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Modeling of large strain hardening during grain refinement

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Strain hardening was modeled at large strains taking into account the geometrically necessary dislocations (GNDs) with the help of a recent grain refinement model. The GND density was studied experimentally with orientation imagining for oxygen-free high-conductivity copper deformed in equal channel angular pressing and in simple shear to the same equivalent strain. The results show that the GND density can be predicted fairly well by the model in accord with experiments, and also affects stage IV hardening.

Keywords: Strain hardening; Geometrically necessary dislocation; OFHC copper; Simple shear; Grain refinement modeling

Experiments and modeling show that strain hardening behavior is microstructure dependent and the most relevant parameter is the heterogeneous dislocation density which develops a cell structure by self-organization of the dislocations [1]. The first widely used model is the Kocks model, which assumes only a homogeneous (average) dislocation density together with the mean free path of dislocation motion [2]. For large strain hardening, Estrin et al. [3] and Tóth et al. [4] considered the composite nature of the dislocation cell structure and showed that the sharpening of the dislocation walls (i.e. the experimentally observed decrease in their volume fraction) can account for stage IV hardening. Rollett and coworkers [5] could explain stage IV by incorporating the role the dislocation debris in strain hardening. Pantleon has shown that by incorporating the geometrically necessary dislocations (GNDs) in the Kocks approach, stage IV can also be obtained [6,7]. At large strains, where grain refinement is in progress, the GNDs are of great importance as they provide a continuous increase of subgrain boundary misorientations. It is therefore important to study the effect of GNDs on hardening simultaneously with grain refinement.

Recently a quantitative polycrystal grain refinement (GR) model was proposed which is capable of predicting texture, grain size, strain hardening and next-neighbor disorientations from the refined grains in a single modeling frame [8]. The model is based on the lattice curvature that develops mostly near the grain boundaries as the result of a slow-down of the strain-induced lattice rotation of an embedded crystal. Several applications of the model proved its pertinence [9–12].

In the present work, we aim to investigate the hardening behavior predicted by the GR model. During simulation, the only parameter that controls the rate of the grain refinement process – called μ – is the retardation of the lattice rotation at the grain boundary. Its value can be in the range between 0.5 and 1; $\mu = 1$ was used here. The GR model predicts the geometrically necessary dislocations that have to be present in the crystal to develop the curvature of the lattice. The necessary populations of GNDs for the described mechanism of the lattice curvature were named curvature-induced dislocations (CIDs) in Ref. [8]. Another population of GNDs are those redundant dislocations that build disorientation across dislocation cell walls. Their origin is stochastic, made by the bias of the dislocation fluxes coming to the wall from two opposite directions [6,13]. Pantleon showed that such GNDs affect stage III only slightly and do not affect stage IV at all [7]. The density of both kinds of GNDs can be obtained quantitatively from the GR model. The CID-made lattice curvature can be extracted from electron backscatter diffraction (EBSD) orientation maps and can be compared to the prediction.

Oxygen-free high-conductivity copper was heat-treated at 650 °C for 2 h, resulting in an average grain size of about 24 μm. The billet of the annealed copper was

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processed by one-pass equal channel angular pressing (ECAP). The EBSD measurements were performed using a JEOL 7001F with an HKL detector with a step size of 0.1 μm. Boundaries were identified using a minimum disorientation angle of 5° between adjacent pixels. In order to obtain a strain hardening curve in the intersection plane of the channels in the ECAP die, torsion tests were carried out on cylindrical samples of 6 mm diameter and 15 mm length to simulate the simple shear deformation mode of ECAP by torsion. To obtain the stress–strain curve from the measured twisting angle and the torque in torsion, the Nadai formula [14] was used.

The GND scalar density can be defined as the entry-wise norm of the Nye dislocation density tensor (α) [15] divided by the Burgers vector length:

$$\rho_{\mathrm{GND}} = \frac{1}{b}\sqrt{\alpha_{ij}\alpha_{ij}} \tag{1}$$

Five components of the Nye tensor can be determined from two-dimensional mapping. From them, a truncated scalar value of ρ_{GND} can be calculated, which we call $\rho_{\mathrm{GND}}^{(2D)}$:

$$\rho_{\mathrm{GND}}^{(2D)} = \frac{1}{b}\sqrt{\alpha_{12}^2 + \alpha_{13}^2 + \alpha_{21}^2 + \alpha_{23}^2 + \alpha_{33}^2} \tag{2}$$

In order to estimate ρ_{GND} for the three-dimensional case, we assume α to be isotropic and obtain $\rho_{\mathrm{GND}} = 3\rho_{\mathrm{GND}}^{(2D)}/\sqrt{5}$ by division of Eqs. (1) and (2). The EBSD map was analyzed using the method proposed by Pantleon [16] to obtain the measurable α_{ij} components. For quantification of GNDs only within the grain interiors, the adjacent pixels across boundaries displaying a disorientation exceeding 5° were not considered. The obtained GND densities using a color code with the help of the EBSDmcf Software [17] are displayed in Figure 1. For densities smaller than 10% of the maximum, the color code was not used; instead, the band contrast was plotted ("BC" in Fig. 1; the total surface where the density is less than 10% of its maximum value represents 49.5% of the total area). It is apparent that the GND density shows a patterning structure in which most of the GNDs are grouping into "walls" where their local density is very high. The approximate average distance between these walls is about 2 μm. These walls are most probably the precursors of new grain boundaries. They are more frequent near the grain boundaries of the original grains (see Fig. 1). The maximum GND density value is $3.35 \times 10^{15}\ \mathrm{m}^{-2}$ in the map and the average value of ρ_{GND} on the map is $4.38 \times 10^{14}\ \mathrm{m}^{-2}$; the entire measured surface was considered in the calculation of the average.

For the simulation of hardening, the GR model was employed in which hardening was simulated with the dislocation cell-based composite model [3,4]. Several populations of dislocations were considered in the model: dislocation density in the cell interior (ρ_c) and in the cell wall (ρ_w), and the CID density (ρ_{CID}). The wall density can be split into two populations ($\rho_w = \rho_{ws} + \rho_{wg}$), where ρ_{ws} is the statistical wall dislocation density and ρ_{wg} is the GNDs that build up misorientation across the cell wall. Transmission electron microscopy measurements show that these cell misorientations are relatively small [18]. Nevertheless, their contribution is present in the dislocation density tensor, which can be measured by the EBSD technique described above. We used the same evolution equations as in Ref. [8] for ρ_c, ρ_{ws} and ρ_{wg}.

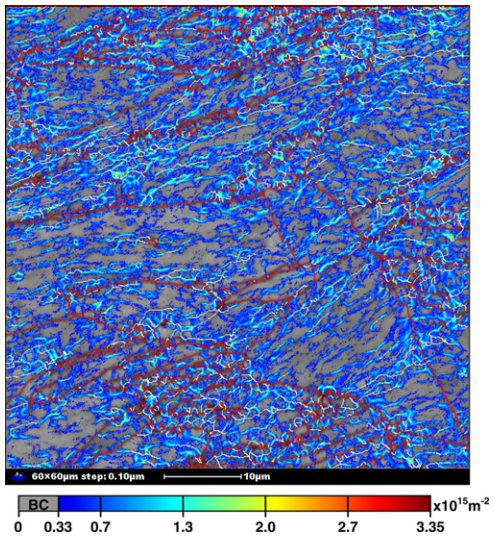

Figure 1. Map of GND density obtained from EBSD measurement after one-pass ECAP on the ND plane. Boundaries with at least 15° disorientation are marked with red lines while those that are between 5 and 15° are colored white. For intensities less than $0.33 \times 10^{15}\ \mathrm{m}^{-2}$, the BC was plotted.

The sharpening of the cell walls is expressed by decreasing their volume fraction according to the formula introduced in Ref. [3]: $f = f_\infty + (f_0 - f_\infty)\exp(-\gamma_r/\tilde{\gamma}_r)$, where f_0 is the initial value of f, and f_∞ is its saturation value at large strains. The quantity $\tilde{\gamma}_r$ describes the rate of decrease of f. The same values of parameters as those used in Ref. [3] were employed in the present study ($f_0 = 0.25$, $f_\infty = 0.06$ and $\tilde{\gamma}_r = 3.2$). There are several parameters that control different dislocation mechanisms (for details, see [8,13]: α^*, β^*, k_0, ξ_1 and ξ_2. ξ_1 and ξ_2 are numerical parameters that describe the fractions of statistical dislocations that contribute to the buildup of cell misorientations. This misorientation can be obtained from the expression $\theta = bd\rho_{wg}$. Finally, the k_0 parameter controls the dislocation annihilation rate. The average dislocation density is defined for the dislocation cell structure as follows:

$$\rho_{\mathrm{average}} = \rho_{CID} + f(\rho_{ws} + \rho_{wg}) + (1 - f)\rho_c \tag{3}$$

The dislocation cell size is related to the total dislocation density according to Holt's formula:

$$d = H/\sqrt{\rho} \tag{4}$$

where the H parameter is about 10 for copper [19].

The density of CIDs is estimated in the present version of the GR model using the basic formula:

$$\rho_{\mathrm{CID}} = C\frac{n}{bR}, \tag{5}$$

where R is the lattice curvature induced by the presence of one grain boundary and n is the number of near grain boundaries that can also induce lattice curvatures. n can be as high as 3 for a "corner" region of the grain, taking an initial cubic shape. For the calculation of R and n, see the original work on the GR model [8]. C is a parameter in Eq. (5), and can take a value of less than 1. This