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# A model of grain fragmentation based on lattice curvature

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**Abstract**

A new model is proposed that aims to capture within a single modelling frame all the main microstructural features of a severe plastic deformation process. These are: evolution of the grain size distribution, misorientation distribution, crystallographic texture and the strain-hardening of the material. The model is based on the lattice curvature that develops in all deformed grains. The basic assumption is that lattice rotation within an individual grain is impeded near the grain boundaries by the constraining effects of the neighbouring grains, which gives rise to lattice curvature. On that basis, a fragmentation scheme is developed which is integrated in the Taylor visco-plastic polycrystal model. Dislocation density evolution is traced for each grain, which includes the contribution of geometrically necessary dislocations associated with lattice curvature. The model is applied to equal-channel angular pressing. The role of texture development is shown to be an important element in the grain fragmentation process. Results of this modelling give fairly precise predictions of grain size and grain misorientation distribution. The crystallographic textures are well reproduced and the strength of the material is also reliably predicted based on the modelling of dislocation density evolution coupled with texture development.


*Keywords:* Grain fragmentation; Severe plastic deformation; Texture development; Strain-hardening; Misorientation distribution

## 1. Introduction

Grain refinement by plastic deformation is a potent way of improving the mechanical properties of metallic materials. In a recent stream of research articles, extreme grain refinement down to micron and sub-micron range by severe plastic deformation (SPD) has been reported. Recent overviews of the area can be found in Refs. [1,2]. Most popular techniques of grain refinement by severe plastic deformation are equal-channel angular pressing, high pressure torsion and accumulated roll bonding, but further SPD-based processing routes are also emerging. While experimental work in this area has produced a significant body of knowledge with regard to microstructure and properties of SPD processed materials, the mechanisms of grain refinement, which is crucial for the property improvement, are far from being unravelled. Important work of the RISØ group [3,4] has led to a comprehensive classification of the grain structures produced by deformation to large strains, but again the underlying mechanisms are not fully understood. Previous work on SPD-induced microstructures [5,6] suggests that a dislocation cell structure formed within a grain can be considered as a precursor of the eventual grain structure. Pantleon [7] and Estrin et al. [8] quantified the notion that fine granularity is attained through gradual accumulation of misorientations across the dislocation cell boundaries with progressing straining. Their calculations of the increase of dislocation cell misorientations are consistent with the observed level of misorientations associated with the incidental grain boundaries (in the terminology of Pantleon and Hansen [3]), but cannot account for the occurrence of a very significant fraction of large-angle grain boundaries found experimentally, e.g. for equal-channel angular pressing (ECAP).

The current situation with modelling SPD processing can be characterized as follows. Whereas the existing

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models based on dislocation density evolution [9–12] can account for strain-hardening associated with severe plastic deformation, the process of grain refinement as such, and the concomitant evolution of misorientations between neighbouring grains, are in need of better modelling. The latter aspect also means that texture simulations of SPD need to be addressed in a more rigorous way.

Existing attempts for understanding grain refinement focused on the effects of the initial orientations of a grain and its neighbours as well as the effects of the deformation field itself. Barnett and Montheillet [13] and Raabe et al. [14] used the asymmetric convergent/divergent nature of the rotation field in orientation space for simulation of orientation gradients within crystals. Raabe et al. [15] carried out finite element simulations and found that grain refinement is much more dependent on the initial orientation of the grain than on the orientations of its neighbouring grains. Disclinations were also employed for modelling orientation gradients [16,17].

To date, the gradual change of the grain population due to grain subdivision is not included in the simulations; cf. Ref. [18], so that an essential feature of the processes is disregarded. The aim of the present article is to develop a model that does account for grain subdivision in considering microstructure evolution, including grain size and local misorientation distributions, overall texture and strain-hardening. A main ingredient of the model, viz. grain subdivision, will be treated as a result of the development of lattice curvature within an individual grain and constraints imposed by its neighbour. The geometrically necessary dislocations associated with the lattice curvature will be considered to give rise to grain subdivision. A simplified model of subdivision of a grain in exactly 27 subgrains, which develop to new grains when a critical misorientation with regard to the neighbouring grains is exceeded, will be constructed. Combined with the strain-hardening modelling frame developed earlier, this element of modelling will be shown to give more than satisfactory predictions of all major features of microstructure and texture evolution, as well as the strain-hardening behaviour of SPD processed copper taken as a representative face-centred cubic (fcc) material.

The paper is structured as follows: In Section 2, the basic assumptions underlying the model are presented. This is followed by a description of the numerical implementation of the model in Section 3. The results of numerical simulations of ECAP processing of copper with regard to grain size and misorientation distributions, strain-hardening and texture are reported in Section 4, along with a comparison with experiment and a discussion of the various aspects of the simulations. A brief concluding section contains an overall assessment of the results and the predictive potential of the model.

## 2. Basic assumptions

### 2.1. Lattice distortion

A polycrystal is considered which is deformed plastically to large strains. Deformation changes the grain shape, the lattice orientation, the dislocation density and, in general, the microstructure. In the initial undeformed state, the lattice planes can be considered to be perfectly planar, i.e. not distorted, as depicted in Fig. 1. However, during deformation the orientation of an individual crystallite undergoes a change. It is reasonable to assume that the concomitant rotation of the crystallographic planes of the crystallite is impeded near the grain boundaries (GBs) so that the lattice rotation is smaller there than in the middle part of the grain. In the simplest case, we can divide the grain interior into two zones: a zone near the GB where lattice rotation is slower and another one, situated in the middle part of the grain, which is not affected by the GB. Because of the differences in the amount of lattice rotation, a crystallographic plane would be curved within the outer, near-boundary, zone. Lattice curvatures can be readily observed experimentally by EBSD in plastically deformed grains [19–22], as seen in an example in Fig. 2.

Following the arguments presented above, if we look at the distorted plane from the direction of the lattice rotation vector, the lattice plane is expected to be of a near S-shape, see Fig. 1. In reality, a plane becomes three dimensional

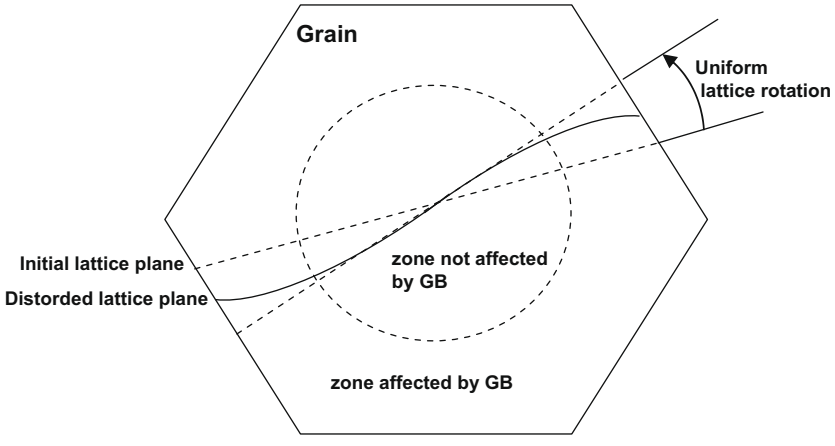


Fig. 1. Lattice curvature in a grain.