Modeling of inelastic deformation of f.c.c. single- and polycrystalline materials with low stacking fault energies.

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ABSTRACT

A new rate-independent constitutive model for plastic deformation of crystalline materials deforming by slip and twinning has been formulated, and implemented in a finite-element program. We have simulated *three different structural levels* by choosing representative volume elements (RVEs) as *(i)* a small part of a single crystal for the analysis of the heterogeneity of plastic deformation in single crystals, *(ii)* a whole single crystal for polycrystal simulations, and *(iii)* a group of crystals for a Taylor-type model of polycrystals. We show that the predictions for the texture and stress-strain response from the model are in reasonably good agreement with experiments in plane-strain compression for a different single crystal and polycrystalline f.c.c. materials.

INTRODUCTION

The two main mechanisms for the plastic deformation of metals are crystallographic slip and deformation twinning. Twinning plays an important role in the plastic deformation of high symmetry materials with low stacking fault energy. The analytical modeling and computational accounting for twinning as a mechanism of plastic deformation is in its nascent stages. Review of the early considerations of twinning in crystal plasticity models is given by Chin (1975). In these early models the shear due to twinning was treated as pseudo-slip, but the rotation due to twinning was not accounted for, and hence these models were not capable of predicting crystallographic texture evolution. Evolution of texture due to slip and twinning has been considered by Van Houtte (1978), and more recently by Lebensohn and Tome (1994). However, their considerations have been targeted for the rigid-plastic, non-hardening case, and have been limited to polycrystalline materials.

We focus our attention on developing an elastic-plastic constitutive model and attendant computational procedure to simulate the stress-strain response and texture evolution in f.c.c. metals which deform by slip on twelve $\{111\} < 110 >$ slip systems and by twinning on twelve $\{111\} < 11\bar{2} >$ twin systems[1].

The overall plastic deformation of a crystal is always inhomogeneous at length scales associated with slip and twinning, and should be defined as an average over a volume element that must contain enough dislocation loops and twins to result in an acceptably smooth process at the continuum level of interest here. The smallest such volume element above which the plastic response can be considered smooth, is labeled as a representative-volume element. In our model we shall take a *small part of a crystal* as a representative-volume element (RVE) for single crystal analysis and a *whole crystal* for polycrystal simulations.

[1]Note that unlike slip, which can occur in either the positive or negative $< 110 >$ slip direction, twinning, because the underlying atomic arrangement is polar in nature, can occur in only one $< 11\bar{2} >$ type direction on a $\{111\}$ plane.

In this paper we report results of finite element modeling to predict the operative twinning-dominated deformations and crystallographic texture evolution during plane-strain compression of f.c.c. (*i*) *single crystals* which have been experimentally studied by Chin *et al.* (1969), and (*ii*) *polycrystalline structure*. We also report our results on Taylor-type simulation of polycrystalline α-brass. We show that our model is able to reproduce well the experimentally measured pole figures and stress levels. Thus, the crystal plasticity based elastic-plastic model is able to predict material behavior on different structural levels: from single crystal inhomogeneity to overall polycrystalline responce.

CONSTITUTIVE EQUATIONS

The two major kinematic issues in modeling twinning are: (*i*) accounting for the shear associated with twinning; and (*ii*) accounting for the reorientation of the crystal lattice due to twinning. Here we follow Van Houtte (1978) idea that the shear due to twinning is first accumulated as a pseudo-slip, that is, the shearing rate on the twin systems is taken to be given by $\dot{\gamma}^i = \dot{f}^i \gamma_0$, where γ_0 is the amount of twinning shear, and the crystal lattice is given the twinning-related orientation only if a probabilistic criterion, based on the relative volume fractions of the twinned and non-twinned parts of a crystal, is met.

The governing variables in the constitutive model are taken as: (*i*) The Cauchy stress, $\mathbf{T}$. (*ii*) The deformation gradient, $\mathbf{F}$. (*iii*) Crystal slip and twin systems labeled by integers i. Each system is specified by a unit normal $\mathbf{n}_0^i$ to the slip/twin plane, and a unit vector $\mathbf{m}_0^i$ denoting the slip/twin direction. The slip and twin systems $(\mathbf{m}_0^i, \mathbf{n}_0^i)$ are assumed to be known in the reference configuration. The amount of shear, γ_0, and the lattice rotation accompanying twinning, $\mathbf{R}^{tw}$, are also assumed to be known. (*iv*) A plastic deformation gradient, $\mathbf{F}^p$, with $\det\mathbf{F}^p = 1$. This represents the cumulative effect of dislocation motion and shear due to twinning on the active slip and twin systems in the crystal. (*v*) The slip and twin system deformation resistances $s^i > 0$, with units of stress. (*vi*) The twin volume fractions $f^i \geq 0$, with $\sum_i f^i \leq 1$ and $\dot{f}^i \geq 0$, which means the absence of detwinning events.

The elastic deformation gradient is defined by $\mathbf{F}^e \equiv \mathbf{F}\,\mathbf{F}^{p-1}$ with $\det \mathbf{F}^e > 0$, and it describes the elastic distortion of the lattice; it is this distortion that gives rise to the stress $\mathbf{T}$. Then, $\mathbf{E}^e \equiv (1/2)\left\{\mathbf{F}^{eT}\mathbf{F}^e - \mathbf{1}\right\}$ and $\mathbf{T}^* \equiv (\det \mathbf{F}^e)\, \mathbf{F}^{e-1}\mathbf{T}\mathbf{F}^{e-T}$ the Green elastic strain measure and the symmetric second Piola-Kirchoff stress tensor relative to the relaxed configuration.

Elastic stretches in metallic single crystals are generally small. Accordingly, the constitutive equation for the stress in a metallic single crystal is taken as the linear relation

$$\mathbf{T}^* = \mathcal{C}\left[\mathbf{E}^e\right], \tag{1}$$

where $\mathcal{C}$ is a fourth-order anisotropic elasticity tensor, where $\mathbf{E}^e$ and $\mathbf{T}^*$ are the strain and stress measures defined above.

Let $\mathbf{S}_0^i = \mathbf{m}_0^i \otimes \mathbf{n}_0^i$ denote the Schmid tensors, and let $\tau^i = (\mathbf{C}^e\,\mathbf{T}^*)\cdot\mathbf{S}_0^i$ denote the resolved shear stress on the ith slip/twin system. Then, the conditions for slip and twinning are taken as

$$\phi^i = \left|\tau^i\right| - s^i \leq 0. \tag{2}$$

During plastic flow the following consistency conditions must be satisfied: $\dot{\gamma}^i\,\dot{\phi}^i = 0$ if $\phi^i = 0$. The consistency conditions serve to determine the shearing rates $\dot{\gamma}^i \geq 0$ on the slip and twin systems. The shearing rates also are restricted by Kuhn-Tacker complementarity conditions $\dot{\gamma}^i\,\phi^i = 0$.

The evolution of the plastic deformation gradient is

$$\dot{\mathbf{F}}^p = \mathbf{L}^p\,\mathbf{F}^p, \quad \text{with} \;\; \mathbf{L}^p = \sum_i \dot{\gamma}^i\,\text{sign}(\tau^i)\,\mathbf{S}_0^i. \tag{3}$$

Here $\mathbf{L}^p$ given by the sum of the shearing rates on all the slip and twin systems.

The evolution equations for slip and twin resistances may be generically taken as $\dot{s}^i = \sum_j h^{ij}\,\dot{\gamma}^j$, where h^{ij} are the hardening moduli.

For the twin systems, evolution equations for twin volume fractions is given as $\dot{f}^i = \dot{\gamma}^i/\gamma_0 \geq 0$, where γ_0 is the twinning shear. The twinning shear corresponding to a twin system may be written as $\mathbf{S} = \mathbf{1} + \gamma_0\,\mathbf{m}_0 \otimes \mathbf{n}_0, \quad \mathbf{m}_0 \cdot \mathbf{n}_0 = 0, \quad \gamma_0 = 1/\sqrt{2}$, where $\mathbf{m}_0$ is a unit vector in a $< 11\bar{2} >$ direction, and $\mathbf{n}_0$ the unit normal to the associated $\{111\}$ plane. The corresponding twinning rotation is given by $\mathbf{R}^{tw} = 2\,\mathbf{n}_0 \otimes \mathbf{n}_0 - \mathbf{1}$.

During the "pseudo-slip" phase, the slip and twin system deformation resistances will be taken as constant. Leffers and co-workers (e.g., 1991, 1993) have reported that during plane-strain compression of brass, twins form thin lamellae which cluster to form bundles in grains, and that subsequent slip is restricted to planes which are parallel to these twin bundles. We have modeled this important kinematic restriction on the activity of the slip systems as follows. When the fraction $f = \max\{f^\alpha\}$, the maximum value of f^α taken over all twin systems, reaches a value $\lambda \approx 0.05$, slipping and twinning in systems whose slip/twin planes are not parallel to the plane of the twin system with maximum f^α are restricted by choosing appropriate values of slip and twin resistances.

The lattice reorientation condition is that if $f > \xi$, with $\xi \in [0.2; 1]$ a random number, then the orientation of the RVE be replaced by the twin related orientation. That is, if $\{\mathbf{e}_i^c | i = 1, 2, 3\}$ denotes a local orthonormal basis associated with the crystal lattice in the old relaxed configuration, then once this criterion is met the crystal basis in the new relaxed configuration of the crystal be taken as $\mathbf{e}_i^{c\,*} = \mathbf{R}^{tw}\mathbf{e}_i^c$.

Further, if the lattice reorientation condition is met, then the f^i are reinitialized to zero, and subsequent twinning in the RVE is suppresed by setting the twin system deformation resistances to a large value. However, subsequent slip in this RVE is allowed, and the values of all slip system resistances are set equal to the value of the resistance for the slip system(s) parallel to the twin system with the maximum f^i prior to the reorientation.

The constitutive equations and the time-integration procedure have been implemented in the finite-element program ABAQUS/Explicit (1995) by writing a "user material" subroutine.

PLANE-STRAIN DEFORMATION of F.C.C. Co-8% Fe SINGLE CRYSTAL

We shall simulate plane-strain compression of $(110)[\bar{3}34]$[2] specially oriented single crystals Co-8%Fe tested by Chin *et al.* (1969). The single-crystal calculations shown in this section were carried out by modeling a part of a single crystal as a single finite element. For the numerical simulation of plane-strain compression, 900 two-dimensional ABAQUS-CPE4R elements (continuum, plane-strain, 4-noded, reduced integration) were assigned to the single crystal. It is important to note that our 2-D finite element simulations incorporate the full 3-D slip and twin system structure. Plane-strain compression was modeled by constraining the top and bottom boundaries of the mesh to remain straight, with the bottom boundary subjected to zero displacement in the Y-direction, and top boundary subjected to

[2] These initial crystal orientations may alternatively be described in terms of the Euler angle notation $\{\theta, \phi, \omega\}$.

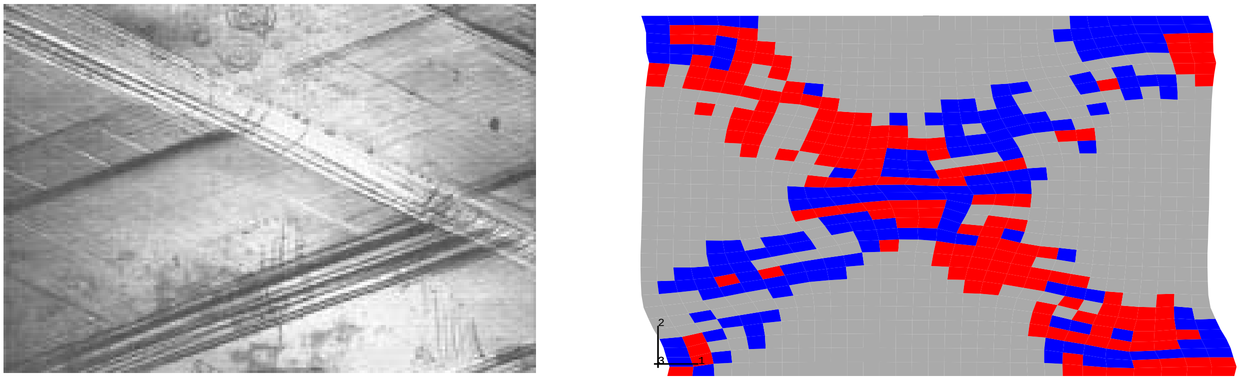

Figure 1: (a) Micrograph of the $(110)[\bar{3}34]$ oriented crystal showing twin bands (from Chin *et al.*, 1969). (b) The deformed FEM mesh with calculated twin bands.

a negative displacement in the Y-direction for a total compressive strain of 20%. For the vertical boundaries we imposed periodic boundary conditions, defined as follows. Let $\mathbf{u}_l$ and $\mathbf{u}_r$ respectively denote the displacements for a node on the left boundary and another on the right boundary which is at the same horizontal level in the initial mesh, and let $\mathbf{d} = \mathbf{u}_r - \mathbf{u}_l$ denote the relative displacement for this pair of corresponding nodes on the left and right boundaries. Then, partially periodic boundary conditions are specified by requiring that $\mathbf{U}_{right} - \mathbf{U}_{left} = \mathbf{d}$, where $\mathbf{U}_{left}$ and where $\mathbf{U}_{right}$ are the vectors of displacements of all the nodes for the left and right boundaries, respectively.

In the numerical simulations reported below, we have used the following values for the initial slip and twin resistances: $s_0^{twin} = 70\,\text{MPa}$; $s_0^{slip} = 40\,\text{MPa}$. A micrograph of the deformed specimen taken from Chin *et al.* (1969) is shown in Fig. 1a. This picture shows that a mixture of slip and twinning has occurred on the (111) and $(11\bar{1})$ planes. Our corresponding finite element simulation is shown in Fig.1b.

Our calculations also predict that slip occurs on the $(111)[\bar{1}01]$ and $(11\bar{1})[0\bar{1}\bar{1}]$ systems, and twinning occurs on the $(111)[1\bar{2}1]$ and $(\bar{1}\bar{1}1)[\bar{1}21]$ systems. The elements twinned by the $(111)[1\bar{2}1]$ system are shaded black, and those twinned by the $(\bar{1}\bar{1}1)[\bar{1}21]$ system are shaded dark grey. The calculated twin bands intersect at an angle close to that observed in the experiments (Fig. 1a).

Texture evolution is one of the most important characteristics of slip/twin systems activity. Fig.2(a) presents the {111} stereographic pole figure of the crystal in its initial orientation. The pole figure predicted by the finite element calculations is shown in Fig.2(b), together with the experimentally measured (Chin et al., 1969) pole figure in Fig. 2(c). The agreement between numerically predicted and experimentally measured texture is very good.

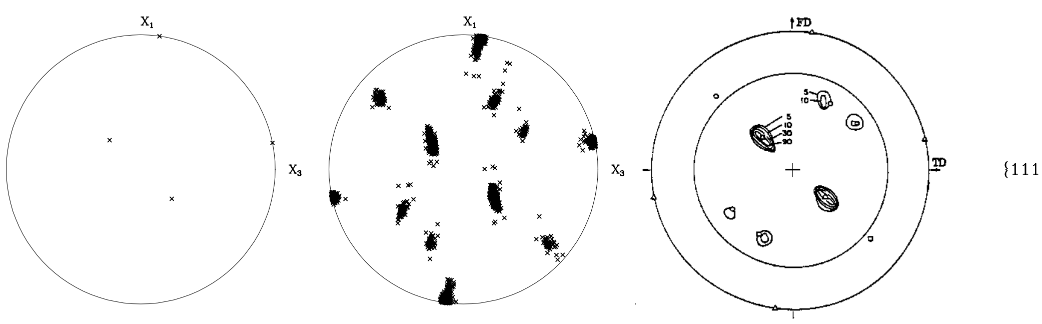

Figure 2: {111} pole figures for $(110)[\bar{3}34]$ oriented crystal. Initial (a), FEM calculated after plane-strain compression to 20% (b), and experimentally measured (Chin et al., 1969) (c).

PLANE-STRAIN DEFORMATION of F.C.C. α-BRASS POLYCRYSTAL

Finite-element calculations for plane strain compression of an aggregate of 225 initially randomly-oriented grains were carried out with various values of the material parameters. Each grain was considered as RVE and modeled as plane strain finite element. The results of plane strain finite element calculations are very close to the full 3D plane strain simulations with 343 (cube $7 \times 7 \times 7$) ABAQUS brick elements (for details of this see Staroselsky and Anand 1998). The process of curve-fitting the plane strain compression stress-strain data to obtain the value of the hardening parameters yields $s_0^{slip} = 25$ MPa, $s_0^{twin} = 155$ MPa,

The quality of the curve-fit is shown in Figure 3. One can see that the calculated stress-strain response is very close to the experimentally observed one. The jumps on the numerically calculated curve at strains greater than ≈ 0.5 are due to the crystal lattice rotations of the grains during twinning.

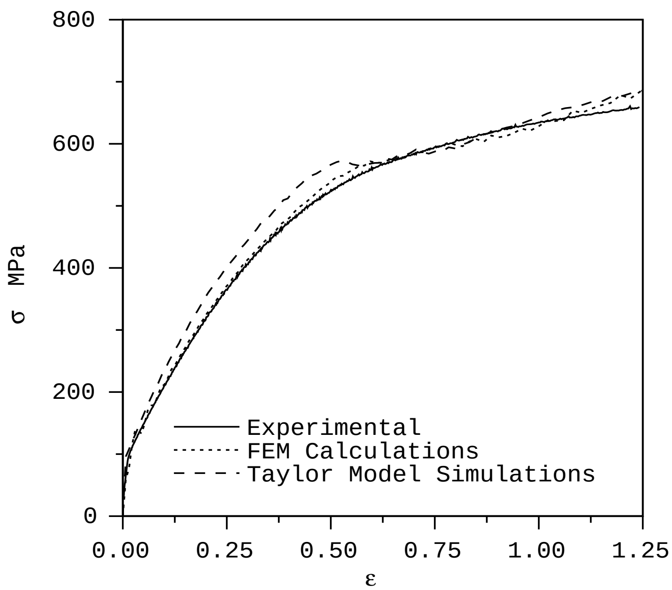

Figure 3: Comparison of the experimentally-measured stress-strain curves for plane strain compression of α-brass against a finite element model as well as against a Taylor model.

The numerical calculations show that because of the different values of slip and twin resistances, in the initial stages of deformation the grains deform by crystallographic slip only. The slip deformation resistances increase due to strain-hardening, and at a level of macroscopic strain of approximately 10%-15%, the first threshold, for the twin fraction used to restrict slip, is reached in some grains. At this stage the slip resistances increase very fast for all systems other than those which are co-planar with the dominant twin system; dominant crystallographic shearing occurs along the chosen crystallographic plane in a given crystal. When the second threshold for the twin fraction $f = \max\{f^\alpha\}$ is reached, $f > \xi$, with ξ a random number distributed over the interval $[0.2; 1]$, the crystal lattice is replaced with a twin-related one, and as discussed previously, all twin system deformation resistances and all slip system resistances are set to the values corresponding to those for the active twin system. With our choice of material parameters, the crystal lattice rotation due to twinning starts at about 45% macroscopic strain. Before this level of deformation, the calculated pole figures are very close to those typical for f.c.c. materials deforming by slip alone. Experimentally measured and numerically predicted equal area $\{111\}$ and $\{100\}$ pole figures for plane strain compression after 100% of compression are shown in Fig. 4.

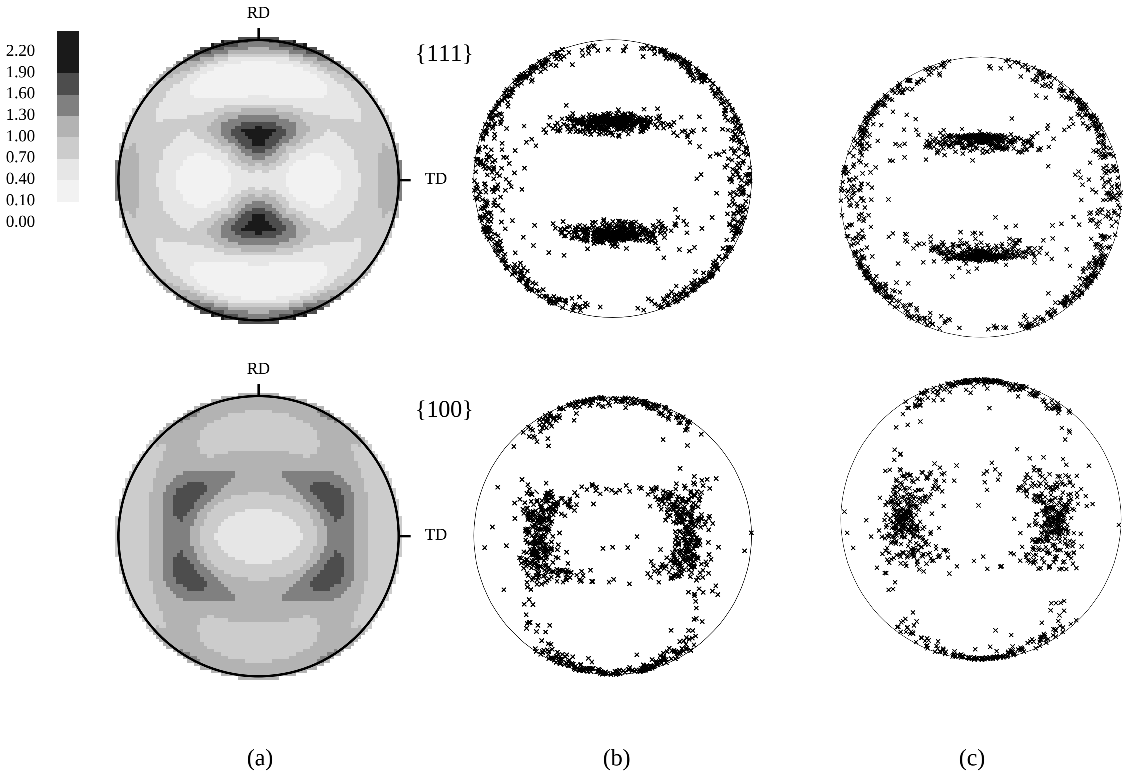

Figure 4: Comparison of the (a) experimentally-measured pole figures after 100% plane strain compression of α-brass against (b) finite element model predictions and (c) Taylor model predictions.

Our numerical experimentation shows that the "brass-texture" is a result of both mechanisms: constrained slip, *and* the lattice reorientation due to twinning. Each of these mechanisms alone is insufficient for accurate model predictions.

A very large body of literature exists on application of the Taylor model for texture prediction. The main assumption of this model for a polycrystal is that the deformation gradient in each grain is homogeneous and equal to the macroscopic one at a material point. If, in addition, we assume that all grains have equal volume, then the average Cauchy stress at each macroscopic continuum point is simply the number-averaged stress (Asaro and Needleman, 1985). With the material parameters calibrated for the finite-element model of the polycrystal, our Taylor model simulations slightly overpredict the stress-strain responses in both plane strain compression and simple compression. The texture predictions from the two modeling schemes are very similar. Thus, the Taylor model may be used for obtaining computationally inexpensive and reasonably accurate predictions of both the stress-strain curve and the crystallographic texture of f.c.c. materials deforming by combined slip and twinning.

CONCLUDING REMARKS AND FUTURE DIRECTIONS

Our calculations clearly demonstrate the ability of our constitutive model and computational procedure to capture the major features of plastic deformation of crystalline f.c.c. material due to slip and twinning at different scales: from a part of a single crystal to a large polycrystalline aggregate.

However, as formulated, the constitutive model has a number of limitations: (i) The important role of twin-boundary energy is neglected in the model. (*ii*) There is no length scale in the model. Much work needs to be done to improve our understanding of the slip and twin hardening and hardening interactions, and their mathematical representation. For this and for the analysis of the width of the twin bands, a suitable length scale associated with non-local effects of twinning needs to be introduced into the constitutive model.

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