Materials Science & Engineering A 658 (2016) 490–502

Contents lists available at ScienceDirect

Materials Science & Engineering A

journal homepage: www.elsevier.com/locate/msea

A three-scale crystal plasticity model accounting for grain refinement in fcc metals subjected to severe plastic deformations

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ARTICLE INFO

Article history:
Received 16 October 2015
Received in revised form
27 January 2016
Accepted 28 January 2016
Available online 12 February 2016

Keywords:
Crystal plasticity
Severe plastic deformation
Grain refinement

ABSTRACT

A new three-scale model of polycrystal accounting for grain refinement is proposed. The model is embedded into the crystal plasticity framework. With the experimental reference to the development of the dislocation induced cell substructure, a single crystallite in the representative grain aggregate is initially subdivided into subdomains with the crystallographic orientations slightly misoriented with respect to the nominal orientation of a parent grain. The predicted misorientation evolution of subgrains with respect to the reference orientation of a crystallite is an indicator of grain refinement. The correlation between the increase of a misorientation angle and a slip activity pattern is analyzed. The model predictions are compared with available experimental data.

1. Introduction

It is well known that materials subjected to severe plastic deformation (SPD) processes can develop ultra fine-grained (UFG) structures (cf. [1]). Many research has been made in order to unravel the mechanisms governing the grain refinement. Qualitative description of the phenomenon can be found in the papers such as [2–8]. Authors discuss the formation of deformation induced cell substructure schematically shown in Fig. 1. Two types of boundaries are distinguished: geometrically necessary boundaries (GNBs) and incidental dislocation boundaries (IDBs). The former divide grains into cell blocks in which plastic deformation occurs by means of different slip systems or with a different level of accumulated strain. The latter form by mutual trapping of dislocations. Plastic strain accumulation is accompanied by a cell size decrease to some saturation value, followed by an increase in misorientation angles across the grain boundaries and in a fraction of high angle boundaries.

One of the simplest and most powerful SPD techniques is the ECAP process, Fig. 2. It was invented by Segal et al. in 1972 and first described in [9]. The process is characterized in many works, e.g. in [6,10,11]. Depending on sample rotations between subsequent passes, there are four fundamental routes of the process, namely A, Ba, Bc and C. Langdon in [7] has dealt with grain refinement in the ECAP process. He concluded that the most equiaxed refined grains form in Route Bc. It is due to the fact that in this route shearing takes place on different planes in subsequent passes, contrary to routes A or C in which the shearing plane does not change throughout the process.

Although the significant research effort has been undertaken to describe and predict the grain refinement phenomenon there is not well-established model yet. Mainly three modeling frameworks can be distinguished among existing proposals.

A macroscopic phenomenological approach was proposed by Beygelzimer [12] and Petryk and Stupkiewicz [13]. Beygelzimer in [12] postulated that accumulation of dislocations leads to the micropore or high angle boundary formation. Hydrostatic pressure limits the former phenomenon, therefore SPD leads to grain refinement rather than material fracture. Petryk and Stupkiewicz in [13] have studied quantitatively the effect of SPD on grain refinement and strain hardening. Within the model the size of dislocation cells and cell blocks is expressed as a function of the effective plastic strain. The standard definition of the effective plastic strain is modified to account for the strain path changes.

The other method to tackle the problem of grain refinement is to apply the crystal plasticity framework enhanced by some additional features [14–19]. With experimental reference to subdivision into cell blocks, Leffers [14,15] has proposed the subdivision of grains into two families of parallel bands. In the model the intragranular strain continuity between bands is maintained by the relaxed constraint model, while the intergranular strain continuity is ensured by imposing identical strains in all grains. The disadvantage of the approach lies in the fact that the orientation of bands is an input data in the computations and it must be established on the basis of some experimental evidences. The Leffers

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http://dx.doi.org/10.1016/j.msea.2016.01.101
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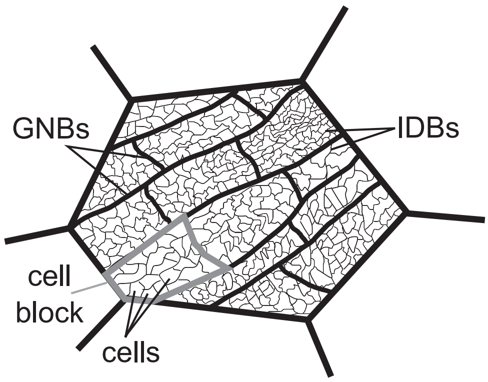

Fig. 1. The schematic drawing of the dislocation induced cell substructure of a grain observed in fcc materials for small to medium accumulated plastic strain according to [4].

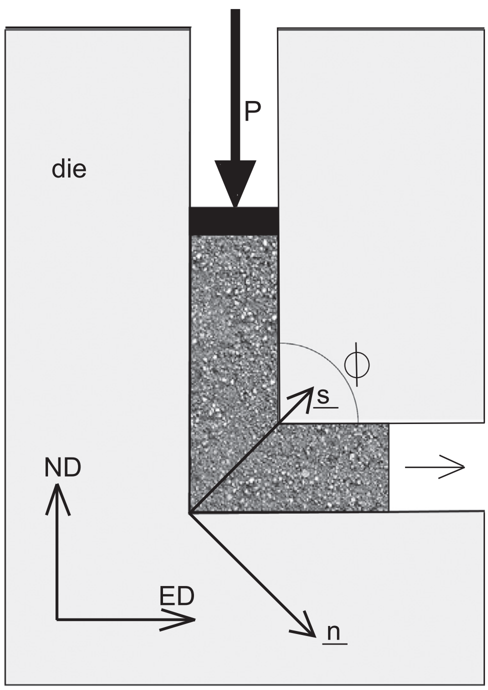

Fig. 2. Scheme of the ECAP process [1].

idea shares common features with the LAMEL and ALAMEL models [20,21]. However, the latter models were not dedicated to study the grain refinement but to improve the Taylor model predictions by relaxing the strong constraints imposed on the aggregate by the iso-strain assumption.

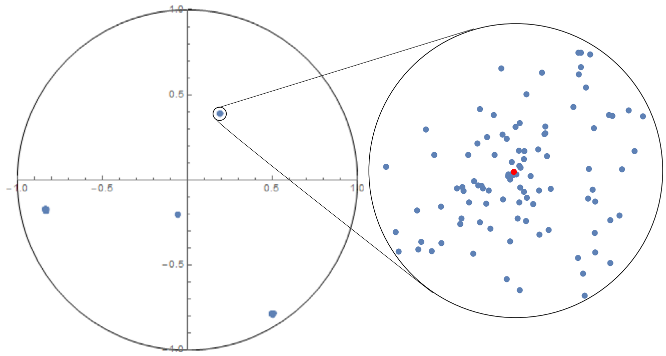

Fig. 4. ⟨111⟩ pole figure presenting initial distribution of orientations in a single metagrain (the nominal orientation of a metagrain is marked by the red point). (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

A simplified model of grain refinement was proposed by Beyerlein et al. [16]. The condition for grain fragmentation is based only on the change of a grain shape. The model uses the visco-plastic self-consistent (VPSC) scheme [22,23] in which every grain is represented by a deforming ellipsoid. If one axis of the ellipsoid becomes considerably longer than the other two (the grain is elongated) then the grain is divided into two new grains. If the middle-length axis becomes additionally much longer than the shortest one (the grain is flattened) the grain is subdivided into four new grains.

In the disclination model for substructure formation proposed in [17,18], which is also set in the crystal plasticity framework, it is assumed that splitting of a grain is possible only when the grain is deforming more slowly than the surrounding medium. This criterion is checked based on the calculated strain rates of the grain and the homogeneous equivalent medium in the VPSC model. Therefore, the splitting occurs for the grains least favourably oriented with respect to the applied strain. After each subdivision the number of grains is increased by one.

In [19,24] another physically sound model is presented. Authors assume that grain rotation is impeded near the grain boundaries which causes the development of a lattice curvature. The latter leads to the increase of misorientation inside a grain and the grain fragmentation as a result. In the model the grain is represented as a 'Rubik-cube' subdivided into $3 \times 3 \times 3$ subgrains. Following the basic assumption of the model, depending on the location of a subgrain with respect to the 'Rubik-cube' outer surface the crystallographic lattice of a subgrain rotates differently. If the misorientation angle between the subgrains reaches a threshold value the subgrain is treated as a new grain and is again subdivided into $3 \times 3 \times 3$ domains. The Taylor hypothesis [25] about an equal deformation gradient in each grain/subgrain is used. Due

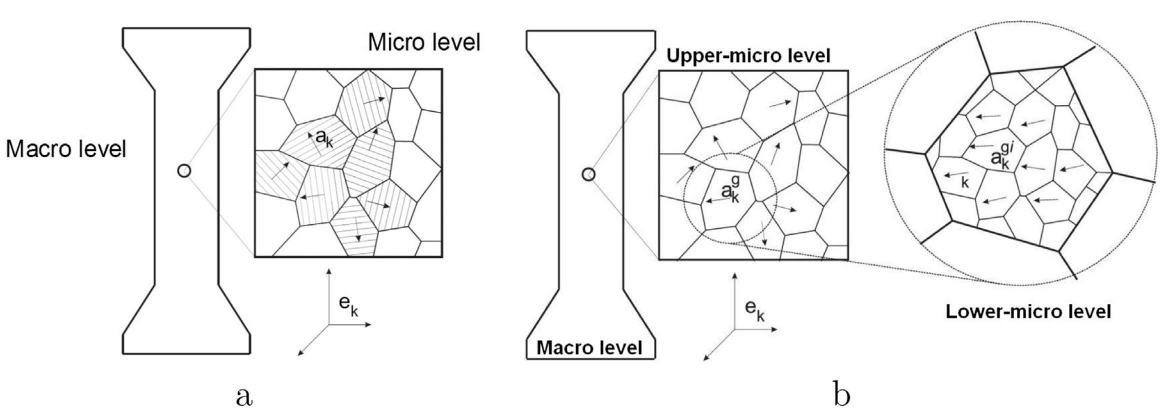

Fig. 3. Schematic view of (a) the two- and (b) the three-scale model.