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Modelling microstructure evolution toward ultrafine crystallinity produced by severe plastic deformation

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Abstract The significance of severe plastic deformation by equal channel angular pressing (ECAP) as a promising technique for extreme grain refinement down to sub-micrometer and sometimes nanometer scale is generally recognised. We present a modelling frame for describing ECAP based on microstructure evolution. Following a particular scenario of grain refinement, in which a dislocation cell structure is considered as a 'precursor' of the developing grain structure, the variation of the cell size with the number of ECAP passes is traced. Finite element simulations based on the model compare favourably with the experimental data. Further features of the model such as a provision for modelling the variation of the misorientation angle distribution and texture evolution are also discussed.

Introduction

Among the severe plastic deformation techniques used as a means of extreme grain refinement in bulk metallic materials [1, 2], equal channel angular pressing (ECAP) has emerged as arguably the most promising one. While a large amount of experimental data have been collected over the past decade, often supported by finite element calculations based on simplified constitutive models, microstructure based modelling has been relatively scarce. The present authors, together with colleagues, have been working in the field of ECAP modelling for some five years. This article outlines the general frame of their modelling approach and gives a summary of results, along with an outlook for outstanding problems.

Among the possible scenarios of grain structure evolution under ECAP processing, we select a gradual transformation of the dislocation cell structure to a new, refined grain structure. This involves accumulation of misorientation between neighbouring dislocation cells with strain turning low angle boundaries to large angle ones [3–5]. Prangnell et al. [6] proposed a picture in which a decrease of lateral dimensions of elongated grains terminates in their subdivision into smaller grains once the grain thickness drops down to the dislocation cell size. Basically, in their model, too, it is the dislocation cell size that determines the final grain size in the material undergoing large strain deformation by ECAP.

The ECAP model providing a description of the dislocation cell size evolution goes back to the strain hardening model for large strains [7]. A brief outline of the model, as well as a description of some recent developments, are given in the subsequent sections. Experimental data validating numerical simulation results are also presented there.

Outline of the microstructure evolution model

The model of large strain deformation [7] underlying our approach applies to dislocation cell-forming

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materials. The initial stage of the process when a 'primordial' cell structure is formed is not considered. The cells of average size d are assumed to have a cubic shape. The volume fraction of the cell walls is given by:

$$f = \frac{d^3 - (d-w)^3}{d^3}, \tag{1}$$

where w denotes the wall thickness. The evolution of the dislocation densities in the cell walls and the cell interiors, denoted respectively ρ_w and ρ_c, is described by the set of coupled differential equations

$$\frac{d\rho_w}{d\gamma} = \frac{6\beta^*(1-f)^{2/3}}{bdf} + \frac{\sqrt{3}\beta^*(1-f)\sqrt{\rho_w}}{fb} - k_0\left(\frac{\dot{\gamma}}{\dot{\gamma}_0}\right)^{-1/n}\rho_w, \tag{2}$$

$$\frac{d\rho_c}{d\gamma} = \alpha^*\frac{1}{\sqrt{3}}\frac{\sqrt{\rho_w}}{b} - \beta^*\frac{6}{bd(1-f)^{1/3}} - k_0\left(\frac{\dot{\gamma}}{\dot{\gamma}_0}\right)^{-1/n}\rho_c. \tag{3}$$

In the above equations it was assumed that the shear strain γ in the cell walls and the cell interiors are the same. The quantity $\dot{\gamma}_o$ denotes a reference shear rate and b the magnitude of the Burgers vector. The quantities α^* and β^* are numerical constants. The physical origin of the various terms in the evolution equations representing possible dislocation reactions involved (such as loss of cell interior dislocations to become entrapped in the walls given by the first term of Eq. 1 and the second term of Eq. 2) has been explained elsewhere [3–5, 7]. The exponent n in the last, *dynamic recovery*, terms in both equations can be taken to be inversely proportional to the absolute temperature, given the fact that ECAP processing is typically conducted below half the melting temperature, while the coefficient k_o can be considered constant.

Whereas Eqs. 2 and 3 describe the detail of the evolution of the dislocation density, that of the other microstructural variables, d and f, involves certain assumptions. Following Ref. [7] we assume that the average grain size d scales with the inverse square root of the total dislocation density

$$\rho = f\rho_w + (1-f)\rho_c, \tag{4}$$

$$d = K/\sqrt{\rho}, \tag{5}$$

where K is a constant. With the variation of the average grain size thus defined, a description of the variation of f requires the knowledge of the evolution of the wall thickness w. The latter quantity undergoes a gradual decrease with straining, as the cell walls, initially fuzzy due to the abundance of geometrically 'unnecessary'' statistical dislocations, become sharper. This effect outstrips the concurrent increase of the total grain boundary area, so that the volume fraction of the wall material turns out to be a decreasing function of strain, which can be represented [2, 3] by

$$f = f_\infty + (f_o - f_\infty)\exp(-\gamma/\tilde{\gamma}) \tag{6}$$

This function was chosen to fit available experimental data for Cu and describes the variation with strain γ of the volume fraction f from an initial value f_o to an asymptotic value f_∞, which is smaller than f_0. The parameter $\tilde{\gamma}$ represents the inverse of the rate of this variation.

Strain hardening is considered by relating the equivalent resolved shear stresses τ_c^r and τ_w^r in the cell interiors and the cell walls, respectively, to the equivalent resolved plastic shear rates in these 'phases' (both assumed equal to $\dot{\gamma}$) and the respective dislocation densities:

$$\tau_c^r = \alpha G b\sqrt{\rho_c}\left(\frac{\dot{\gamma}}{\dot{\gamma}_0}\right)^{1/m}, \tag{7}$$

$$\tau_w^r = \alpha G b\sqrt{\rho_w}\left(\frac{\dot{\gamma}}{\dot{\gamma}_0}\right)^{1/m}. \tag{8}$$

Here G is the shear modulus, $1/m$ is the strain rate sensitivity parameter and α is a numerical constant. The strain hardening behaviour of the 'composite' is defined by a scalar quantity, τ^r, that is obtained by applying the rule of mixtures:

$$\tau^r = f\tau_w^r + (1-f)\tau_c^r\ . \tag{9}$$

The model outlined was shown to describe strain hardening behaviour of dislocation-cell forming metallic materials, including late stages of hardening, very well [7]. It is particularly suited for simulating ECAP processing, in which very large strains are involved.

In the scenario of grain refinement adopted, the smallest dislocation cell size achievable for a given material pre-determines the eventual grain size. With the highest dislocation density not exceeding 2.5×10^{15} m^{-2}, *cf.* [8], and K of the order of 10, the smallest grain size in copper ECAP can produce would be, as predicted by Eq. 5, of the order of 250 nm—a value found experimentally [4]. Equation 5 can roughly be re-written as

$$\frac{d}{b} = KM\alpha \cdot \frac{G}{\sigma}, \tag{10}$$

where σ is the flow stress and M is the Taylor factor. From this relation it is easily seen that for the grain size to become smaller than a 100-fold of the lattice parameter, say, the stress should become higher than one tenth of the theoretical strength, which is hardly possible with common metallic materials.

A typical example of an ultrafine grained structure produced in copper by ECAP is shown in Fig. 1. The grain size distribution evolving during the ECAP (but basically fairly stable already after the first ECAP pass) is seen in Fig. 2.

While the evolution of the dislocation cell size leading to the average grain size as seen in Fig. 1 is described by the above model, an extra model was developed in Ref. [9] to account for the grain size distributions.

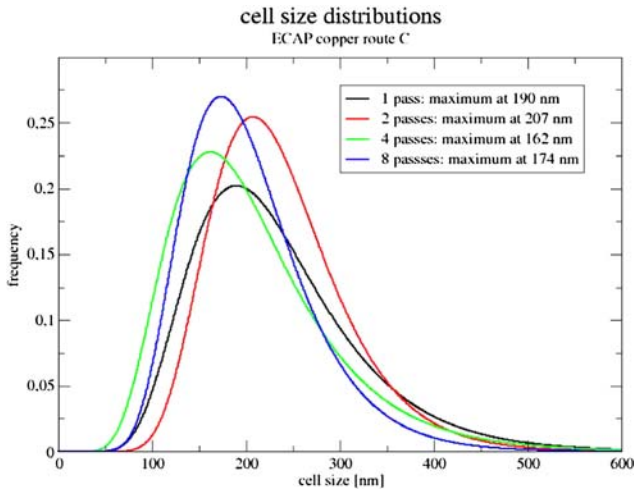

Fig. 2 Grain size distribution in copper for different numbers of equal channel angular pressing (ECAP) passes (Route C [9])

Modelling of texture evolution

To describe texture evolution, the above microstructure evolution 'module' can be combined with a crystal plasticity model [7]. A first variant of the model used so far is admittedly oversimplified. Thus, misorientations between the dislocation cells within an individual grain are disregarded, so that the grain can be characterized by a single equivalent resolved shear strain rate. This approach was developed at a time when no model for the evolution of misorientations was available. Still as illustrated below, reasonably good results with regards to texture prediction were obtained [3]. The equivalent resolved shear strain rate was expressed in terms of the resolved shear strain rates $\dot{\gamma}_s^r$ on the active slip systems s:

$$\dot{\gamma}^r = \left[\sum_{s=1}^{N} \dot{\gamma}_s^{r\,\frac{m+1}{m}}\right]^{\frac{m}{1+m}}, \tag{11}$$

where N is the number of active slip planes. Using the full-constraint Taylor approach, and employing a technique of random selection of five slip systems from among the 12 potentially active ones in each grain, finite element calculations with ABAQUS were performed. With 300 grains per node (initially randomly oriented), pole figures were determined by aggregating the grain orientations. A typical result for copper is presented in Fig. 3. Similarly good predictive capability of the model was also proven for Al and IF steel.

Now that models for the evolution of the misorientation angle distributions for the dislocation cell structure within a grain are available (see next section), further development of the texture 'module' has become possible. One can envisage a procedure for updating the cell/grain population at each simulation step that would account for the fact that part of the cells develop into new grains by acquiring sufficiently large misorientations with the adjacent cells.

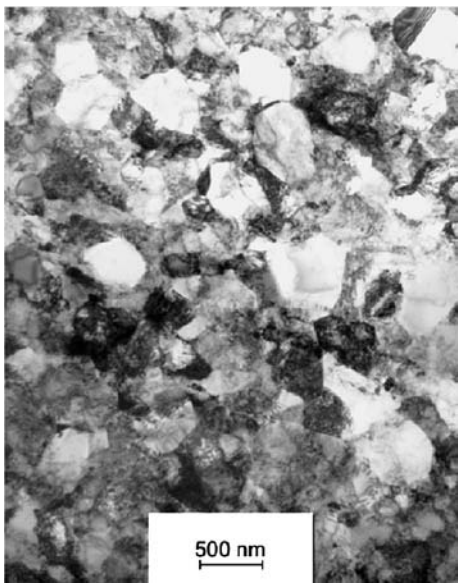

Fig. 1 TEM micrograph of the grain structure in copper after eight equal channel angular pressing (ECAP) passes (Route B_c [10])

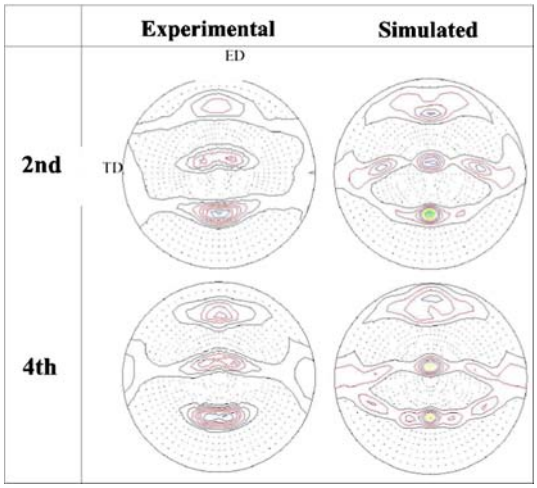

Fig. 3 Simulated (right) and experimental (left) (111) pole figures for the uniform part of a copper billet deformed by two and four equal channel angular pressing (ECAP) passes (Route A [11])

Modelling of the evolution of dislocation cell misorientations

Recently, a modification of the model presented in ''Outline of the microstructure evolution model'' was proposed [12] with the aim of tracing the average misorientation angle. To that end, the dislocation density in the cell walls was divided in two distinct groups. Dislocations of the first group contribute to an imbalance in the Burgers vector in a dislocation cell wall and thus produce a misorientation across the wall. Accordingly, they are referred to as geometrically necessary ones, their density being ρ_w^g. The other group are statistical dislocations, which are redundant in the sense that they do not produce misorientation across the boundary. (Their density is denoted ρ_w^s). The absolute value of the misorientation angle between the neighbouring cells is then given by

$$\theta = \arctan\left(b\sqrt{\rho_w^g}\right) \cong b\sqrt{\rho_w^g}. \tag{12}$$

The main assumption made in Ref. [12] was that a certain fraction ξ of the dislocations incoming into cell walls from the cell interiors contribute to *local* imbalance in the Burgers vector by build-up of the density of geometrically necessary dislocations and thus misorientation. The rate of growth of ρ_w^g was written in the form

$$\dot{\rho}_w^g = \xi\frac{6\beta^*\dot{\gamma}_c(1-f)^{2/3}}{bdf}. \tag{13}$$

It should be noted that this evolution equation does not include any recovery terms, as geometrically necessary dislocations are assumed to be unrecoverable. Adjustments of the evolution equations for the statistical dislocation density in the walls and the total dislocation density in cell interiors are straightforward [12]. A very simple equation,

$$\frac{d\theta}{d\gamma} = \frac{\chi}{2}\frac{1}{\theta}, \tag{14}$$

that follows from Eqs. 12 and 13 can easily be solved. Here the notation

$$\chi = 6\beta^*\xi\frac{b}{d}\frac{(1-f)^{2/3}}{f}, \tag{15}$$

was used. For sufficiently large strains when d and f approach their saturation values, χ tends to a constant, and the solution of Eq. 14 yields a 'parabolic' law of the kind observed experimentally [13]. Using reasonable parameter values, the model equations can be solved numerically, yielding the dependence of the average misorientation angle for copper. It was recognised, however, that the predicted misorientation angles were significantly smaller than the observed ones. This discrepancy can be eliminated by a slight modification of the model [12]. We consider that with the progress of misorientation accumulation the efficiency of cell walls as places for storage of incoming cell interior dislocations increases. This is taken into account by making β^* an increasing function of θ, e.g. by replacing the old β^* with the function $\beta^{**} + (\beta^* - \beta^{**})\exp(-12\theta/\pi)$. This function describes the evolution of this 'efficiency parameter' from an initial value of β^* to a saturation value of β^{**}, the characteristic rate of this evolution being determined by a misorientation angle of 15° ($\pi/12$)—a value that is commonly accepted to signify transition from small angle to large angle case. Figure 4 shows the predicted variation of θ as well as the measurement data. While reasonable agreement was found for a particular choice of the parameter values ($\beta^{**} = 6\beta^*$), the validity of the above *ansatz* needs to be investigated further. One issue that requires experimental clarification before possible modifications are considered is whether the average misorientation angle saturates with the number of ECAP passes. The current version of the model does not predict saturation within a practicable number of passes.

Of great interest for modelling the effects of ECAP on the material microstructure is the misori-

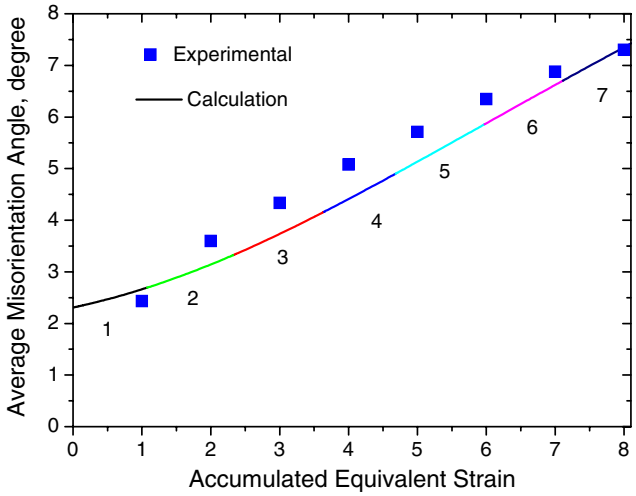

Fig. 4 Evolution of the average misorientation angle with strain (or the number of equal channel angular pressing (ECAP) passes in a 90° ECAP die) for copper: calculation results for ($\beta^{**} = 6\beta^{*}$) vis-à-vis experiment [13]

entation angle *distribution*. A provision for a probabilistic description involving distribution functions can be made in terms of a Fokker–Planck equation [12, 14]. A particular form of the Fokker–Planck equation, derived using the Langevin approach [12], reads

$$\frac{\partial P(\theta,\gamma)}{\partial \gamma} = \frac{kT}{\eta}\frac{\partial^2 P(\theta,\gamma)}{\partial^2 \theta} - \frac{\partial}{\partial \theta}\left\{\frac{1}{\eta} F P(\theta,\gamma)\right\}, \tag{16}$$

where $P(\theta,\gamma)$ represents the misorientation angle distribution function for a given value of the shear strain γ, while the quantities η and F are given by

$$\eta = \frac{\chi}{2\theta^2}. \tag{17}$$

and

$$F = \frac{1}{2\theta}\frac{d\chi}{d\gamma}. \tag{18}$$

A discussion of this probabilistic approach and an analysis of the ECAP history on the misorientation angle distribution will be given elsewhere.

Conclusion

In a 'snapshot' presentation of our research on the evolution of the microstructure and texture during severe plastic deformation by equal channel angular pressing, we attempted to show the recent successes of modelling and also indicate some outstanding problems. These involve particularly the understanding and modelling of the evolution of misorientation angles in the dislocation cell structure and the effect of this evolution on texture development. It is the belief of the authors that these aspects of modelling of ECAP deformation should be among the main targets of research in this area in a near future.

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