ being the overall shear strain. We assume that $\mathbf{s}^T = (\cos\varphi, \sin\varphi, 0)$, $\mathbf{m}^T = (-\sin\varphi, \cos\varphi, 0)$ and all dislocation lines are parallel to the x_3-axis, so $\rho = |\nabla\beta\cdot\mathbf{s}|/b$. If the deformations are uniform such that

$$\mathbf{F} = \bar{\mathbf{F}} = \mathbf{I} + \gamma\mathbf{e}_1 \otimes \mathbf{e}_2, \quad \mathbf{F}^p = \mathbf{I} + \beta\mathbf{s} \otimes \mathbf{m},$$

with γ and β being the constants, then the energy (3) normalized by $\mu|\mathcal{V}|$ and minimized with respect to β turns out to be non-convex for $\varphi \in (-\pi/2, 0)$ as shown in Fig. 1 (see [8]).

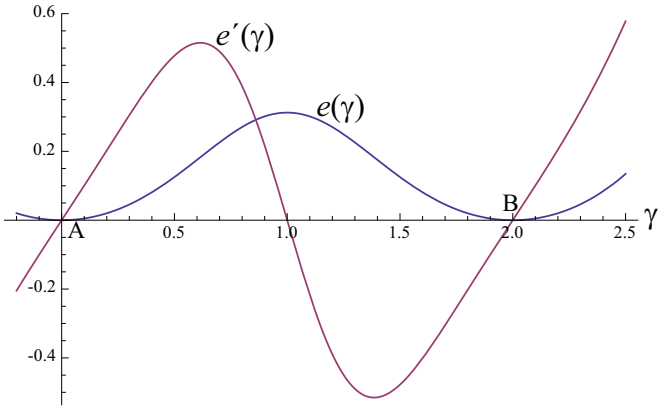

Fig. 1. Condensed energy $e(\gamma)$ and the dimensionless shear stress $e'(\gamma)$ for $\varphi = -45°$.

In view of this non-convexity, we proposed in [8] the energy minimizing sequence consisting of layers having the uniform states A and B according to

$$\gamma_A = 0, \quad \gamma_B = -2\cot\varphi,$$
$$\beta_A = 0, \quad \beta_B = 2\cot\varphi,$$

such that the volume fraction of the layer B is given by $s = -\gamma/(2\cot\varphi)$. It has been shown in [8] that such candidates for the minimizer satisfy the equations of equilibrium in each layer as well as the outer boundary conditions except at the side boundaries $x_1 = 0, L$ of the specimen. Besides, the energy of such lamellar structure is equal to zero which is the minimal possible value. However, if the boundaries between layers are sharp interfaces, these candidates do not belong to the set of admissible fields of our original variational problem (2) and (3) due to the jumps of $\mathbf{F}$ and β on those interfaces, so they fail to be the energy minimizers of (2) and (3).

To correct the behavior of those candidates for minimizers we assume now that the layers corresponding to the states A and B are separated by a thin layer of small thickness h in which the placement and plastic slip change smoothly from state A to state B (see Fig. 2). Since this boundary layer is thin (h is much smaller than $sH, (1-s)H$, and the sizes of the specimen), it is reasonable to assume that the displacement in the x_2-direction is zero, while the displacement in the x_1-direction and the plastic slip depend only on x_2:

$$y_1 = x_1 + u(x_2), \quad y_2 = x_2, \quad \beta = \beta(x_2).$$

With this Ansatz it is easy to show that the determination of functions $u(x_2)$ and $\beta(x_2)$ as well as the unknown boundary layer reduces to minimizing the following functional: