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AUTHOR(S): U. Fred Kocks, CMS; J. D. Embury, McMaster University; J. D. Cotton, MTL-
S. R. Chen, MTL-5; A. J. Beaudoin, Reynold Metals Co; S. I. Wright, MTL-6
A. D. Rollett, DIR

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ATTEMPTS TO MODEL THE GENERATION OF NEW GRAIN BOUNDARIES
DURING THE DEFORMATION OF POLYCRYSTALS†

U. F. Kocks¹, J. D. Embury², J. D. Cotton¹, S. R. Chen¹

A. J. Beaudoin³, S. I. Wright¹, and A. D. Rollett¹

¹Los Alamos National Laboratory, Los Alamos, NM 87545 USA

²McMaster University, Hamilton, Ont. L8S 4L7, CANADA

³Reynold Metals Co., Richmond, VA 23219 USA

Abstract

We explore ways by which new orientations ("nuclei") can arise during essentially homogeneous deformation in polycrystals. All of these can be categorized as generating new large-angle boundaries: one is due to excessive storage of dislocations of one sign parallel to existing grain boundaries; another is due to reactions of cell walls with grain edges; and in the last, new boundaries are created surrounding a domain of different slip system distribution.

Introduction

It is generally realized that the "nuclei" for recrystallization must be already present in the deformed structure. The flat regions of new orientations generated by heterogeneous deformation in kink bands and shear bands are possibilities, and have been clearly identified as early recrystallization sites, in both mono- and polycrystals [1]. However, even in the absence of such macroscopic heterogeneities, recrystallization does occur. In polycrystals, grain boundary regions might provide sufficiently special sites and have indeed been so identified, especially during dynamic recrystallization [2,3]. Some of these effect may relate to the occurrence of grain boundary sliding, others to a higher level of local stored energies (whose gradient provides the driving force for the motion or perhaps "bulging" of high-angle grain boundaries). The concern in "nucleation" is not so much with the *motion* of high-angle boundaries as with their *generation*.

The purpose of our current investigation is to further explore ways by which new orientations ("nuclei") can arise due to mechanisms specifically connected with deformation in polycrystals. All of these can be categorized as generating new large-angle boundaries - either parallel to an existing grain boundary, or around a grain edge, or surrounding a domain near a grain boundary; these three will be addressed in turn.

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Excess Dislocation Storage Near Grain Boundaries

Plastic deformation in polycrystals of homogeneous materials with a sufficient number of easy deformation modes proceeds in an essentially uniform manner on a macroscopic scale [4]. One may expect a somewhat higher rate of dislocation accumulation near grain boundaries [5,6]. This could have two effects. First, the rate of energy storage could be locally higher; however, while this would provide a greater driving force for the motion of existing boundaries, it is not clear how a greater stored energy should help in the generation of new boundaries. Second, one may expect a higher excess of one sign of dislocation on one side of the boundary, and the other sign on the other side (much as in cell walls [7,8]). This has been observed in Cu [9]. It could lead to a greater tendency for polygonization into subgrains with, perhaps, a somewhat greater misorientation than normal subboundaries would exhibit. These special subboundaries should be more or less parallel to the grain boundaries.

One such case has been observed: Figure 1 shows a TEM micrograph, Fig. 2 the misorientations as a function of distance. The cell walls are sharper near the grain boundary, and the misorientations accumulate. Continuing this process would be tantamount to continuous polygonization or "progressive lattice rotation" [3]. Fig. 1 was taken from a copper specimen that had already undergone some dynamic recrystallization; its stress/strain history is shown in Fig. 3 [10]. In non-cell-forming materials like Al-Mg alloys at high temperature, the same process would occur without the intermediary of recovering cell walls [11,12]. Note that the sharp cell walls in Fig. 1 are not only parallel to the boundary but retain their equi-axed nature; this could be the reason for the scalloping or neck-lacing often observed at boundaries [2].

It is also interesting to note that, in cyclic deformation at low strain amplitudes, the opposite effect has been observed (in Ni at 600°C)[13]: the cell walls are more diffuse near a grain boundary than in the grain interior; but also, dynamic recrystallization is much more difficult under these conditions.

For subboundaries to become possible sites for new large-angle boundaries, they would have to lose any debris accumulated in them during their formation, for example, by diffusive annihilation of dipoles. Once they are clean, they could move and associate into larger-angle subboundaries parallel to grain boundaries. Note that all subboundaries that form near one side of a boundary would have the same sign, so that mutual annihilation would be much less likely than an increase in misorientation.

Interaction of Subboundaries with Grain Edges

Recrystallization is often observed to begin near grain edges [14]. An interesting situation of this kind was observed by TEM in a copper polycrystal foil from specimen A in Fig. 3: Fig. 4(a). One can recognize a former "triple point" (a two dimensional section of a grain edge) where three straight grain boundaries met. In its neighborhood a new grain (B) appears to have formed. Its boundaries are curved out toward grains C and D; the boundary to grain A is straight. Detailed determination of the orientations by Kikuchi diffraction pattern analysis (Fig. 4b) revealed that the A/B boundary is a small-angle tilt boundary, of about 5° misorientation. This observation is supported by the presence of a visible, fine dislocation array in this boundary.

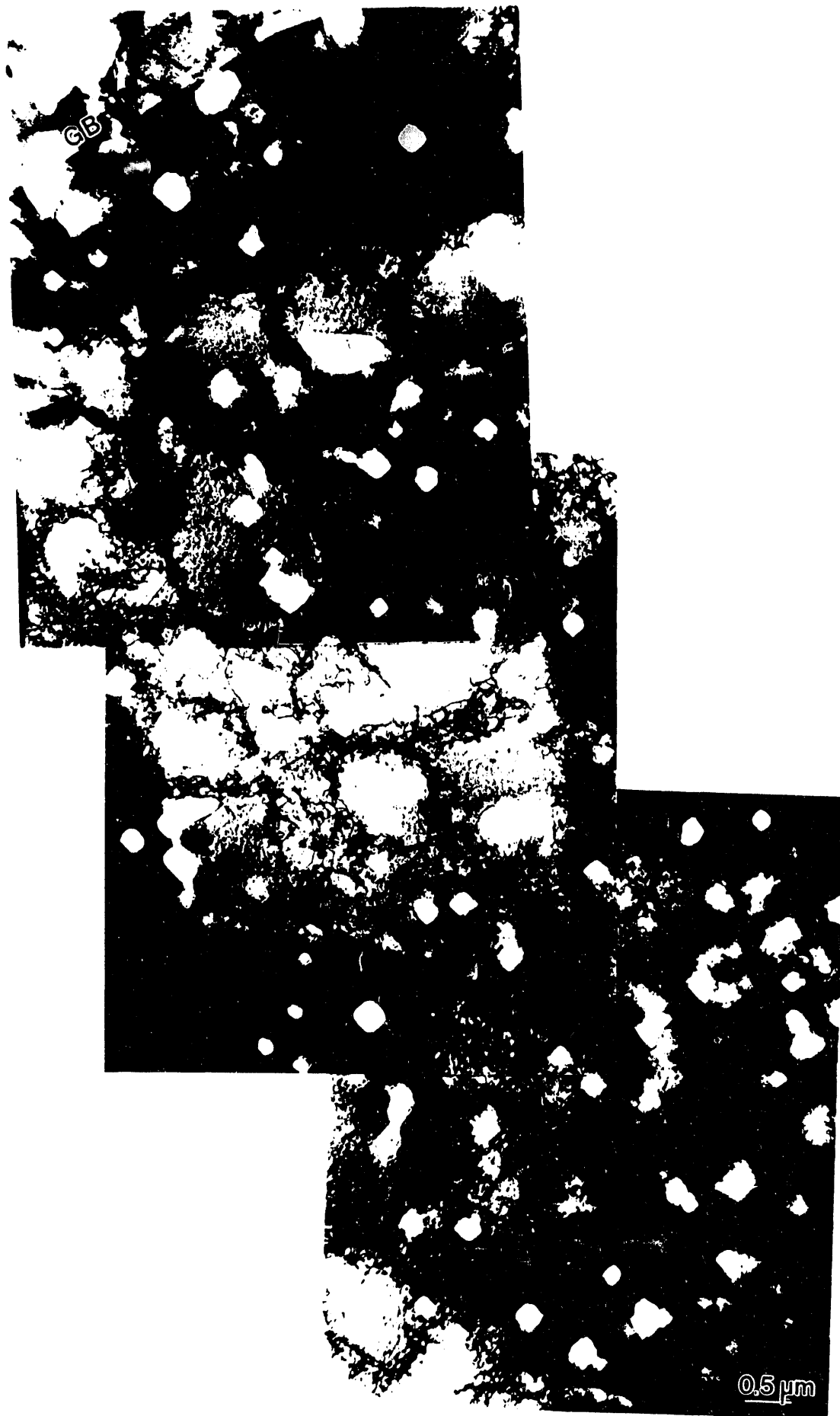


Fig. 1 - TEM micrograph demonstrating that the cell walls in a copper sample become sharper as a grain boundary (GB) is approached. History: B in Fig. 3.

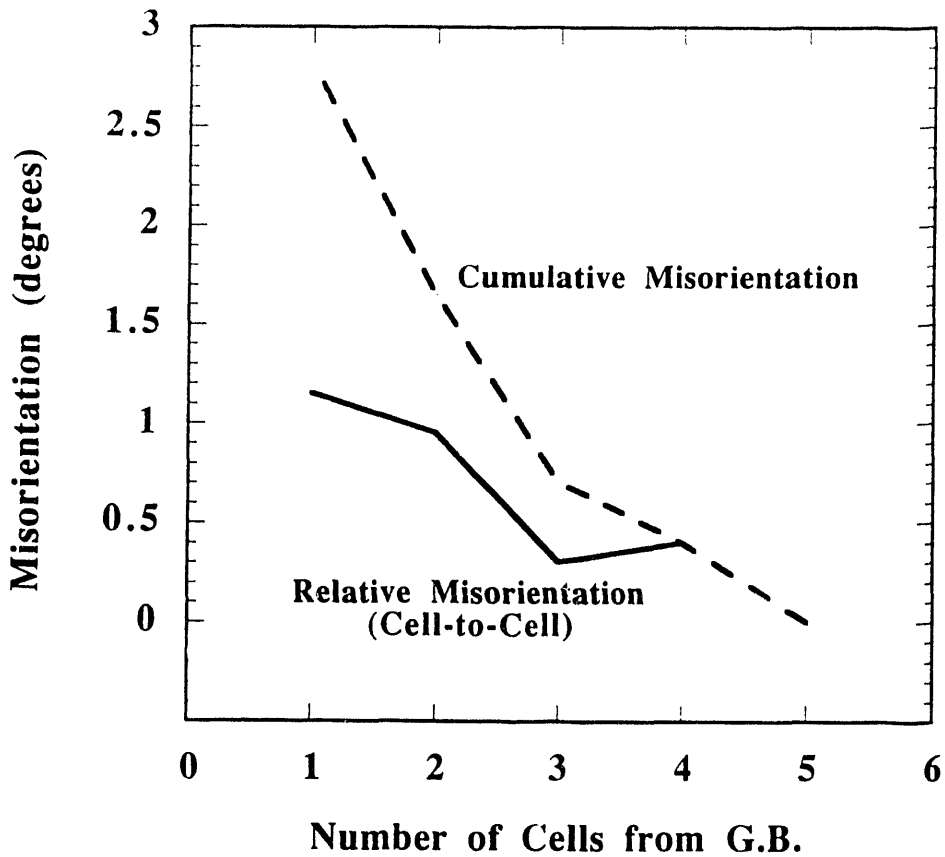


Fig. 2 - Relative and cumulative misorientation between cells in a sample similar to Fig. 1.

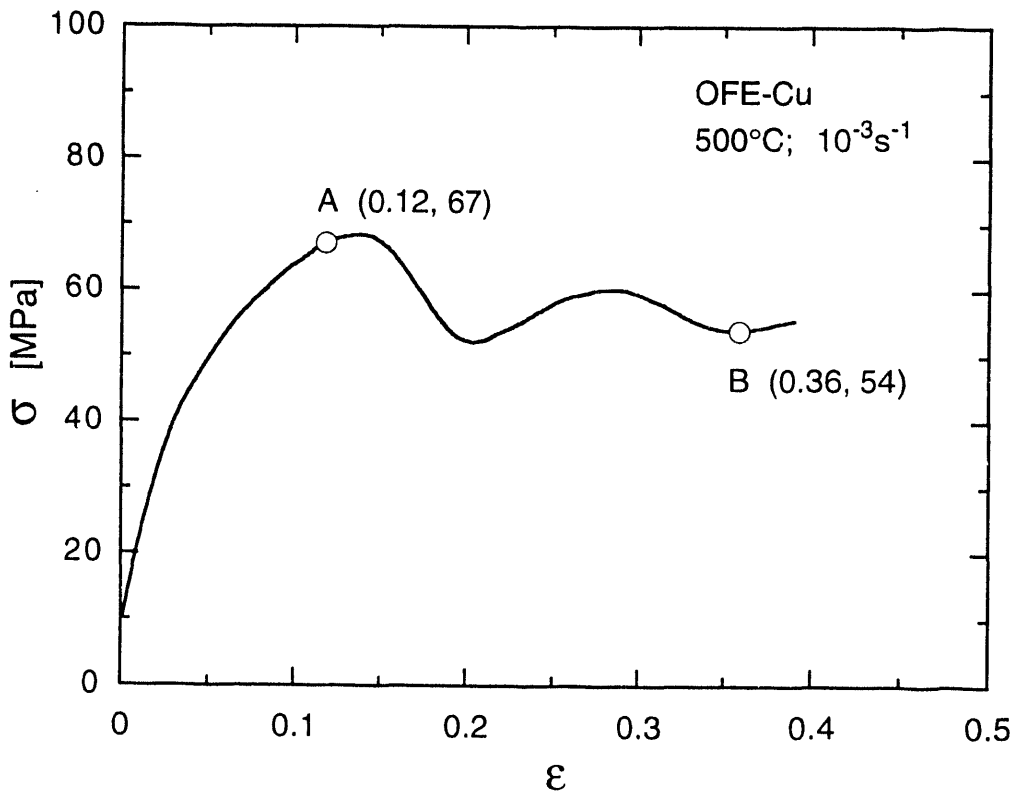


Fig. 3 - True stress strain curve of deformed copper polycrystal [10]. Sample B was used for Fig. 1, sample A for Fig. 4.

It was observed that the dislocation density is high and approximately equal in grains A, C, and D, but apparently lower in grain B. We surmise that the sequence of events was as follows. A subboundary formed in grain A, near one of its edges. The region between it and the edge was relatively free of dislocations. How and why these two steps occurred (in sequence or simultaneously) is not clear. However, once this situation arises, the standard thermodynamic argument for motion of boundaries into grains of higher stored energy density would explain why the boundaries B/C and B/D obviously moved into grains C and D, respectively, by a fair amount. Note that their curvature varies: it is higher where cell walls intersect the boundary. Thus, it is perhaps not necessary to claim the region between the A/B subboundary and the original grain edge to have been free of dislocations: only free of cell walls, which is easy to accept. The remaining question is: why did the A/B subboundary not move? First, its small misorientation presumably prevents its motion by non-mechanical driving forces. Second, any stress on it would presumably act such as to move it away from the center of grain A; perhaps it is anchored too much by its integration into the dislocation network in A, or by internal debris.

In conclusion, the processes near grain edges could be initiated by the same mechanism discussed above: the formation of small-angle boundaries of somewhat higher-than-normal misorientation near grain boundaries. Conversely, they might also be formed by the mechanism to be discussed next.

The Formation of Domains of Different Slip Activity

A different reason for the possible generation of large-angle subboundaries lies in the variation of slip system combinations in different parts of the same grain [9]. This can occur both under exactly uniform deformation (when there are redundant slip systems - especially in unstable orientations), or because of slight non-uniformities in the deformation within a grain [16,17]. The result, in either case, is a local variation in the plastic rotation. Different such "domains" must develop boundaries between them. The term "transition band" has been associated with such boundaries [18], although this term implies a double boundary, with the "band" between them. We shall here treat the possibility that it may not be a *nucleus* which arises *within* a band [18], but rather a domain *boundary* which becomes a large-angle boundary: one side of a nucleus.

One would expect such domain boundaries to be more nearly perpendicular to grain boundaries than parallel to them; perhaps, they would be likely to end near grain *edges*. This is because the slip system combination should be influenced by the specific neighboring grain, or by the specific orientation of the boundary with respect to the external stress state.

We have explored the possibility of developing domain misorientations by finite-element-method (FEM) simulation (following [19,20]) of a cube-shaped grain of 10x10x10 elements, embedded in an environment consisting of 3096 elements, which had a single, relatively stable orientation. The whole assembly was subjected to approximate plane-strain boundary conditions. Plotted in Fig. 5 are the orientations of finite elements composing the embedded grain, after 30% deformation. Also shown is the reorientation predicted for the entire grain by a Taylor calculation (using LApp, the Los Alamos polycrystal plasticity code [21]). The FEM predictions show not only large, non-random deviations; they also exhibit the grain breaking up into two regions of different average orientation.

Displayed in Fig. 6 are sections through the FEM mesh of the embedded grain: Fig. 6(a) parallel to the rolling plane, Fig. 6(b) perpendicular to the transverse direction. Two types of shading are employed: the interior of each element is shaded according to one of the Euler angles (the polar angle θ); the boundary between two elements is darker the higher the misorientation across it. The combination of the two types of shade helps in the analysis: there are essentially two domains of very different orientation, separated by a rather sharp boundary. We have studied a variety of cases; in some, the transition is smoother; in some, a band of orientation which is different from that on either side starts at a grain edge. (It is wider than the mesh length.) The large spread in orientations within a single grain was a feature common to all.

It is worth noting that the new orientation starts at a boundary of the embedded grain, and the domain boundary runs into an edge: much like the behavior postulated above. In summary, it is certainly possible that the large misorientations characteristic of large-angle grain boundaries develop from "slip domain boundaries". An interesting question that needs exploring is whether the scale of the misoriented domains is proportional to the grain facet size, or the grain edge size, or what other parameter, for different grain shapes.

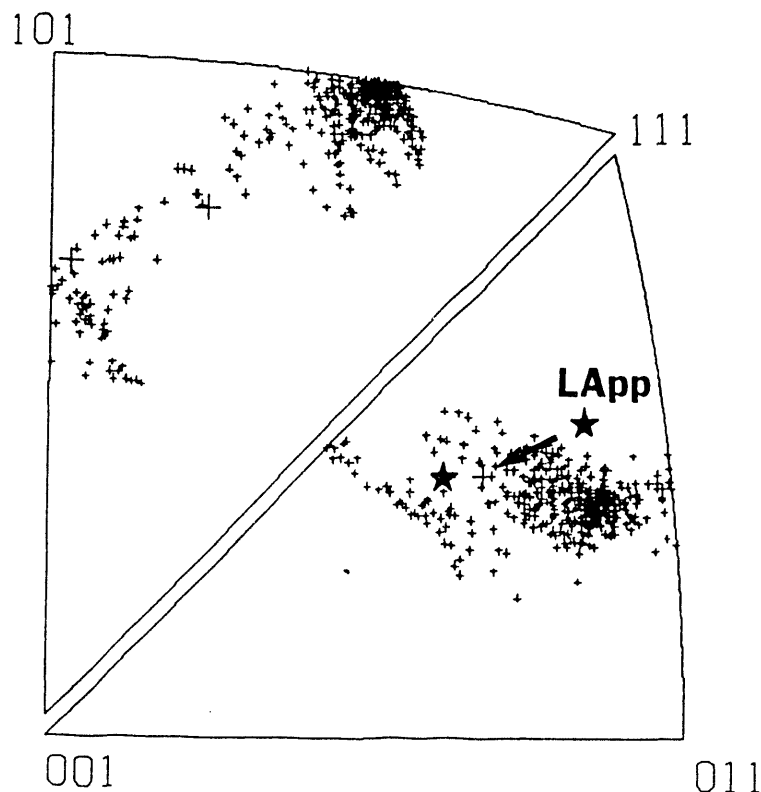


Fig. 5 - Spread of orientations of the "rolling plane normal" (right triangle) and the "rolling direction" (left triangle) in a single grain, completely embedded in another (stable) grain, after 30% deformation. The LApp prediction is shown as two stars, with an arrow indicating the direction of reorientation.

→ RD

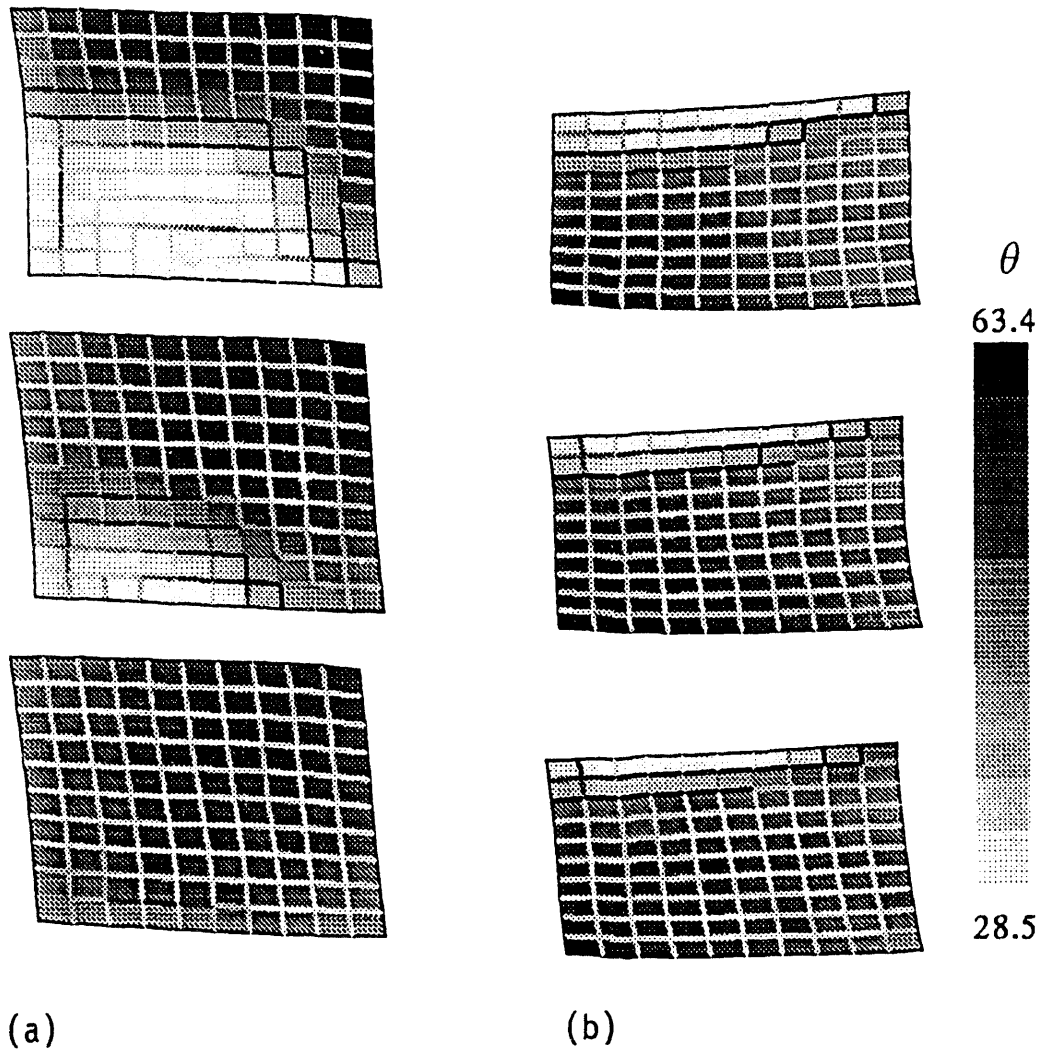


Fig. 6 - Sections through the finite-element mesh of the central grain after deformation: (a) parallel to the rolling plane; (b) perpendicular to the transverse direction. Interior shading of each element is proportional to its Euler angle θ . Shading of the element boundary indicates its misorientation with the neighbor; solid black denotes a misorientation of $>10^\circ$.

The Role of Stresses and Diffusion

In the above discussion, we have emphasized the generation of microstructural features that could, from a geometric point of view, lead to the formation of large-angle grain boundaries. This process need not occur smoothly. If a subboundary were "clean", i.e. consisting of "geometrically necessary" dislocations only, then it might well move rapidly under the action of ever-present local stresses [22,23]. If it were to accumulate, by association with other such subboundaries, a sufficiently large angle of misorientation, it would then become a real grain boundary that moves under thermodynamic, non-mechanical driving forces. What is needed to get to this stage, is a disappearance of the debris associated with the generation of the subboundary from a cell wall, the redundant dislocations. This is where diffusion must play its major role. We surmise that this conversion from a diffuse cell wall to a sharp subboundary may happen at any misorientation. This picture agrees with the experimental fact that intermediate-angle subboundaries are rarely observed.

The subboundaries that arise from developing misorientations between domains of different slip activity, may in fact attempt to form with a spatially varying angle of misorientation; it is tempting to think of them as disclinations, which move under couple stresses, and of the whole "nucleation" phenomenon as a typical example of non-local effects.

Summary

In summary, the essence of "nucleation" in recrystallization may well be the generation of new large-angle boundaries out of small-angle boundaries that are formed even during quasi-homogeneous deformation. The initial generation of subboundaries may be due to an extra accumulation of dislocations near boundaries, and their dynamic recovery. In addition, and perhaps more commonly, it may be due to the generation of boundaries or transition bands between domains of different slip activity. In either case, the onset of diffusion could lead to a loss of dipolar debris, and then these subboundaries might move rapidly under local stresses. They would be more likely to accumulate misorientations than to annihilate each other. In this way, they could form new large-angle boundaries that move under thermodynamic rather than mechanical driving forces. At grain boundaries, this may lead to "necklace" structures; at grain edges or corners they may supply the anchor from which a subgrain can expand into neighboring higher-energy grains.

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