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Dynamic subgrain coalescence during low-temperature large plastic strains

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Large plastic strains of polycrystals, from a substructural point of view, are characterized by the development of subgrains. It is proposed that, once a subgrain structure with low content of redundant dislocations in the boundaries is formed, the election of active sets of slip systems among those minimizing the expended plastic work tends to minimize the increment of internal energy associated with the presence of low-angle boundaries in a grain; this selective choice could contribute to the observed dynamic subgrain annihilation and average misorientation stabilization at large strains. Some tests about the capability of this hypothetical contribution to substructural evolution have been made taking the simple case of axisymmetric elongation of close-packed arrays of up to 27 hexagonal ⟨1 1 1⟩ f c c fibres. For the particular ideal example chosen, the proposed contribution for dynamic subgrain coalescence is very strong. Even if only 1% of the total amount of crystallographic slip responds to the tendency of energy minimization, noticeable effects are registered.

1. Introduction

Large plastic strains of polycrystals, from a substructural point of view, are characterized by the development of subgrains, whose size evolves with strain in a manner that can be formally accounted for by assuming the prevalence of wall annihilation over cell multiplication [1]. Average misorientation across subgrain boundaries increases steadily with strain but the misorientation growth rate decreases when the large strain stage is attained [2, 3]. The development of a structure of domains enclosed by bidimensional dislocation low-angle boundaries – subgrains – replacing the cellular substructure induced by small and moderate strains and constituted of tridimensional dislocation walls, appears to be essential for the transition from a high to a low work hardening rate, also typical of the large strain stage; the work hardening transition is independent of the static or dynamic origin of the substructural transition [4].

The driving force for subgrain coalescence arises from the reduction of the surface energy of the walls. Subgrain boundary annihilation implies rotation of adjacent volumes to a common orientation. In heavily strained metals at low temperature – a regime of slip controlled by a critical resolved shear stress – different rotation of adjacent volumes means different active slip systems across the boundary, and rotation to a common orientation means a selective choice of active slip systems in neighbouring subgrains. It is proposed that, once a subgrain structure with low content of redundant dislocations in the boundaries is formed, the election of active sets of slip systems among those minimizing the expended plastic work tends to minimize the increment of internal energy associated with the presence of low-angle boundaries in a grain; this selective choice should contribute to the observed dynamic subgrain annihilation and average misorientation stabilization at large strains.

Many arguments may be raised against the relevance of this assumption; it is not more than a second-order effect in the choice of the set of operative slip systems and the choice possibilities are probably very limited in real situations, [1, 5]. Anyhow, some numerical tests about the

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capability of this hypothetical contribution to substructural evolution have been made.

2. A simulation

The simplest possible case, axisymmetric elongation of fcc grains containing subgrains with a common ⟨1 1 1⟩ axial orientation, has been considered. The grains are assumed to have undergone large previous strain, e.g. by wire drawing, and are modelled as close-packed arrays of long hexagonal ⟨1 1 1⟩ fibres, ⟨1 1 1⟩ being the principal final stable orientation of the axisymmetric elongation texture of high stacking-fault energy metals. The behaviour of arrays of up to 27 fibres has been simulated. The fibres of an array, i.e. a grain, are assumed to be subgrains, their mutual misorientation being a small random rotation around the common ⟨1 1 1⟩ direction.

The fibres are supposed to increase their mutual misorientation with a rate proportional to its actual value (i.e. exponentially):

$$\theta_{ij} = |\omega_i - \omega_j| \qquad (1)$$

$$d\omega_{ij} = k\omega_i d\epsilon \rightarrow d\theta_{ij} = k\theta_{ij} d\epsilon$$

$$\theta = \theta_0 \exp(k\Delta\epsilon) \qquad (2)$$

where ω_i is a rotation around ⟨1 1 1⟩ defining the orientation of the i fibres, θ_{ij} the misorientation across the wall separating the i and j fibres and θ the average misorientation between neighbouring fibres in a grain after an axisymmetric strain increment $\Delta\epsilon$ starting with an initial misorientation value of θ_0.

A value of $k = 2$ has been taken; it determines a misorientation increase with strain of the same order as that found experimentally in copper for low and moderate rolling strains [2].

After some critical strain it is assumed that the suggested process of energy minimization is superimposed to the process tending to produce a monotonous average misorientation increase. The specific energy of the dislocation boundaries has been made to follow the Read and Shockley formula,

$$E_{ij} = E_0\theta_{ij}[1 - \ln(\theta_{ij}/\theta_M)] \qquad (3)$$

with E_0 and θ_M being two constants; θ_M has been taken as 25° (0.436 rad) in the numerical calculations. For a small misorientation change,

$$dE_{ij}/d\theta_{ij} = E_0 \ln(\theta_M/\theta_{ij}). \qquad (4)$$

The fully constrained axisymmetric elongation of ⟨1 1 1⟩ fcc crystals gives way to a multiplicity of mechanically equivalent sets of slip systems allowing for a crystallographic rotation rate of $-0.87 \leqslant \Omega \leqslant 0.87$ rad per unit strain around the ⟨1 1 1⟩ stable axial direction. Now, for a small strain increment, the orientation of a particular fibre is able to change within the limits,

$$[-0.87f + (1-f)k\omega_i]\ d\epsilon \leqslant d\omega_i \leqslant [0.87f + (1-f)k\omega_i]\, d\epsilon \qquad (5)$$

where f is the fraction of the total amount of crystallographic slip in the fibre responding to the tendency of minimization of the energy stored in the grain.

For the whole grain, after a small strain increment, the stored energy increment is

$$d\xi = \Sigma(S_{ij}dE_{ij} + E_{ij}dS_{ij}) \qquad (6)$$

with S_{ij} the surface of the wall separating the i and j subgrains; the summation is extended to all the walls contained in the grain. The function $d\xi/d\epsilon$ is to be minimized on the basis of the allowed rotation values of the fibres, given by Equation 5. For the particular example chosen, no relative changes of the surface of the walls occur and the problem is reduced to find the combination of rotation increments, $d\omega_i$, minimizing ΣdE_{ij}. Minimization has been performed by a numerical procedure. The behaviour of arrays of 12, 19 and 27 fibres has been studied, starting with a random distribution of orientations in the range $-0.1 \leqslant (\omega_i)_0 \leqslant 0.1$ rad (± 5.7°). Strain is applied by small increments and the evolution of the orientation of the fibres, the average misorientation in the grain and the fraction of initial subgrain walls remaining are computed. Figs. 1 to

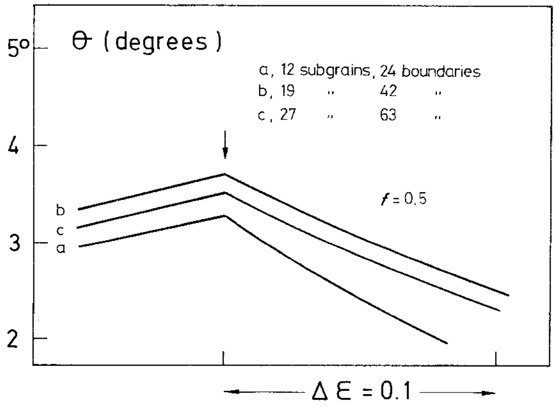

Figure 1 Average mutual misorientation evolution during axisymmetric elongation of three ⟨1 1 1⟩ fcc arrays of 12, 19 and 27 hexagonal fibres. From the strain indicated by the arrow, a selective choice of 50% of the crystallographic slip tends to minimize the sub-boundary energy storage in the array.

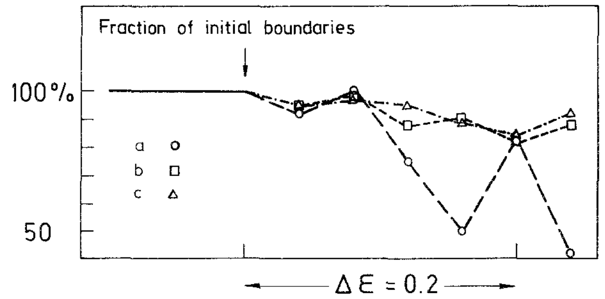

Figure 2 Fraction of initial boundaries remaining as plastic deformation goes on. Meaning of the symbols as in Fig. 1. The rebuilding of previously annihilated walls has been allowed.

4 show results for $f = 0.5$ and $f = 0.01$. It can be seen that for the hypothetical case studied strong substructural effects are predicted. Even if only 1% of the total amount of slip in a grain tends to minimize the rate of energy storage, the effects are far from negligible.

3. Discussion

From the case studied, some factors influencing the substructural effect considered stand out. First of all, it is exclusively a dynamic effect: it will only operate if plastic deformation goes on. Its effectiveness will be dependent on the instantaneous grain size but this dependence will only be noticed for small grain to subgrain size ratios; from the limited tests run it appears that second-order neighbours are the farthest subgrains influencing the choice of rotations in a particular subgrain. The crystallographic system should be another important factor: this hypothetical contribution to dynamic recovery at large strains will be much less important in bcc than in fcc metals as the mechanical indetermination in the choice of the operative set of slip systems among those equivalent is very infrequent in the former compared with the latter (totally absent under the pencil glide assumption). Crystallographic orientation of the grain and deformation mode are obviously other influencing factors; it must be pointed out that the orientation and the deformation mode chosen for the simulation are not only the simplest case to treat but also a very favourable one from the point of view of coalescence. It is a case where the allowable strain-induced rotation range is uniaxial, around ⟨111⟩ and covering both rotation senses, and where the misorientations have been artifically chosen to be rotations about the same ⟨111⟩ elongation axis. Moreover the assumed rotations maintain the grain permanently in its final stable orientation. In general, the situation will be much more constrained: both the available rotation rate range and the misorientation spectrum will be three-dimensional. Multiaxial misorientations will not be covered by the range of rotation rates available and the continuous growth of such misorientations will be unaffected by the process.

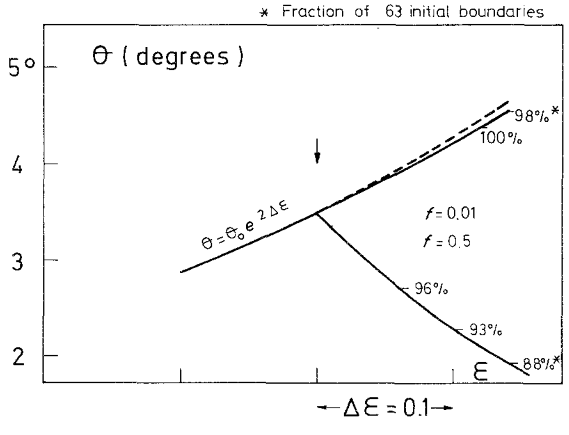

Figure 3 Average misorientation as a function of strain for a fcc grain with 27 ⟨111⟩ fibre subgrains and two values of f. The dotted line represents the monotonic growth of θ without the assumed selective choice of slip systems.

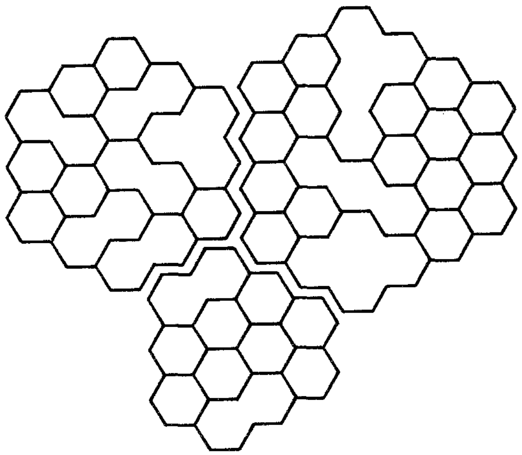

Figure 4 Cross-section of the three different sized grains of Figs. 1 and 2 ($f = 0.5$) after a strain increment $\Delta\epsilon = 0.2$ beyond the critical strain.

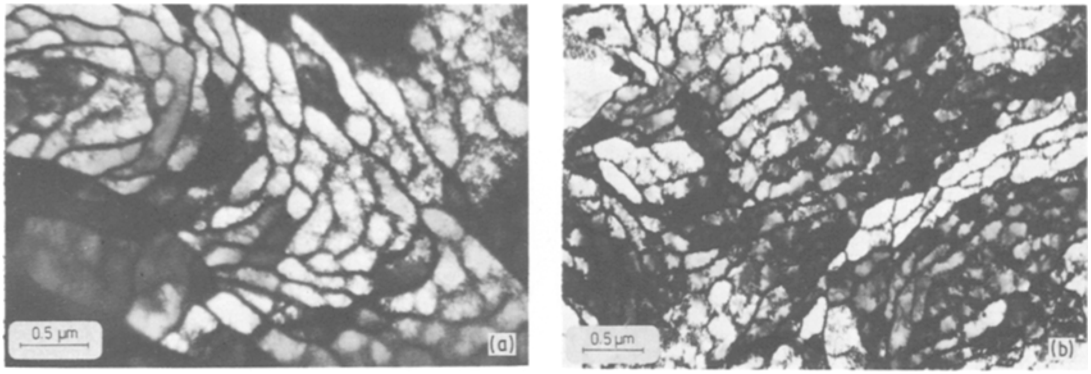

Figure 5 TEM micrographs (J. M. Alberdi, unpublished work) of transverse sections of wire-drawn copper, (a) $\bar{\epsilon} = 2.0$ and (b) $\bar{\epsilon} = 3.1$. Regions of $\langle 001 \rangle$ axial orientation constitued of subgrains with polygonal cross-sections whose morphology strongly suggests the action of a coalescence process (compare with Fig. 4). The ideal $\langle 001 \rangle$ orientation allows for an axial orientation rotation rate of $-0.5 \leqslant \Omega \leqslant 0.5$ rad per unit axisymmetric strain, although its whole rotation rate range is three-dimensional and covers any direction of the space of rotations.

An influence of temperature and strain rate on the rate of misorientation reduction (determined by the parameter f) cannot be excluded: generation of dislocations on a particular slip system may necessitate cross-slip to be activated. Temperature and strain rate will be very important in relation to the critical strain level determining the action of the proposed process: for the subboundary energy to drive the process of subgrain misorientation reduction, the contribution of inner dislocations and redundant wall dislocations to a strain-induced stored energy increment must be negligible. The critical strain level is perhaps also linked to some critical misorientation across the boundaries, which must be barely penetrable to dislocations to permit an independent activity of slip systems in each grain; furthermore as the subgrain size decreases, the misorientation-related energy increment relative to the expended plastic work increases, and subgrain size should also affect that critical strain level.

In conclusion, although the speculative character of the proposed effect cannot be denied, there is some experimental evidence in support of the conclusions of our geometrical model. Substructures, such as shown in Fig. 5, strongly suggest the action of a subgrain coalescence mechanism active at low temperatures and large strains. It must also be pointed out that Langford and Cohen [6] developed a continuum-plasticity approach to the same problem of surface energy driven dynamic recovery, studying the merging of subgrains by migration of "h" or "y" junctures, an alternative to the subgrain rotation mechanism dealth with here. They assimilate orientation changes to rigid-body rotations produced by local, in the junctures, redundant shear strains; however, the actual existence of such redundant strains is not compatible with the "upper-bound" theorem of plasticity.

4. Conclusions

1. A truly dynamic contribution to the observed subgrain coalescence during low-temperature large plastic strains of polycrystals has been proposed. It is based in a selection of the operative sets of slip systems – among those available to produce a given strain increment with the minimum plastic work – in order to minimize the increment of stored energy associated with the presence of low-angle boundaries.

2. Some numerical simulations of the action of such selective choice of slip systems during the straining of a particular orientation suggest that the proposed contribution to dynamic subgrain coalescence may be of importance.

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