Microstructure evolution in the equal channel angular extrusion process

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Abstract

We apply a theory of single-crystal plasticity with microstructure to the simulation of the ECAE process. The specific microstructures considered in the simulations are of the sequential lamination type. The size of the microstructure is estimated a posteriori by means of a nonlocal extension of the theory which accounts for dislocation energies. Texture evolution is calculated simply by recourse to Taylor’s hypothesis. Calculations concerned with an FCC material (Al–Cu alloy) and 90° ECAE reveal a wealth of information regarding the geometry, size, and texture evolution of subgrain microstructures. The predicted sizes and textures are in good quantitative agreement with the available experimental data.

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1. Introduction

The recent years have witnessed the re-emergence of severe deformation processing methods for the introduction of subgrain grain microstructures in the metallic alloys. The re-emergence was initiated by addressing some key difficulties faced in the traditional mechanical processing techniques. The objective of this processing is to induce high angle grain boundaries that act as grain subdividing and strength and ductility enhancing mechanism. Several new novel deformation techniques have surfaced in the recent past apart from the traditional cold-rolling and wire drawing process used for specific purposes of metal-working. Some such techniques are equal channel angular extrusion (ECAE) [30,37,5], severe plastic
torsion straining (SPTS) [35], multi-axis compression [32], accumulative roll bonding (ARB) [29] and cyclic extrusion compression (CEC) [28] each with specific advantage over the others in metal processing. All these techniques focus on grain refinement that are primarily initiated by heterogeneous plastic flow. The shear bands that form during this extreme plastic deformation processing are precursors to the grain subdivision in the form of high-angle grain boundary creation in the subgrains.

ECAE [30,37,5] is one of several metal forming processes that utilize severe plastic deformations (SPD) in order to impart special properties to the metal, including severe plastic torsion straining (SPTS) [35], multi-axis compression [32], accumulative roll bonding (ARB) [29] and cyclic extrusion compression (CEC) [28]. A schematic of the ECAE setup is shown in Fig. 1. In its simplest form, it consists of two channels of equal cross section joined together at a certain angle $\varphi$ to each other. Depending on the material processed, this angle varies between $90^\circ$ and $157.5^\circ$. Since the channels are of equal cross section, the cross-sectional shape of the specimen does not change during the process. This enables the process to be repeated several times, with each run called a pass. There are several possible sequences of passes, or routes, which differ on the re-orientation of the specimen's shear plane relative to the die's shear plane (see Fig. 1).

The specimen goes through severe shear deformation at the die's shear plane before going out the tail channel. The sharp discontinuity in the deformation at the die's shear plane is the principal mechanism by which severe plastic deformation is imparted to the specimen. This process of severe plastic deformation induces a nanostructure into the metal in the form of lamellar structures which simultaneously the enhances ductility and strength of the material, properties which have been regarded as mutually exclusive in traditional metallurgy.

Figs. 2 and 3 show the observed evolution of the lamellar structures which develop in aluminum and copper specimens with increasing number of passes ($N$) of the continued shearing route [18,30]. Several striking aspects of the evolution of the microstructure with increasing deformation are evident in these figures. Thus, the relatively uniform and equiaxed grains in the specimens prior to processing become elongated and aligned along the direction of shearing after processing. The extent of the shear deformation

Fig. 1. Equal channel angular extrusion die.
Fig. 2. Evolution of lamellar structures in aluminum specimens undergoing multiple ECAE passes [18].

Fig. 3. Evolution of lamellar structures in copper specimens undergoing multiple ECAE passes [18,30].
is observed to increase with increasing number of passes. After a sufficient number of passes, the microstructure attains a fibrous or lamellar morphology of the type which is commonly observed in highly deformed metals, e.g., cold-rolling [9,7,10–12,8,13].

The optimal design of the ECAE process, including such processing parameters as the dye angle, the number of passes and the processing routes, require a precise and quantitative understanding of the mechanics of deformation-induced subgrain microstructure. In particular, the theory must allow the structures to form under applied stress, and it must predict its geometry, layout, the orientation of the dislocation boundaries and of the intervening cells, the spacing between boundaries, and the attendant macroscopic behavior of the crystal. Ortiz et al. [22,23] have proposed a theory of single crystal plasticity which meets these requirements. In this theory, the formation of dislocation structures is the result of strong latent hardening, namely, the fact that crystals exhibit substantially higher hardening rates when deforming in multiple slip than when deforming in single slip. The presence of strong latent hardening implies that the crystal has a clear incentive, in work of deformation terms, to deform in single slip and avoid multiple slip. More precisely, the work of deformation expended in deforming a crystal into a deformation field composed of regions of single slip is always less than the work or deformation required to attain the same average or macroscopic deformation by multiple slip. As also noted by [22,23], microstructure-size predictions can be additionally achieved by the consideration of the self-energy of the dislocations, e.g., through a simple line tension model. This additional source of energy renders the model nonlocal and, therefore, sensitive to the size and shape of the crystal.

Crystals possessing infinite latent hardening provide a particularly simple and computationally convenient limit of the theory [3]. Mathematically, the infinite latent hardening property means that the crystal must necessarily deform in single slip at all material points. This requirement introduces a nonconvex constraint which renders the incremental problem nonconvex. Materials can attain plastic deformations other than single slip—and thus beat the single-slip constraint—by developing deformation microstructures. These microstructures may be expected to involve ‘patchy slip’ [25,1], i.e., the activation of different slip systems or ‘variants’, in the parlance of martensite—over different regions of the crystal, possibly arranged in complex spatial patterns.

In this paper we apply the theory of single-crystal plasticity with microstructure of Ortiz and Repetto [22,23] in the limit of infinitely strong latent hardening [3] to the simulation of the ECAE process. The specific microstructures considered in the simulations are of the sequential lamination type. In order to generate and evolve these deformation microstructures we use the sequential lamination algorithm proposed by Aubry et al. [2]. The size of the microstructure is estimated a posteriori by means of a nonlocal extension of the theory which accounts for dislocation energies [22]. Texture evolution is calculated simply by recourse to Taylor’s hypothesis at the undeformed grain level.

The paper is arranged as follows: After a brief description of the model that predicts the subgrain microstructure formation and evolution, severe plastic deformation processing applications with special focus on equal channel angular extrusion (ECAE) are described and typical simulation results are presented and discussed.

2. A simple model of finite-deformation single-crystal plasticity with microstructure

We begin by reviewing some general aspects of single-crystal plasticity and, more specifically, investigating the limiting case of crystals exhibiting infinite latent hardening. In this limit, the local kinematics of plastic deformation is restricted to processes of single slip. This results in a constrained theory, in the sense that the possible directions of the plastic rate-of-deformation tensor $\dot{\mathbf{F}}\mathbf{F}^{-1}$ are restricted to a small set of values determined by crystallography.
2.1. Constitutive basis of the constrained theory

Much of the phenomenology targeted by the present theory occurs at large deformations. These circumstances require the theory to account for full finite-deformation kinematics. To this end, we assume a conventional multiplicative decomposition of the deformation gradient \( F \) of the form [17]:

\[
F = F^e F^p,
\]

(2.1)

where \( F^e \) is the elastic component of the deformation gradient and \( F^p \) is the plastic part. Using the polar decomposition the elastic part of the deformation gradient can be further decomposed as

\[
F^e = R^e U^e,
\]

(2.2)

where \( U^e = U^e^T \) is the elastic stretch tensor and \( R^e \in SO(3) \) is the rotation of the crystal lattice.

For metallic crystals, the elasticity and heat capacity of the crystal may be assumed to be structure insensitive, i.e., independent of the internal processes, to a good approximation. The free energy of the crystal is thus of the form [27]:

\[
A = W^e(C^e, T) + W^p,
\]

(2.3)

where \( W^e \) is the elastic strain-energy density, \( W^p \) is the stored energy of cold work, \( T \) is absolute temperature, and \( C^e = F^e^T F^e \) is the elastic right Cauchy–Green deformation tensor. Throughout this paper we shall restrict our attention to isothermal processes and will omit any subsequent reference to \( T \). The first Piola–Kirchhoff stress tensor follows from the free energy as:

\[
P = A_{,F} = W^e_{,F} F^p^{-T}.
\]

(2.4)

For simplicity, we shall assume that the crystal exhibits infinite latent hardening [22,3]. In this limiting regime, processes of multiple slip are barred altogether and the crystal is constrained to deform locally in single slip. Thus, locally at every material point \( x \), we must necessarily have

\[
\hat{F}^e(x) F^p^{-1}(x) = \hat{\gamma}(x) s(x) \otimes m(x),
\]

(2.5)

where \( (s(x), m(x)) \in \mathcal{S} \) is the sole slip system which is active at material point \( x \) and \( \hat{\gamma}(x) \) is the corresponding shear strain. Here and subsequently, we denote by \( \mathcal{S} \) the set of all slip systems of the crystal, defined by the slip direction \( s \) and the normal to the slip plane \( m \). For instance, fcc crystals possess 12 slip systems consisting of \{111\} slip planes and \{110\} slip directions, see Table 1, whereas the slip-system set \( \mathcal{S} \) in bcc crystals is potentially larger and includes slip planes of the type \{211\} and \{110\} and the slip direction \{111\}.

Evidently, the crystal may still accommodate general macroscopic deformations plastically by developing microstructures, as discussed subsequently. In addition, we note that we express the single-slip assumption (2.5) incrementally and, consequently, we allow for the local active slip system to vary over time. We regard slip as irreversible and, in consequence, we shall enforce the plastic irreversibility condition:

\[
\hat{\gamma} \geq 0.
\]

(2.6)

This tacitly implies that the slip directions \( \pm s \) are regarded as defining two different slip systems.

### Table 1

<table>
<thead>
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<th>System</th>
<th>B2</th>
<th>B4</th>
<th>B5</th>
<th>A3</th>
<th>A2</th>
<th>A6</th>
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<tr>
<td>( \sqrt{3} m )</td>
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<table>
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<tr>
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<th>C3</th>
<th>C5</th>
<th>D4</th>
<th>D1</th>
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<td>±[0 1 1]</td>
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We shall additionally idealize processes of single-slip as being ideally plastic, i.e., we take \( \tau_c \) to be constant. This implies that the critical resolved shear stress is assumed to be insensitive to the deformation. The critical resolved shear stress can thus be directly attributed to the statistically stored dislocations present in the crystal prior to the deformation. It should, however, be noted that all the hardening that occurs is directly assumed to be related to the formation and evolution of dislocation structures. The local value of the stored energy then follows by integration of resolved shear stress acting on the slip system \( \alpha \) over the slip strain path and takes the simple form

\[
W^\alpha(x) = \tau_c \gamma(x),
\]  

(2.7)

where we write

\[
\gamma(x) = \int \dot{\gamma}(x) dt.
\]  

(2.8)

Since the instantaneous local slip-strain rate \( \dot{\gamma}(x) \) is constrained by (2.6) to be nonnegative, it follows that \( \gamma(x) \) must itself be nonnegative at all material points. All the hardening is attributed directly to the formation and evolution of dislocation structures.

As noted earlier, the single-slip constraint forces crystals to develop microstructures in order to accommodate general macroscopic deformations. Following [22, 23] our aim here is to understand the formation and evolution of these microstructures in variational terms, or, more precisely, as manifestations of non-attainment of a non-convex minimum principle. A powerful device enabling the formulation of incremental minimum principles in transient and inelastic problems is time-discretization [26, 22, 24]. Thus, we consider a local material neighborhood of the crystal and we assume that the local deformation is known at discrete times \( t_0 = 0, \ldots, t_n, t_{n+1} = t_n + \Delta t, \ldots \) The problem is to determine the corresponding evolution of the state of the crystal. Assume, in particular, that the state of the crystal is known at time \( t_n \), and that the deformation mapping \( y_{n+1} : \Omega \rightarrow \mathbb{R}^3 \) is subject to the boundary condition

\[
y_{n+1}(x) = \bar{F}_{n+1} x, \quad x \in \partial \Omega,
\]  

(2.9)

where the macroscopic deformation \( \bar{F}_{n+1} \) is given at time \( t_{n+1} \). The problem now is to determine the full state of the crystal at time \( t_{n+1} \).

Following [26, 22, 24], we introduce the incremental work-of-deformation density function

\[
f_n(F_{n+1}, y_{n+1}; (s, m)) = W^\alpha(F_{n+1} F_{n-1}^{-1}) + \tau_c \Delta \gamma,
\]  

(2.10)

where

\[
F_{n+1} = (I + \Delta \gamma s \otimes m) F_n,
\]  

(2.11)

and \( \Delta \gamma = \gamma_{n+1} - \gamma_n \). Then, the deformation mapping \( y_{n+1} \) and the distribution of slip \( y_{n+1} \) follow from the variational problem

\[
\inf_{y_{n+1}, \gamma_{n+1} : (s, m) \in \mathcal{Y}} \int_{\Omega} f_n(Dy_{n+1}, \gamma_{n+1}; (s, m)) dx,
\]

\[
\Delta \gamma(x) \geq 0, \quad in \ \Omega,
\]

\[
y_{n+1}(x) = \bar{F}_{n+1} x, \quad on \ \partial \Omega,
\]  

(2.12)

where \( Dy_{n+1}(x) = F_{n+1}(x) \) is the local deformation gradient, and \( \gamma_{n+1}(x), s(x) \) and \( m(x) \) are now to be regarded as fields over the domain \( \Omega \) of the crystal. It should be noted that the boundary condition of specifying macroscopic deformation in Eq. (2.9) is directly related to the notion of quasi-convexification.

Thus, the initial condition \( y_0 = 0 \) implies that they are.

The remainder of this section is devoted to constant time discretization.

2.2. Selection of dislocation structures

Unlike in the case of materials treated in the previous section, we can simulate the evolution of dislocation structures [22] with this formulation. As in the previous section, we define the deformation mapping \( y_{n+1}(x) \) by

\[
y_{n+1}(x) = \bar{F}_{n+1} x, \quad x \in \Omega.
\]  

(2.10)

where

\[
F_{n+1} = (I + \Delta \gamma s \otimes m) F_n,
\]  

(2.11)

and \( \Delta \gamma = \gamma_{n+1} - \gamma_n \). Then, the deformation mapping \( y_{n+1} \) and the distribution of slip \( y_{n+1} \) follow from the variational problem

\[
\inf_{y_{n+1}, \gamma_{n+1} : (s, m) \in \mathcal{Y}} \int_{\Omega} f_n(Dy_{n+1}, \gamma_{n+1}; (s, m)) dx,
\]

\[
\Delta \gamma(x) \geq 0, \quad in \ \Omega,
\]

\[
y_{n+1}(x) = \bar{F}_{n+1} x, \quad on \ \partial \Omega,
\]  

(2.12)

where \( Dy_{n+1}(x) = F_{n+1}(x) \) is the local deformation gradient, and \( \gamma_{n+1}(x), s(x) \) and \( m(x) \) are now to be regarded as fields over the domain \( \Omega \) of the crystal. It should be noted that the boundary condition of specifying macroscopic deformation in Eq. (2.9) is directly related to the notion of quasi-convexification.
Thus, for any other boundary conditions, quasi-convexification may be done only on the affine boundary condition and other details of the boundary condition may be left the same as the original problem since they are not directly related to the notion of quasi-convexification.

The connection between deformation fields and dislocation structures may be established by recourse to the theory of continuously distributed dislocations [20]. While the deformation gradient field $\mathbf{F}(x)$ is subject to compatibility requirements, the plastic deformation field $\mathbf{F}^p(x)$ need not be compatible in general. Following Nye [21] (see also [20]), the dislocation density tensor is defined as

$$ A = \text{curl} \mathbf{F}^p $$

or, in components, $A_{iK} = F_{iJ}^p \delta_{JK}$, with $\delta_{JK}$ denoting the components of the permutation tensor. Following [22,23], the theory may be rendered nonlocal through an appropriate accounting of dislocation energies. Thus, a simple isotropic line-tension model, consisting of according the dislocations an energy per unit length $T$, leads to the modified variational problem

$$ \inf_{\gamma_{n+1} : (s,m)} \int_D \left[ f_n(Dy_{n+1}; \gamma_{n+1}; (s,m)) + (T/b)(|\text{curl} \mathbf{F}^p| - |\text{curl} \mathbf{F}^p_p|) \right] \, \, dx $$

subject to constraints in (2.12) and (2.11). The introduction of the dislocation energy term introduces a characteristic length in the form of the Burgers vector length $b$, with the result that the dislocation structures and the macroscopic effective behavior depend sensitively on the domain size and shape.

### 2.2. Sequential laminates

Unfortunately, a general procedure for solving problems just formulated is not available at present. Instead, we content ourselves with investigating special microstructures which lend themselves to analytical treatment. Specifically, we consider microstructures which may be described as simple or sequential laminates [15,14,22,23,3]. While other types of microstructures cannot be ruled out a priori, sequential laminations does appear to suffice for the purpose of mathematically describing the vast majority of dislocation structures which are observed in the ECAE process.

Following [14], a laminate of rank-$k$ is a layered mixture of two rank-$(k-1)$ laminates, which affords an inductive definition of laminates of any rank. Sequential laminates have a binary-tree structure. Indeed, with every sequential laminate we may associate a graph $G$ such that: the nodes of $G$ consist of all the sub-laminates of rank less or equal to the rank $k$ of the laminate; and each sub-laminate of order $l \leq l \leq k$ is joined with its two constituent sub-laminates of order $l-1$. The root of the graph is the entire laminate.

Let $i = 1, \ldots, n$ be an enumeration of the nodes of $G$. Then, to each node $i$ we may associate a deformation $\mathbf{F}_i$. The root deformation is the average or macroscopic deformation $\bar{\mathbf{F}}$. Each node in the tree has either two children or none at all. Nodes with a common parent are called siblings. Nodes without children are called leaves. Nodes which are not leaves are said to be interior. The deformations of the children of node $i$ will be denoted $\mathbf{F}_i^\pm$. Each generation of nodes is called a level. The root occupies level 0 of the tree. The number of levels is the rank $k$ of the tree. Level $n$ contains at most $2^n$ nodes.

Compatibility demands that each pair of siblings be rank-one connected, i.e.,

$$ \mathbf{F}_i^+ - \mathbf{F}_i^- = \mathbf{a}_i \otimes N_i, \quad i \in \mathcal{S}_G $$

for some $\mathbf{a}_i \in \mathbb{R}^3$, $N_i \in \mathbb{R}^3$, $|N| = 1$, is the normal to the interface between $\mathbf{F}_i$ and $\mathbf{F}_i^+$, and $\mathcal{S}_G$ denotes the set of all interior nodes. Let $\lambda_i^\pm$,

$$ \lambda_i^- + \lambda_i^+ = 1, \quad \lambda_i^+ \in [0,1] $$
denote the volume fractions the variants $F_i^+$ within node $i$. Then, the deformation of the parent variant is recovered in the form

$$F_i = \lambda_i F_i^+ + \lambda_i^+ F_i^-, \quad (2.17)$$

If $F_i$ and $\{a_i, \lambda_i^+, N_i\}$ are known for an interior node $i$, then the deformation of its children is given by:

$$F_i^- = F_i - \lambda_i^- a_i \otimes N_i,$$

$$F_i^+ = F_i + \lambda_i^+ a_i \otimes N_i. \quad (2.18)$$

Therefore, $F$ and $\{a_i, \lambda_i^+, N_i, i \in \mathcal{F}\}$ define a complete and independent set of degrees of freedom for the laminate. A recursive algorithm for computing all the variant deformations $F_i$, $i = 1, \ldots, n$ from $F$ and $\{a_i, \lambda_i^+, N_i, i \in \mathcal{F}\}$ is given in [23].

It is also useful to introduce the global volume fractions $v_l$ of all leaves $l \in \mathcal{L}_G$, where $\mathcal{L}_G$ denotes the collection of all leaves of $G$. These volume fractions are obtained recursively from the relations:

$$v_i^+ = \lambda_i^+ v_i, \quad i \in \mathcal{F}_G \quad (2.19)$$

with $v_{\text{root}} = 1$ for the entire laminate, and satisfy the relation:

$$\sum_{l \in \mathcal{L}_G} v_l = 1. \quad (2.20)$$

Thus, $v_l$ represents the volume occupied by leaf $l$ as a fraction of the entire laminate. The Young measure (e.g., [19]) of the laminate consist of the convex combination of atoms $\partial \mathcal{F}(F)$ with weights $v_l$, $l \in \mathcal{L}$.

For a sequential laminate the macroscopic work-of-deformation function (2.12) is of the form:

$$\bar{W}_n(F_{n+1}) = \min_{\{a_i^{n+1}, N_i \in \mathcal{F}_G\}} \sum_{i \in \mathcal{F}_G} v_i W_n(F_i^{n+1}). \quad (2.21)$$

The Euler–Lagrange equations, or equations of equilibrium corresponding to this minimization problem are readily verified to take the form

$$[P_i^{n+1}] N = 0, \quad i \in \mathcal{F}_G, \quad (2.22)$$

which expresses the requirement of continuity of tractions across dislocation walls. The average stress of the laminate can be expressed as

$$P_{n+1} = \frac{\partial \bar{W}_n}{\partial F_{n+1}} = \sum_{i \in \mathcal{F}_G} v_i P_i^{n+1}, \quad (2.23)$$

where

$$P_i^{n+1} = \frac{\partial W_n}{\partial F_i^{n+1}}(F_i^{n+1}), \quad l \in \mathcal{L}_G \quad (2.24)$$

are the stresses in the leaves. A recursive algorithm for computing the average stress $P$ from $\{P_l, l \in \mathcal{L}\}$ and $\{\lambda_i^+, i \in \mathcal{F}_G\}$ is given in [23].

2.3. Microstructural evolution

Suppose that a microstructure is already established at time $t_n$ in the form of a sequential laminate. We wish to ascertain whether a leaf in the microstructure branches upon further deformation. Let $\tilde{F}_n$ be the deformation of the leaf at time $t_n$ and $\tilde{F}_{n+1}$ the new deformation in the leaf at time $t_{n+1}$. The work-density cost incurred as a result of a uniform deformation is $W_n(\tilde{F}_{n+1})$. Imagine now that the leaf branches instead into two branches.

$$W_n(\tilde{F}_{n+1}) = \min_{\{a_i^{n+1}, N_i \in \mathcal{F}_G\}} \sum_{i \in \mathcal{F}_G} v_i W_n(F_i^{n+1}).$$

Branching is avoided if

$$W_n(\tilde{F}_{n+1}) = \min_{\{a_i^{n+1}, N_i \in \mathcal{F}_G\}} \sum_{i \in \mathcal{F}_G} v_i W_n(F_i^{n+1}),$$

Minimizing the functional for $\tilde{F}_{n+1}$

$$\tilde{F}_{n+1} = \lambda_i^- F_i^- + \lambda_i^+ F_i^+, \quad (2.25)$$

where

$$\tilde{P}_n = \sum_{l \in \mathcal{L}_G} v_l P_l^{n+1}, \quad (2.26)$$

The left hand side represents the work associated with the force acting on

$$a_n = \sum_{l \in \mathcal{L}_G} v_l a_l, \quad (2.27)$$

which minimizes the characteristic energy

$$W_n(\tilde{F}_{n+1}) = \min_{\{a_i^{n+1}, N_i \in \mathcal{F}_G\}} \sum_{i \in \mathcal{F}_G} v_i W_n(F_i^{n+1}). \quad (2.28)$$

2.4. Notation

In order to determine the stress emanating from a dislocation, we need to know the local energy density of the dislocation. The nature of slip associated with a dislocation is usually determined by $\Delta_{\gamma}$ and $\Delta_{\alpha}$ of the slip system.

Thus, we can compute the stress emanating from a dislocation through...
into two new variants with volume fractions $\lambda^\pm$ separated by a dipolar dislocation wall of unit normal $N$. The energy density of the best possible branched configuration is

$$W_a(F_{n+1}) = \min_{\lambda^\pm, a_{n+1} \cdot N} \{\lambda^- W_a(F_{n+1} - \lambda^+ a_{n+1} \otimes N) + \lambda^+ W_a(F_{n+1} + \lambda^- a_{n+1} \otimes N)\}. \quad (2.25)$$

Branching is assumed to occur provided that

$$W_a(F_{n+1}) < W_a(F_{n+1}). \quad (2.26)$$

Minimization with respect to $\lambda^\pm$ and $N$ may be regarded as the enforcement of equilibrium of configurational forces and torques acting on the dislocation walls. Thus stationarity of $W_a(F_{n+1})$ with respect to $\lambda \equiv \lambda^\pm$ requires

$$[W_a] - \bar{F}_{n+1} \cdot [F_{n+1}] = 0, \quad (2.27)$$

where

$$\bar{F}_{n+1} = \lambda^- \bar{F}_{n+1} + \lambda^+ \bar{F}_{n+1}. \quad (2.28)$$

The left-hand side of (2.27) is the normal component of Eshelby's energy-momentum tensor and thus represents the configurational force conjugate to parallel displacements of the dislocation wall. Likewise, stationarity of $W_a(F_{n+1})$ with respect to $N$ requires

$$a_{n+1} \cdot [P_{n+1}] \times N = 0. \quad (2.29)$$

which may be interpreted as a configurational torque conjugate to rotations of the dislocation walls.

The system of equations (2.22), (2.27) and (2.29) may now be solved for the unknowns $a_{n+1}$, $\lambda^\pm$ and $N$ characterizing the nascent pair of leaves.

### 2.4. Nonlocal extension and microstructural size evolution

In order to estimate the microstructural size and its evolution, e.g., the evolution of lamellar width with deformation, we resort to the nonlocal extension (2.14). As noted by [22, 23, 3], within this extension the size of the microstructure results from the competition of two energy terms: the dislocation wall energy; and the energy of the intervening boundary layers between laminates. In order to simplify calculations we make the assumption that the essential geometry of the microstructure, namely, the graph $G$, and the deformation-jump amplitudes, dislocation wall orientations and variant volume fractions $(a_i, \lambda_i^\pm, N_i, i \in F_G)$, are set by the local model, and we regard the dislocation wall energy as a perturbation whose main effect is to set the lamellar width.

The calculation of the dislocation-wall energy is particularly simple under the conditions of local single slip assumed here. Consider dislocations sweeping through a lamella of thickness $l$ bounded by two parallel dislocation walls. This fixes the travel distance of the dislocations to be $l$. In order to increase the slip strain by $\Delta \gamma$, a certain additional mobile dislocation density $\Delta \rho$ needs to be generated. These considerations lead to the simple relation [3]

$$W_{n+1} = W_n + \left(\tau_c + \frac{T}{bl}\right)\Delta \gamma. \quad (2.30)$$

Thus, we reach the exceedingly simple result that, under conditions of local single slip, the effect of the dislocation wall energies is to increase the yield strength of the lamella in the amount $Tbil$. It should be carefully noted that the effective yield strength thus becomes explicitly dependent on the size of the microstructure through the lamellar thickness $l$. 


Fig. 4. Schematic of interpolation boundary layer and scheme used to estimate misfit energy.

An additional source of energy is the boundary or misfit layers which separate the different sublattices which form the microstructure. A schematic of one such boundary layer is shown in Fig. 4. A simple estimate of the boundary layer energy has been provided by Aubry and Ortiz [3], namely,

$$W^{BL} = \lambda^+ W^e(F^{BL+}) + \lambda^+ W^e(F^{BL-}) - \overline{W}_e(\overline{F}),$$

(2.31)

where

$$F^{BL\pm} = \frac{1}{2}(F^\pm + \overline{F})$$

(2.32)

with

$$\overline{F} = \lambda^+ F^- + \lambda^+ F^+. $$

(2.33)

Combining these estimates, it follows that the total excess or nonlocal energy due to the dislocation walls and the misfit boundary layers contained within a region of the laminate is

$$E^{NL} = L^2 \left\{ \frac{T}{bF} (\gamma^- + \gamma^+) + \frac{F}{l} W^{BL+} \right\}. $$

(2.34)

This excess energy may now be minimized with respect to $l^c$, with the result

$$F^c = \sqrt{\frac{T}{b} (\gamma^- + \gamma^+) \overline{F}^{BL+}}, $$

(2.35)

which affords an estimate of the lamella size $l^c$. We note that the lamella widths are not constant but depend sensitively on deformation. For the particular case of a simple laminate contained within a domain of size $d$, the lamella width scales as $F^c \sim \sqrt{bd} / \gamma$, i.e., as the geometric mean of the intrinsic lengthscale $b$ and the extrinsic lengthscale $d$ [22,23,3].

2.5. Solution strategy

The solution strategy adopted in the examples presented here is as follows. For fixed microstructure $G$, the unknowns $\{a_i, i \in \mathcal{I}_c\}$ are determined from the equilibrium Eq. (2.22) by a Newton–Raphson iteration. At the start of each time step, the condition of branching (2.26) is checked at each of the leaves of the laminate and for every pair of slip systems. This entails the solution of the minimization (2.25) for the unknowns $\{a_{i+1}, \lambda^+, N\}$. An iterative solution of this problem requires a careful choice of initial values of the unknowns. An appropriate choice of the initial orientation $N$ is particularly important, as it determines the orientation of the dislocation walls. An estimate for $N$ is obtained by assuming that the elastic strains are small, i.e., $C^e = F^{eT} F^e \approx I$. Under these conditions, the elastic deformation reduces to a rotation, i.e., $F^e \approx R^e \in \text{SO}(3)$. Ortiz and Repetto [22] have determined and tabulated all possible interfaces which can

be formed from the different intergranular orientations, and this set of solutions has been used to initialize the computation. Each solution has the form

$$\mathbf{F} = \mathbf{R} \mathbf{D},$$

where

$$\mathbf{D} = \mathbf{I} - \mathbf{R} \mathbf{R}^T,$$

and

$$\mathbf{R} \in \text{SO}(3).$$

This approach has been found to be effective for a wide range of problems.

3. Application

Deflection of a plate due to thermal loading

The deflection of a plate $\mathcal{X} = (X_1, X_2, X_3)$ subjected to a temperature field $T(X_1, X_2)$ is given by

$$N(x_1, x_2, x_3) = 0,$$

where $x \in \mathcal{X}$. The problem is then to find the deformation $F: \mathcal{X} \rightarrow \mathcal{X}$ such that

$$a \cdot \nabla \nabla \cdot F = 0,$$

where $a \in \mathbb{R}^3$. The solution is

$$F = a \cdot \nabla \nabla \cdot F = 0,$$

for some $a \in \mathbb{R}^3$. This solution is unique and satisfies the boundary conditions.
be formed by twinning deformations in this class. The admissible interfaces belong to a small set of crystallographic planes. Once the iteration is seeded in this way, the system of Eqs. (2.22), (2.27) and (2.29) is solved for \( \{a_{n+1}, \lambda^2, N\} \) by means of Spellucci’s DONLP2 sequential quadratic programming algorithm [31]. Rank-one convexification used in this work render the work of deformation function convex and thus computational problems that may arise due to lack of convexity are totally avoided. This numerical scheme now has the advantage of dealing only with a well-posed minimization problem and, consequently, their orientation is held fixed in the reference configuration of crystal. The lamellar sizes are computed a posteriori from Eq. (2.35).

3. Application to the ECAE process

Deformation structures such as those shown in Figs. 2 and 3 are the principal conduits for grain boundary formation in ECAE samples. As is evident from this figures, after a sufficient number of passes the deformation structures exhibit a clear lamellar morphology. Thus, ECAE is ideally suited to the application of the model of microstructure evolution described in the foregoing.

3.1. Kinematics of the ECAE process

The deformation gradient undergone by the specimen in one run can be derived by assuming that all deformation occurs instantaneously at the die’s shear plane (Fig. 1). In the referential coordinate frame \((X_1, X_2, X_3)\) shown in Fig. 1, the normal to the shear plane is

\[
N = \begin{bmatrix}
\cos \varphi / 2 \\
-\sin \varphi / 2 \\
0
\end{bmatrix}.
\]  

(3.1)

The Hadamard compatibility condition requires

\[
F - I = a \otimes N,
\]

(3.2)

where \( F \) is the total deformation in the specimen after passing through the shear plane. Assuming further that only shear deformation occurs across the shear plane, we have

\[
a \cdot N = 0,
\]

(3.3)

where \( a \) is a polarization vector. In addition, the boundary conditions require that

\[
F \begin{bmatrix}
0 \\
-1 \\
0
\end{bmatrix} = \lambda \begin{bmatrix}
\sin \varphi \\
\cos \varphi \\
0
\end{bmatrix}
\]

(3.4)

for some stretch \( \lambda \). Solving for \( a \) and \( \lambda \) from (3.2), (3.3) and (3.4) we obtain

\[
F = \begin{pmatrix}
2 + \cos \varphi & -\sin \varphi & 0 \\
(1 + \cos \varphi) \cot \varphi / 2 & -\cos \varphi & 0 \\
0 & 0 & 1
\end{pmatrix},
\]

(3.5)
which gives the total deformation resulting from the passage of the material points through the shear plane. In the processing route considered here, the specimen is rotated by an angle $\varphi$ about $X_3$-axis and $180^\circ$ about $X_2$-axis. The resulting total rotation is

$$
R = \begin{pmatrix}
-1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & -1
\end{pmatrix}
\begin{pmatrix}
\cos \varphi & -\sin \varphi & 0 \\
\sin \varphi & \cos \varphi & 0 \\
0 & 0 & 1
\end{pmatrix} =
\begin{pmatrix}
-\cos \varphi & \sin \varphi & 0 \\
\sin \varphi & \cos \varphi & 0 \\
0 & 0 & -1
\end{pmatrix}.
$$

(3.6)

Hence, the deformation undergone by the specimen after $n$ passes is

$$
F_n = (RF)^n.
$$

(3.7)

All the calculations presented here are carried out for the case $\varphi = 90^\circ$, whence (3.5) reduces to

$$
F = \begin{pmatrix}
2 & -1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 1
\end{pmatrix}.
$$

(3.8)

The specimen undergoes a shear deformation of order two at the shear plane. As is expected, $\det(F) = 1$, i.e., there is no volume change in the specimen after deformation. The shear plane is at $45^\circ$ to the $X_1$-axis. In calculations, the deformation $F$ corresponding to one ECAE pass is subdivided into 50 equal incremental steps.

3.2. Sample calculations for an FCC material (Al–Cu alloy)

For purposes of illustration we consider an Al–Cu alloy with elastic constants $C_{11} = 168.4$ GPa, $C_{12} = 121.4$ GPa, $C_{44} = 75.4$ GPa. Due to the cubic symmetry of the FCC crystal structure, a set of three elastic constants only are necessary to completely determine the elastic moduli $C_{ij}$. Thus, the values $C_{11}$, $C_{12}$ and $C_{44}$ fully determine the elastic moduli for this material. The initial critical resolved shear stress is $\tau_0 = 100$ MPa. The line tension is taken to be $T = 7.5$ pN. The length of the Burgers vector is $b = 2.5$ nm and the grain diameter is assumed to be $d = 10$ µm for all grains unless specified. The small number of parameters of the model is noteworthy. The slip systems of the material, which crystallizes in the FCC class, are collected in Table 1.

3.3. Subgrain microstructural evolution

We begin by tracking the evolution of a single grain of orientation

$$
Q = \begin{pmatrix}
0.774 & 0.463 & -0.432 \\
-0.601 & 0.324 & -0.730 \\
-0.198 & 0.825 & 0.529
\end{pmatrix}.
$$

(3.9)

relative to the die coordinate system. As the specimen goes through the shear plane, three slip systems are activated: $\mbox{B}_2$, $\mbox{A}_2$, $\mbox{C}_5$ (cf Table 1 for Schmid–Boas nomenclature). The attendant lamellar structure predicted by the theory is of rank 2 and is shown in Fig. 5. The geometry and evolution of the lamellar structure is further shown in Fig. 6. The faces of the representative volume in this figure are chosen parallel to the coordinate planes. The morphological similarity of the predicted and observed microstructures, (Figs. 2 and 3), is noteworthy.

The evolution of local slip strains in the lamellae with the increasing deformation is plotted in Fig. 7a. The predicted pattern of slip activity is complex and shifts between systems. Thus, whereas the $\mbox{B}_2$ system
Fig. 5. Graph of the lamellar structure predicted after one ECAE pass in a randomly oriented grain.

Fig. 6. Geometry of lamellar microstructure at different stages of deformation.
Fig. 7. (a) Evolution of local slip strains with deformation and (b) evolution of lamellar thickness with deformation.

may be regarded a fragmentation of the original grains into lamellar subgrains. The misorientation angle between two adjacent lamellae having undergone lattice rotations \( R_i \) and \( R_j \) is the angle of the relative rotation \( R_i R_j^{-1} \). As noted at the introduction, the chief objective of the ECAE process is to simultaneously enhance the ductility and strength through deformation-induced grain refinement into the nanoscale. The resulting grain fragmentation introduces a range of low and high-angle subgrain boundaries. The optimal ECAE process should be such that the number of low angle boundaries is minimized. The evolution of these misorientation angles across lamellar boundaries is shown in Fig. 8. The figure shows the variation of misorientation angle between the pair of regions in each of two sets of laminates (A2–B2 and A2–C5). It should be noted that reduction in misorientation angles owing to the symmetry of the crystal is not performed for this plot. The misorientation between A2–B2 shows a rapid initial relative rotation followed by a gradual increase while a gradual increase is observed for A2–C5 relative rotation. Experimental trends show rapid initial increase in average misorientation angle followed by a steady increase with deformation.

Fig. 8. Misorientation angles across lamellar boundaries.
Fig. 9. (111) pole figures for Al, 90° ECAE: (a) initial random texture, (b) predicted texture half way through a pass, (c) predicted texture after one entire pass and (d) measured texture [36].

mation. The statistics of misorientation angles in polycrystalline metals predicted by the theory has been investigated by Aubry and Ortiz [3], who found good agreement with between theory and experiment.

The predicted evolution of lamellar sizes which increasing deformation is shown in Fig. 7b. As noted in the foregoing, the lamellar size is determined by a competition between the dislocation wall energy, which favors coarse microstructure, and the misfit boundary layers, or pileups, between grains and between twinned lamellae, which favors fine microstructure. The lamellar size $l$ roughly scales with the geometrical mean of two characteristic lengths, the grain diameter $d$ and the Burgers vector length $b$. The power-law behavior of the microstructural size predicted by the theory is evident Fig. 7b. Indeed, a simple estimate [22,23,3] gives the scaling relation $l \sim \sqrt{bd}/\gamma$, where $\gamma$ is the shear deformation experienced by material points as they cross the shear plane. This scaling relation is indeed roughly consistent with the power-law behavior observed in Fig. 7b, which is well-approximated by the relation $l \sim d^{0.45} \gamma^{-0.6}$. An analysis of the micrographs in Figs. 2 and 3 reveals a relation between grain size refinement with respect to deformation approximated by $l \sim \gamma^{-0.65}$ which is quite close the simulation results. The statistics of lamellar sizes in polycrystalline metals predicted by the theory has also been investigated by Aubry and Ortiz [3], who found good agreement between theory and experiment.
3.4. Polycrystal behavior

Texture measurements can also be conveniently used as a basis for the validation of the theory. We specifically consider the data provided by Vogel et al. [36], who have conducted a systematic investigation of texture evolution during ECAE in a variety of materials using neutron diffraction techniques.

In calculations we assume the polycrystal to obey Taylor’s hypothesis [33], i.e., each grain is assumed to undergo an average deformation equal to that undergone by the polycrystal. However, it should be noted that the deformation fields undergone by the grains differ at the microstructural level, owing to the formation of microstructure. This has the effect of enriching and diffusing the texture pattern relative to Taylor calculations without consideration of microstructure. An obvious improvement over the Taylor calculations would be the use of self-consistent models or other models of polycrystalline behavior accounting for grain-to-grain interactions (e.g., [6,16,5]), but such enhancements will not be considered here. However, as stated above, at the subgrain level, the lamella-to-lamella interactions that occur after the formation of microstructure are fully considered.

The initial texture of the sample is assumed to be random, Fig. 9a. Fig. 9b and 9c show the predicted (1 1 1) pole figures half way through one pass and after one entire pass, respectively. All plots are made using program POLE [34]. Finally, Fig. 9d shows the texture measured by [36] for aluminum. The gradual sharpening of the texture components can be observed in 9b. A comparison between Fig. 9c and 9d shows that the theory closely matches all observed texture components and their amplitudes.

The texture for a simulation of Taylor calculations without considering microstructure [4] is shown in Fig. 10 to show the sharpness of its texture pattern in comparison with the diffused texture pattern obtained in the calculations with the consideration of microstructure (Fig. 9c). This diffused texture pattern may be attributed to the fact that the subgrain lamella-to-lamella interactions are considered in the microstructure simulation as the lamellar microstructure forms.

4. Conclusions

We have applied the theory of single-crystal plasticity with microstructure of Ortiz and Repetto [22,23] in the limit of infinitely strong latent hardening [3] to the simulation of the ECAE process. The specific microstructures considered in the simulations are of the sequential lamination type [2]. The size of the microstructure has been estimated a posteriori by means of a nonlocal extension of the theory which accounting for textures in calculations.

Calculations assume a form of the microstructure that is a good qualitative representation of the grain size, grain boundary area, and grain boundary energy. Textures are calculated with a rotation of the random microstructure between 20° and 30°. This process is repeated for each pass.

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accounts for dislocation energies \([22]\). ECAE induces grain fragmentation in the form of fine lamellar structures in polycrystalline samples and is thus ideally suited to simulation by means of such tools of analysis. Texture evolution has been calculated simply by recourse to Taylor's hypothesis.

Calculations concerned with aluminum and 90° ECAE reveal a wealth of information regarding the geometry, size, and texture evolution of subgrain microstructures. The predicted sizes and textures are in good quantitative agreement with the available experimental data. In particular, we find that the lamellar widths \(I\) obey a power law of the form \(I \sim d^{0.45} \gamma^{-0.6}\) as a function of grain diameter \(d\) and shear deformation \(\gamma\). Texture evolution during ECAE is found to be the result of the overall grain rotation as well as relative rotations, or misorientation, between the various lamellae which form at the subgrain level. Owing to this subgrain contribution, the deformation textures are found to be more diffuse and have more structure than otherwise predicted by a Taylor conventional calculation.

The ability of the theory to predict these effects, despite its reduced number of parameters, suggests that it may be useful as a design tool for optimizing key aspects of the ECAE process such as the number of passes required to achieve a certain microstructural size, the optimal channel angle, and the optimal processing route.

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Abstract

This paper presents a formulation for modeling the deformation behavior of polycrystalline materials with emphasis on the development and description of anisotropic microstructure evolution models for modeling deformation and microstructure evolution in the simulation of Earth's crustal deformation. The results are presented in the context of anisotropic extension and compression.

Keywords: Adaptive, Geomechanics, Anisotropy, Microstructure evolution

1. Introduction

1.1. Related Work

Salt deformation processes, as well as the behavior of polycrystalline materials, have been extensively studied in the geological and geophysical communities.

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