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Development of local shear bands and orientation gradients in fcc polycrystals

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ABSTRACT: A finite element formulation which derives constitutive response from crystal plasticity theory is used to examine localized deformation in fcc polycrystals. The polycrystals are simple, idealized arrangements of grains. Localized deformations within individual grains lead to the development of domains that are separated by boundaries of high misorientation. Shear banding is seen to occur on a microscopic scale of grain dimensions. The important consequences of these simulations are that the predicted local inhomogeneities are meeting various requirements which make them possible nucleation sites for recrystallization.

1 INTRODUCTION

Efforts that combine the finite element method with crystal plasticity models are often applied to problems of macroscale deformations. In such applications, polycrystal plasticity theories provide a useful means of introducing a description of material anisotropy which is both intializable and evolvable. There is however another research path that is providing valuable results: the study of material microstructure. The ability of finite element formulations to address gradients in the deformation field enables the researcher to probe grain-to-grain interactions in the microstructure.

With regard to fcc metals with high stacking fault energy, a question that has been the subject of much labor concerns the origin of recrystallization nuclei. It is well established that aluminum and copper, when rolled to sufficient reduction and then subsequently heat treated, will develop a strong recrystallization texture. Upon heat treatment, strain free grains with orientations different from adjacent grains appear. Growth of these recrystallized grains is aided by the motion of high-angle boundaries (Vandermeer & Juul Jensen 1994). In fcc metals, this recrystallization texture is often dominated by the cube orientation - an orientation that is not predicted when the usual crystal plasticity models are applied to homogeneous plane strain compression.

Looking back (before any heat treatment) to the prior cold working of the metal, it is the intent of this work to assess the potential of a finite element model to develop the mis-orientations, then - possibly - the specific cube orientations which have been the focus of so much experimental work.

1.1 *Development of misorientation in the deformation microstructure of fcc metals*

Generation of large-angle subboundaries may possibly procede from a variation of slip system activity throughout a grain (Kocks *et al.* 1994). Microscopic variations in slip lead to local domains with differences in the plastic rotation. Subdivision occurs within a grain, with some misorientation existing between adjacent domains. Several names have been given to microstructural features of this general kind: dislocation boundaries, dense dislocation walls, microbands, lamellar boundaries (Hansen & Juul Jensen 1992, Hughes & Hansen 1994). From the viewpoint of achieving a nucleus for recrystallization, we will restrict our consideration to "domains", separated by relatively high misorientation, developing within a grain.

1.2 *Generation of cube orientations in plane strain compression*

Numerous researchers have offered experimental evidence showing the presence of cube orientations in deformed microstructures. Inhomogeneity of the imposed strain field due to friction effects and tool geometry leads to mesoscale shearing which produces the rotated cube component (100)[011] (Hansen & Mecking 1975, Fedosseev & Gottstein 1993). For moderate reductions of 80-90%, cube orientations rotated about the sheet normal N have been observed in polycrystals (Doherty *et al.* 1993) and single crystals (Kamijo *et al.* 1993). At reductions of 95% or more, true cube orientations begin to appear from recrystallization (Nes & Dons 1986, Doherty *et al.* 1993)

Kamijo *et al.* (1993) have noted the importance of aspect ratio on the formation of cube nuclei. In experimental studies involving rolling of a single $\mathcal{S}$-orientation, the generation of cube nuclei is enhanced by increasing the crystal length-to-thickness ratio. In addition, the cited work has pointed to the formation of (001)[uv0] (N-rotated cube) due to deformation inhomogeneity required to maintain compatibility amongst neighboring grains.

The Dillamore and Katoh (1974) mechanism provides for divergent rotation within a grain. As the orientation gradient within the grain increases, a cube orientation is formed in a transition band inside of the grain. Recently, Lee *et al.* (1994) have proposed a deformation banding model which produces cube orientations at reductions of 80%.

1.3 *Objective*

The objective of this work is to address two questions:

- can regions of high misorientation be developed due to deformation heterogeneities arising from grain-to-grain interaction, and
- are cube (or near cube) orientations developed in regions of deformation heterogeneity?

Two model arrangements of crystals are developed to study the development of deformation heterogeneity.

2 METHOD

2.1 *Description of the Hybrid Finite Element code*

The hybrid element formulation is a viscoplastic formulation centered on two residuals (treatment of the incompressibility constraint is detailed in Beaudoin *et al.* (1994). A statement of equilibrium is derived from the traction balance between elements, as

$$0 = \sum_e \left[\int_{\mathcal{B}_e} tr(\sigma \mathrm{grad}(\Phi))\, dV + \int_{\mathcal{B}_e} \Phi \cdot \mathrm{div}(\sigma) dV - \int_{\partial\mathcal{B}_t} \Phi \cdot \mathrm{t}\, dA \right] \quad (2.1)$$

where σ is the Cauchy stress, t are tractions, $\mathcal{B}_e$ is the element volume, $\partial\mathcal{B}_t$ is the element surface, and Φ are weighting functions. A second residual is formed for the deviatoric stress derived from the crystal consitutive response

$$\int_{\mathcal{B}_e} \mathbf{T} \cdot \mathcal{C}[\sigma'] dV = \int_{\mathcal{B}_e} \mathbf{T} \cdot \mathbf{D}' dV \quad (2.2)$$

where σ' and $\mathbf{D}'$ are the deviatoric portions of the stress and deformation rate, $\mathcal{C}$ describes the constitutive response, and $\mathbf{T}$ are weighting functions. The combined use of a single orientation (or single polycrystal aggregate, though not utilized here) in each element with piecewise discontinuous shape functions for the deviatoric stress facilitates concurrent (parallel) computations. Hence, these simulations are particularly well-suited to massive parallel architectures. Spectral decomposition of the mesh is used to partition the unassembled global system of equations. Adherence to Fortran-90, with communications performed through library routines allows for porting of the code (even to workstations).

2.2 *A hypothetical bicrystal*

To explore the ability of a particular orientation to accommodate its surroundings in plane - strain compression, a hypothetical bicrystal structure was investigated (Figure 1). A single orientation, representing a grain, was imbedded in an environment consisting of a single $\mathcal{S}$-orientation, $\{123\} < 634 >$. The entire assembly was then subjected to a plane strain compression.[1] Nodes on the two free faces (faces with normal to R) were constrained such that the structure retained a brick shape.

Three interior grains were examined using (ψ,θ,ϕ) in the convention of Kocks: (10,12,22), (35,45,30), and (55,12,22). Mesh configurations of $12 \times 12 \times 12$, $16 \times 16 \times 16$, and $32 \times 32 \times 32$ were used.

[1] To simplify discussion of the resulting texture, the axes of the sample coordinate system for the plane strain compression will be referred to using their rolling counterparts: R (rolling), T (transverse), and N (normal) directions.

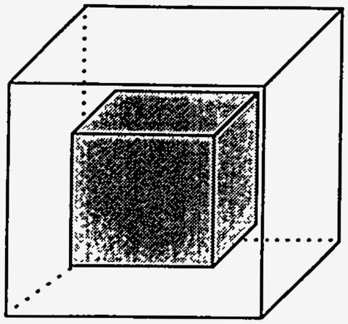

Figure 1. The bicrystal.

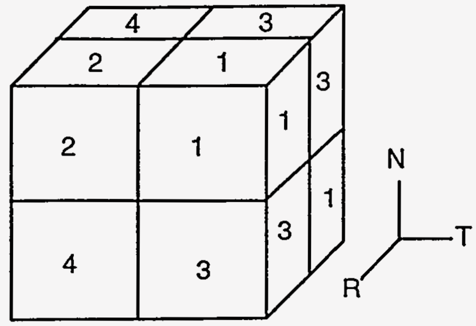

Figure 2. The S-array.

2.3 *Array of S-orientations*

This model was developed with the intention of producing a periodic structure which maintained orthotropic sample symmetry during plane strain compression (at least in the interior, on a local scale). In rolling of a single crystal with an S-orientation, there are two shears produced: ϵ_{RN} and ϵ_{TN}. The positive and negative sense of each of the two shears combine in four combinations for the four respective symmetrical orientations. In our model, the four symmetrical S-orientations were placed in a $2 \times 2 \times 2$ array (Figure 2). The symmetrical orientations were arranged such that the shears balanced along center planes with normals in the R and T directions. This structure will be referred to as the S-array.

Mesh densities of $16 \times 16 \times 16$ and $32 \times 32 \times 32$ were used. For reasons to be described subsequently, simulations were run with two initial geometries. One geometry was initially cube-shaped, the other was brick-shaped with relative proportions in directions of R:T:N as 2:1:$\frac{1}{2}$.

3 RESULTS

3.1 *The bicrystal*

Results for the (35,45,30) and (55,12,22) interior grains are shown in Figures 3 and 4. In these plots, the inside of each element is shaded according to the middle Euler angle, θ. The boundary is shaded in proportion to the misorientation of an element with its neighbor; a solid black border indicates a misorientation of 10° or more.

Distinct structures were observed for each of the three trial orientations. For the orientation (10,12,22), a gradient in orientation was present across the grain, but not so great that any significant misorientation was developed. In contrast, a slice with normal in the T direction for the (35,45,30) orientation shows the development of a distinct boundary near the edge of the grain (Figure 3). The most interesting result was provided by the orientation (55,12,22). Here, a band courses through the grain which is sharply misoriented from the grain bulk (Figure 4). It was the resolution of this band that prompted refinement of the mesh outlined above; the band appeared in the same location for all mesh configurations.

In an effort to rule out hardening as an initiator of the localization, the simulation of the (55,12,22) orientation was re-run with a high hardening rate so as to prevent saturation of the flow stress. Changes in hardening rate did not alter the texture development.

For the bicrystal shown in Figure 4, orientations within the band have the (001) crystal axis quite close to the sheet normal direction: they are close to "cube". These orientations were rotated cube; band orientations with closest coincidence between the crystal (001) axis and the sheet normal were rotated roughly 30° degrees from the sheet rolling direction.

3.2 *S-array*

Initial trials were carried out with a 1:1:1 aspect ratio. Figure 5 shows the mesh after a 50% reduction. The view shown in Figure 5 is a cut through the mid-plane with normal in the T direction. The symmetry designed into the problem, that center-planes with normals T and R would remain plane, was clearly maintained. Shearing deformations are quite severe. Similar to the bicrystal simulation of Figure 4, bands develop within the mesh. Situated in the bands are cube orientations - again, of the N-rotated cube variety.

Kamijo et al. (1993) have suggested that the grain aspect ratio plays a role in the development of cube orientations from an initial S-orientation.

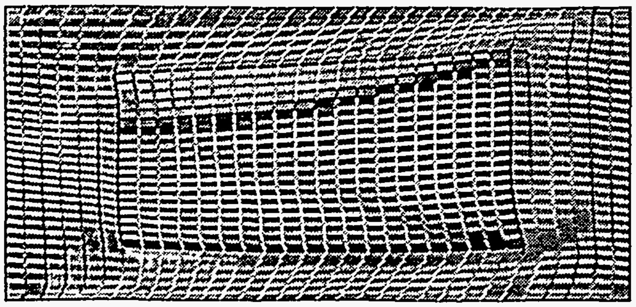

Figure 3. Bicrystal with (35,45,30) interior grain.

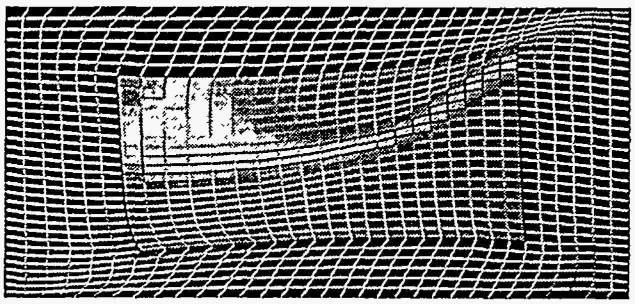

Figure 4. Bicrystal with (55,12,22) interior grain.

Prompted by this suggestion, simulations were re-run with the flattened aspect ratio of 2:1:$\frac{1}{2}$ (R:T:N). Results after a reduction of 80% are shown in Figure 6. Orientations from the light-shaded regions of Figure 6 are also shown in the accompanying < 100 > pole figure. There are clusters of cube orientations which are now within 20° of "true" cube.

The rotations of a single orientation - marked in Figure 6 - from S towards (001)[100] is shown in Figure 7. The rotation of an adjacent orientation is shown in Figure 8. Here, it is seen that the neighboring region re-orients towards a symmetrical orientation.

4 DISCUSSION

It is known that inhomogeneities in deformation may be introduced on a mesoscopic scale in the sense that they are not confined to a single grain as a consequence of the imposed strain field (due to friction effects and tool geometry) or by strain localizations due to instabilities of flow (caused by work hardening characteristics and rate sensitivity). The present paper shows that shear banding occurs also on a microscopic scale (of grain dimensions); it is presumably caused by the reaction forces set up between grains with no regard to the inhomogeneities of either the external strain field or by strain localization. These interactions again produce shear zones with a similar strain geometry to the mesoscopic shear bands and similarly, the rotated cube appears.

Several observations of structure development in these idealized models concur with descriptions made in experimental studies.

- Clearly, the present work points to the possibility of developing domains within a grain that are separated by boundaries of high (> 10°) misorientation. Two distinct structures were observed: a grain breaking up into domains and bands of orientations which are mis-oriented (on both sides of the band) from the grain bulk. These domains follow from slip variations within the grain leading to differential rotation between domains.
- At intermediate reductions, N-rotated cube orientations appear in bands. In the bicrystal and S-array models, the bands are produce by shear deformations initiated through grain interaction.
- To effect a rotation of an element towards true cube requires quite large deformations. Combining the aspect ratio of the initial configuration with reduction of the flattened S-array, a 95 % reduction from an equiaxed substructure was required to produce the near cube sites.

The important consequences of these simulations are that the predicted local inhomogeneities are meeting various requirements which make them possible nucleation sites for recrystallization. First, they are sufficiently narrow so that a nucleus picks up quickly a strong orientation difference with its neighborhood as it expands into its environment; a high-angle, and therefore highly mobile, boundary is formed quickly. Secondly, they are everywhere in the microstructure since they form in every grain at large enough strains and are dispersed throughout the whole volume.

Though the precise (001)[100] cube orientation was not produced in this work, with high grain aspect ratio and reduction orientations with closer rotation towards true cube were developed. In the Dillamore and Katoh (1974) theory, cube orientations form in transition bands generated by the deformation of (001)[uv0] orientated material. The suggestion by Kamijo *et al.* (1993) that a slip rotation from S towards an intermediate (001)[uv0] orientation may arise from to local inhomogeneities in deformation is supported by the present work.

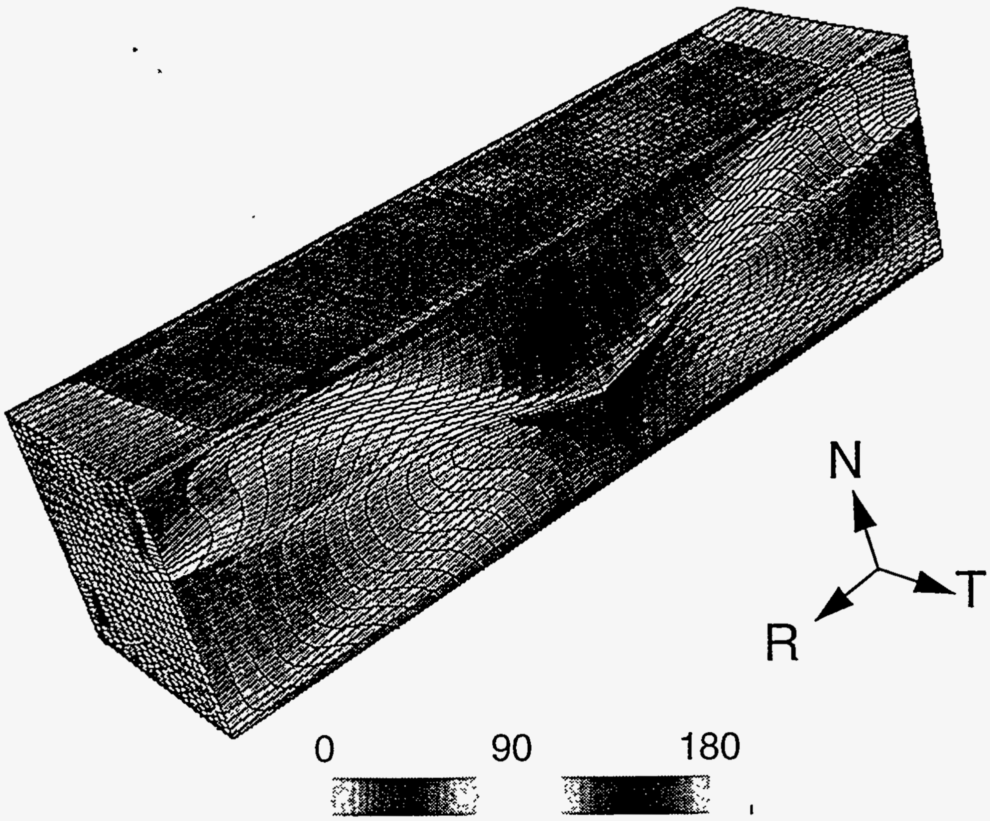

Figure 5. Array of $\mathcal{S}$-orientations shown after 50% reduction. N-rotated cubes lie on shear shear band.

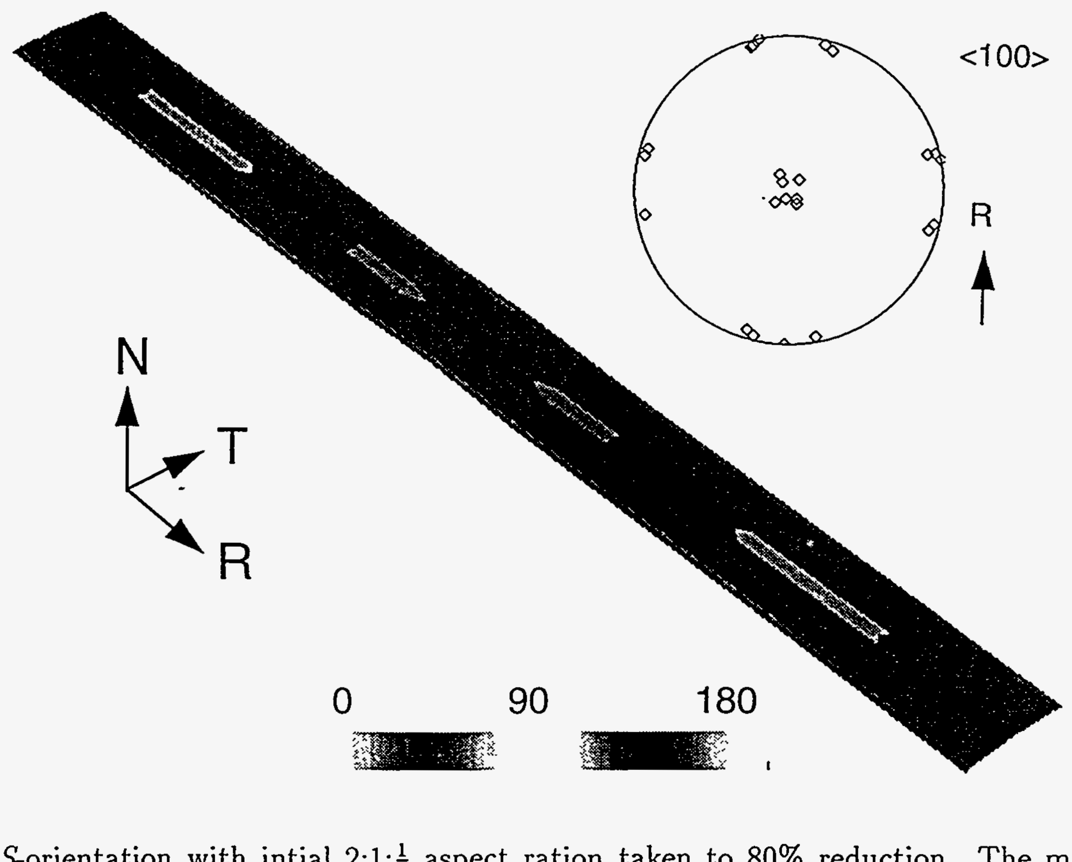

Figure 6. $\mathcal{S}$-orientation with intial 2:1:$\frac{1}{2}$ aspect ration taken to 80% reduction. The mid-plane with normal N is shown.

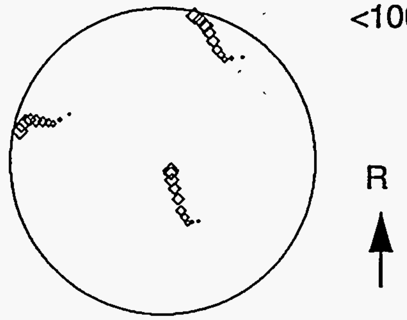

Figure 7. Rotation of an element orientation from "S" to cube.

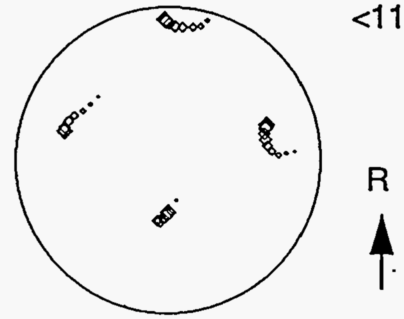

Figure 8. Rotation of an orientation from an element adjacent to that shown in Figure 7. The rotation is toward a symmetrical position.

Finally, a few comments must be made with regard to the numerical aspects of the work. Much effort was placed in refining the mesh to resolve gradients in the texture. In all of the simulations, the pattern of texture development was unchanged with the mesh discretization. For the bands containing the N-rotated cube shown in Figures 4 and 5, it was possible to capture two or more elements at or near rotated cube within the band. This was not the case for the S-array with flattened aspect that produced the truer cubes. Here, the texture gradients appear to be quite severe, with a cube orientation lying in the center of typical rolling orientations. Future efforts will focus on mesh refinement necessary to better capture this gradient and enable studies of higher reduction.

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