On the orientation of cell block boundaries in the grains of a rolled f.c.c. polycrystal

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Abstract. Grains in f.c.c. polycrystals that accommodate imposed deformation purely by slip processes develop a multi-scale dislocation substructure that evolves with deformation. When the polycrystal is subjected to rolling deformation or to channel-die compression, one of the elements of this substructure, called cell block boundaries, are widely reported to align parallel to the transverse direction and close to the macroscopic plane of maximum shear. This observation is explained based on standard rate-independent crystal plasticity augmented by three hypotheses.

Introduction

Grains in f.c.c. polycrystals of medium to high stacking fault energy, which accommodate imposed deformation purely by slip processes develop a multi-scale dislocation substructure that evolves with deformation. At the coarsest scale the grain may divide into lath-shaped regions, each several tens of dislocation mean free paths wide and extending across the domain of the entire grain. The misorientation between such regions may be of the order of tens of degrees [1]. Depending on their morphology, such regions are either termed shear bands or deformation bands. At the intermediate scale, the crystal may divide into regions called cell blocks (CBs), a few dislocation mean free paths wide. Cell blocks are demarcated by dislocation structures called dense dislocation walls and microbands [2], also called cell block boundaries (CBBs). The misorientation across these structures is of the order of a few degrees. Shear band boundaries, deformation band boundaries and cell block boundaries are all geometrically necessary boundaries. Beside these, incidental dislocation boundaries called cell boundaries also subdivide the grain at the finest scale. The nature of the subdivision (presence or absence of each of the three scales of subdivision, microstructural morphology, lattice misorientation across demarcating boundaries, etc.) is depends on the lattice orientation with respect to the imposed deformation.

When either single crystals or polycrystals of medium to high stacking fault energy f.c.c. metals such as Cu, Al or Ni are rolled to less than about 50% reduction, they develop CBBs that are inclined approximately parallel to the transverse direction and make about 45° with the rolling direction [1, 3, 4, 5]. These CBBs are mobile relative to the material of the grain in that their orientation does not evolve according to the shape of the grain [4]. Instead, CBB orientation is thought to be controlled by the distribution of slip amongst the slip systems. At high rolling reductions, CBB mobility is lost so that they align with the rolling plane.

While some understanding has been gained about CBB orientation [6] and the correlation between the distribution of slip activity within a grain and its CBB structure [7], a comprehensive theoretical explanation of CBB structure is still unavailable. In the present work, a theoretical model for the orientation of CBBs is proposed. The proposed model correctly predicts that CBB orientations are concentrated perpendicular to the transverse direction. It also

gives important insight into the relative influence of crystallographic and macroscopic factors on CBB orientation [5].

Theory

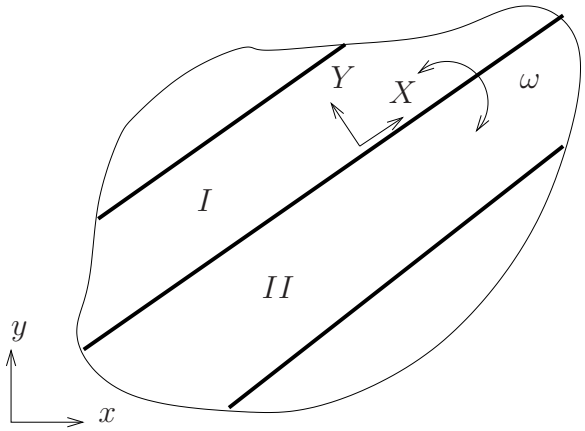

Fig. 1: Schematic diagram of a small part of a grain located well away from the grain boundaries showing two cell blocks, I and II.

As shown in Fig. 1, a pair of neighboring CBs, denoted I and II, equal in volume and each interacting across the intervening planar CBB with the other. Each CB has a uniform lattice orientation. The CBs are, however, mutually misoriented; the misorientation angle is denoted by ω. In accordance with experimental observations [8, 9], the domain of the entire grain, which is much larger than the section shown in Fig. 1, is assumed to be patterned repetitively by CBs of types I and II. The CBB separating two CBs is idealized as a straight and infinitesimally thin dislocation wall that may move relative to the material of the CBs by the collective motion of its constituent dislocations.

Each CB is assumed to deform homogeneously following standard rate-independent rigid plasticity [10, 11]. The strain-rate of material points in CB I and CB II will be denoted $\dot{\boldsymbol{\epsilon}}^{(I)}$ and $\dot{\boldsymbol{\epsilon}}^{(II)}$, respectively. In order to accommodate the externally imposed strain-rate, $\bar{\dot{\boldsymbol{\epsilon}}}$, $\bar{\dot{\boldsymbol{\epsilon}}} = (\dot{\boldsymbol{\epsilon}}^{(I)} + \dot{\boldsymbol{\epsilon}}^{(II)})/2$, where the factor $1/2$ is the volume fraction, assumed equal, of each of the two CB types.

Misorientation and orientation of CBBs are determined by three hypotheses:

1. The deviatoric stress in CB I, $\boldsymbol{\sigma}^{(I)}$ and that in CB II, $\boldsymbol{\sigma}^{(II)}$ are equal. Because of the assumption of repetitious patterning of the entire grain by the two CB types, this amounts to assuming a uniform deviatoric stress state in the entire grain. Further, by the lower bound theorem, this hypothesis implies the minimization of the plastic power density during grain deformation.

2. Of all possible misorientation vectors distributed on the unit sphere, CBs misorient preferentially about the misorientation vector $\boldsymbol{m}$, which minimizes the plastic power density of the grain, $P = (1/2)(\boldsymbol{\sigma}^{(I)} : \dot{\boldsymbol{\epsilon}}^{(I)} + \boldsymbol{\sigma}^{(II)} : \dot{\boldsymbol{\epsilon}}^{(II)})$.

3. The deformation of CBs is generally incompatible across a CBB. A measure of this incompatibility is given by $I = [\![\dot{\epsilon}]\!]^2_{\mathrm{XX}} + [\![\dot{\epsilon}]\!]^2_{\mathrm{YY}} + [\![\dot{\epsilon}]\!]^2_{\mathrm{ZZ}} + 2[\![\dot{\epsilon}]\!]^2_{\mathrm{XZ}}$, where, $[\![\dot{\boldsymbol{\epsilon}}]\!] = \dot{\boldsymbol{\epsilon}}^{(I)} - \dot{\boldsymbol{\epsilon}}^{(II)}$ denotes the jump in strain-rate across a CBB. It is hypothesized that the CBB assumes the orientation that minimizes the incompatibility I. It can be shown that I is minimized

then the CBB has normal either $\boldsymbol{\nu}_1 = (\boldsymbol{v}_1 + \boldsymbol{v}_3)/\sqrt{2}$ or $\boldsymbol{\nu}_2 = (\boldsymbol{v}_1 - \boldsymbol{v}_3)/\sqrt{2}$ where $\boldsymbol{v}_1$ and $\boldsymbol{v}_3$ denote the unit eigenvectors corresponding to the maximum and minimum eigenvalues of $[\![\dot{\boldsymbol{\epsilon}}]\!]$. $\boldsymbol{\nu}_1$ and $\boldsymbol{\nu}_2$ are the normals predicted for the CBBs in the present theory.

Results

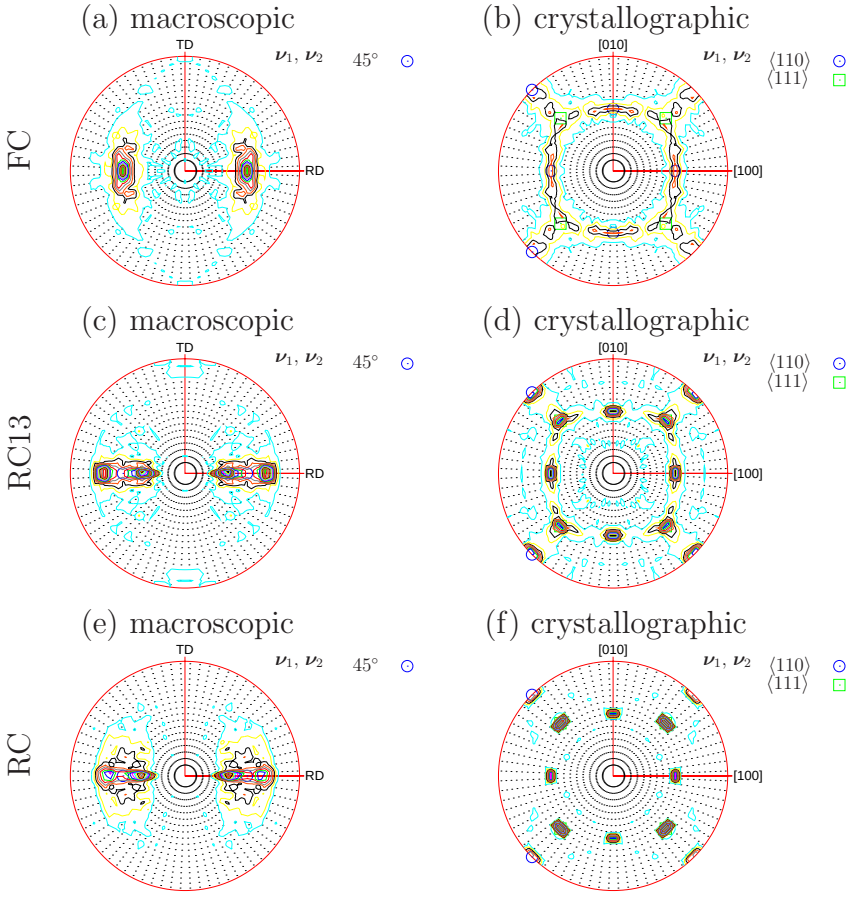

Fig. 2: Equal angle projection of the normals, $\boldsymbol{\nu}_1$ and $\boldsymbol{\nu}_2$, to the two predicted CBBs in each of the 2250 orientations regularly spanning the lattice orientation space in the macroscopic (first column) and crystallographic (second column) systems, corresponding to full, partially relaxed and fully relaxed constraints (different rows). Intensity levels are $1, 2, \ldots$.

We now apply the foregoing theory to predict CBB orientation under rolling deformation in 2250 lattice orientations obtained by regularly sampling the orientation space. The principal directions of rolling deformation: the rolling, transverse and normal directions are abbreviated as RD, TD and ND, respectively. The deformation of a material point in a rolled single crystal or polycrystal may be described by

$$[\bar{\dot{\boldsymbol{\epsilon}}}]_{\mathrm{RD-TD-ND}} = \begin{pmatrix} 1 & \bar{\dot{\epsilon}}_{12} & \bar{\dot{\epsilon}}_{13} \\ \bar{\dot{\epsilon}}_{21} & 0 & \bar{\dot{\epsilon}}_{23} \\ \bar{\dot{\epsilon}}_{31} & \bar{\dot{\epsilon}}_{32} & -1 \end{pmatrix}.$$

Process geometry fully determines the diagonal terms of this matrix, but not the off-diagonal terms. A simple model of the rolling process, called the full constrained (FC) model, assumes that rolling deformation is plane strain in character, i.e., $\bar{\dot{\epsilon}}_{12} = \bar{\dot{\epsilon}}_{13} = \bar{\dot{\epsilon}}_{23} = 0$. Another model,

which treats rolling as flow through a convergent channel is due to Lee and Duggan [12] and assumes that $\bar{\dot{\epsilon}}_{12} = \bar{\dot{\epsilon}}_{23} = 0$ so that only $\bar{\dot{\epsilon}}_{13} = \bar{\dot{\epsilon}}_{31}$ may be non-zero due to geometric and frictional effects. This model is called the partially relaxed constraints model and is denoted RC13. Yet another model which finds common use in modeling channel-die compression experiments is called the fully relaxed constraints model [13] and is denoted RC. In the present calculations a constant misorientation angle $\omega = 0.3^\circ$ between the CBs is assumed. This corresponds to the expected misorientation across an incidental dislocation wall at a strain level of 0.1 according to the scaling law of Hughes et al [14].

CBB orientations calculated in 2250 lattice orientations obtained by regularly sampling the entire orientation space for FC, RC13 and RC constraints are shown in Fig. 2. In agreement with experimental observations [1, 3, 4, 5], it is seen from Fig. 2 (a), (c) and (e) that predicted CBB normals are predominantly clustered close to the RD-ND plane, i.e., CBBs are predominantly parallel to TD in the macroscopic coordinate system, regardless of the constraint imposed.

In the crystallographic coordinate system, as seen from Fig. 2 (b), (d) and (f), CBBs are predominantly aligned near {111} and {110}-type crystallographic planes. The alignment of a CBB with one of these planes, however, becomes closer with decreasing imposed constraint. Thus, CBBs are more densely clustered close to {111} and {110}-type crystallographic planes in Fig. 2 (f) corresponding to RC constraint than in Fig. 2 (d) or (b) corresponding to RC13 and FC constraints, respectively. This indicates that CBB orientation has both crystallographic and macroscopic preferences. The macroscopic preference however, dominates the crystallographic one when grain deformation is highly constrained.

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