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Generalized vertex model of recrystallization – Application to polycrystalline copper

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Abstract

The vertex model is first extended in order to take into account the influence of the stored energy on the recrystallization processes. Some phenomenological laws describing the evolution of grain boundary energy and mobility versus misorientation are used. Nucleation is considered to be site-saturated and no specific misorientation is taken into account in the law describing the grain boundary mobility. The experimentally determined stored energy values, crystallographic orientations and boundary misorientation distributions are used in order to characterize the initial microstructure. The vertex model is then tested to study the recrystallization of 70% and 90% cold rolled polycrystalline copper during annealing treatment. In order to explain the texture evolution in both cases, it is necessary to introduce an energy threshold for grain boundary movement, i.e. a minimal value of the stored energy difference between neighboring grains necessary to cause the grain boundary motion. With both improvements (incorporation of the stored energy and of its threshold), the developed model is shown to predict texture evolutions in good agreement with experimental data.

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1. Introduction

Recrystallization within a deformed metallic material occurs by the formation (nucleation) and subsequent growth of a new, strain-free, structure of grains. The growth process is driven by the stored energy difference between the nuclei and the surrounding deformed microstructure. This difference, which is linked to the difference in dislocation density, is often considered as the main driving force for recrystallization. It is well known that recrystallization can significantly modify the distribution of orientations (texture) inside the material and produce drastic changes of many physical properties (electrical resistance, internal stresses, micro-hardness, etc.). Despite extensive studies on recrystallization over many years, the basic mechanisms of nucleation and growth, which are quite complex, are still not clearly explained. Also, different models were developed in order to describe the recrystallization process. The most important ones are: the Monte-Carlo model [1–3] based on a global energy minimization concept, the vertex model [4–6] in which forces acting on triple junctions are considered, cellular automata algorithms [7], some statistical approaches using a compromise function concept [8,9] or finite elements approach [10]. Each of these models has some advantages and some restrictions. The Monte-Carlo concept is very efficient and relatively easy to apply to complex microstructures.

Abbreviations: SE, stored energy; EBSD, electron back scattered diffraction; BMD, boundary misorientations distribution; ODF, orientation distribution function.

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On the other hand, grain boundary curvature cannot be satisfactorily introduced. The vertex model is usually based on some simple assumptions for grain boundary energy and mobility. Contrary to the Monte-Carlo model, the vertex model is a deterministic one and enables the introduction of a grain boundary curvature. This model was thus successfully used in the past to predict the grain growth [4,5], where boundary energy and boundary types play the most important role. The present authors have extended the vertex model by introducing the intragranular stored energy (SE) parameter into the model [11,12], which allows to describe the primary recrystallization as well.

It is indeed generally accepted that SE plays a key role in recrystallization. Therefore, the knowledge of SE distribution vs. crystallographic orientations is crucial for a tentative explanation (at least qualitatively) of texture transformation during annealing. This energy can be estimated by electron, X-ray, neutron and electron back scatter diffraction (EBSD). In the present calculations, some stored energy data estimated from synchrotron X-ray measurements in the deformed state [13,14] was used.

In this paper, we focus on the recrystallization of cold rolled copper after two levels of deformation – 70% and 90% rolling reductions. It is commonly observed that, in cold rolled polycrystalline copper, there exists a transformation from the copper type rolling texture to the cube recrystallization type texture during annealing after high strains (i.e. higher than 70% strain) and to a mixed "deformation–recrystallization" texture during annealing after low strains. In order to explain this texture transition, both preferred nucleation and oriented growth theories have been evoked in the past, based on somewhat contradictory arguments. From the experimental point of view, some recent and accurate analysis of the data obtained after two strain levels (70 and 90%) clearly indicate that recrystallization in polycrystalline copper takes place by the following mechanisms [13,14]:

- The so-called strain induced boundary migration (SIBM) in recovered grains, especially for crystallites having an orientation close to the cube one,
- some uniform intergranular nucleation (IN) in all other rolling orientations, presumably at grain boundaries, where the gradient of orientation is usually quite high,
- the subsequent growth of nuclei or recovered grains driven by the SE gradient.

The vertex model was generalized in order to account for these facts. Its original version proposed by Kawasaki et al. [4] and later developed by Weygand [5] was, up to now, only used to simulate the grain growth (i.e. the process occurring *after* primary recrystallization). In this case, grain boundary movement leads to the minimization of the total boundary energy. In Kawasaki's 2D model, the evolution of the grain structure is described by movements of the triple points – so-called "real vertices" (at which three grain boundaries meet). The equations of triple point motion are derived from a variational approach. The grain boundary energies and mobilities are taken anisotropic in both models – i.e. they depend on the crystallographic misorientation between adjacent grains. The introduction of the intragranular stored energy into this vertex model by Piekos et al. [11,12] enables then the application of the model to the simulation of primary recrystallization.

The aim of this paper is to describe in details the development of the recrystallization model and to compare predictions with some recent experimental results obtained on polycrystalline copper. It is especially interesting to know whether the mechanisms described above, combined with different stored energy distributions for the two deformed states (after 70% and 90% strain), can explain the observed differences in the final recrystallization texture of copper. In order to get as accurate predictions as possible, the measured initial distributions of orientations (deformation texture), stored energy and boundary misorientations (BMD) were used as input parameters for modelling.

2. Experimental and modelled description of the initial deformed state

2.1. Texture evolution in cold-rolled copper

The development of crystallographic texture during recrystallization after rolling has been a subject of intense study over the last decades, but the strong influence of the deformation level on the recrystallization texture is still not clearly explained. In the present work, the textures of deformed and recrystallized samples have been determined both by X-ray diffraction (for a statistical and quantitative analysis) and by EBSD (for incorporation into the vertex model).

The orientation distribution function (ODF) measured after 70% rolling reduction (Fig. 1a) is composed of the typical so-called "β-fiber" which is composed of the following ideal orientations: C at the (approximated) Euler angles $(\varphi_1, \phi, \varphi_2) = (90°, 35°, 45°)$, $S = (59°, 34°, 65°)$ and $B = 35°, 45°, 90°)$. The cube $= (0°, 0°, 0°)$ and Goss $= (0°, 45°, 0°)$ orientations are also present but in a very small percentage. In the case of 90% reduction, the deformation texture (Fig. 2a) is very similar in terms of main components but is more intense. The ODF of recrystallized polycrystalline copper consists of a strong cube component $(0°, 0°, 0°)$ and of a relatively strong retained rolling texture after 70% reduction (Fig. 1b). On the other hand, in the material previously rolled up to 90% reduction, only the cube component is present after recrystallization (Fig. 2b). The recrystallized samples were obtained by annealing during 15 min at 300 °C (for a more detailed description of these textures, see Refs. [13,14]). The choice of the annealing temperature was selected in order to ensure a complete recrystallization.