Monte Carlo simulation of primary recrystallization in an IF steel

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Abstract

This study presents a contribution to the modeling of primary recrystallization stage in an IF steel that is destined to the automotive industry. A two dimensional Monte Carlo technique is proposed to simulate primary recrystallization. It is well known that recrystallization includes nucleation and growth of nuclei until the consumption of the deformed matrix. The major challenge is the choice of nuclei (locations, orientations, number ...) and conditions of their subsequent growth (speed, final size ....). Nucleation starts in grains that have the highest stored energy of deformation, and then progresses in grains that have lower stored energy. In this work, we used an internal misorientation parameter, calculated from EBSD data, to estimate stored energy in the deformed microstructure. The comparison of primary recrystallization simulation results with the experimental behavior requires initial data for the model development and final data for its validation. For this, a detailed experimental recrystallization study was performed, starting from 75% cold rolled state. This presentation will discuss the effect of using our misorientation parameter for identifying nucleation sites on microstructure and texture evolutions as well as the ability of our model to predict the experimental behavior.

Keywords: Monte Carlo, modeling, recrystallization, IF steel, texture, EBSD.

Introduction

Interstitial Free (IF) steel is important classes of deep drawing quality steels [1-2]. Development of deformation and recrystallizaion texture, in IF steels, provides a high level of scientific interest. Primary recrystallization includes germination and growth of germs and their subsequent growth until the consumption of the deformed matrix. Nucleation involves the formation of small volumes relatively perfect, which are partially bordered by boundaries at high angles, within the deformed matrix [3]. For nuclei viable, these volumes must have sufficient sizes to continue to grow in the hardened matrix. If recrystallization is considered as a phenomenon of nucleation and growth, and controlled by thermally activated process, whose driving force is provided by

the stored energy of deformation. The evolution of the microstructure and texture, during annealing, can be simulated with the Monte Carlo method from an EBSD mapping which is formed of pixels [4]. The primary recrystallization is simulated in 2D, changing the equation site energy [5], adding a term that takes into account the energy stored during the deformation:

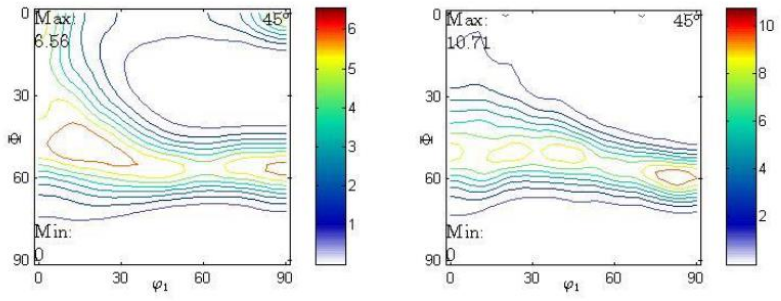
$$E = J \sum_{neihbors} \left(1 - \delta Q_{site}(i)\, Q_{neighboring\ site}\right) + H\, \theta(Q_{site})$$

Where J is a constant that defines an energy scale of the grain boundary per unit length, δ is the Kronecker function, Qsite(i) the value of the orientation of the chosen site and Qsite voisin is the numbers corresponding to the orientation of the sites that are neighbors of the site chosen Qsite(i). H is the stored energy per unit area in 2D, θ(Qsite) is a function which is 1 for non-recrystallized grains and 0 for the

recrystallized grains. After initializing the microstructure, nucleation is simulated by adding small nuclei in the material.
The objective of this study is simulation of microstructure and texture evolution during primary recrystallization of 75% cold rolled IF steel, using the Kernel Average Misorientation (KAM) [6-7] as a semi quantitative indicator for the stored energy and for identifying nucleation sites.

Results

As in previous studies [8,9], textures of steel are discussed mainly considering the α (RD//<110>) and γ (ND//<111 >) fiber components.
Texture of the 75% cold rolled sample is characterized by the presence of both α and γ fibers (Fig.1a), with α-fiber more intense than γ-fiber. The trend reversed during recrystallization; the evolution of the texture is marked by a reinforcement of γ-fiber at the expense of α-fiber (Fig.1b).

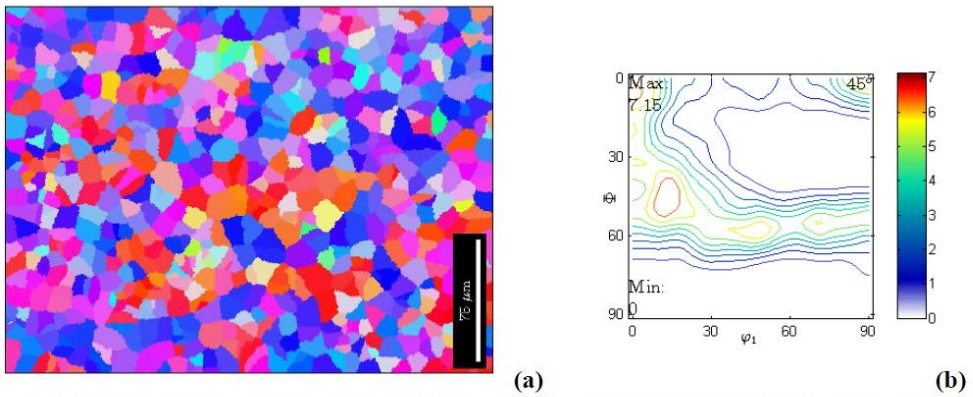


(a) (b)

Figure 1: φ_2 = 45° ODF sections showing: (a) texture of 75% cold rolled sample, (b) texture of the fully recrystallized sample.

In our Monte Carlo technique, we have used real (experimental) microstructures, obtained from EBSD analyses, to initialize the simulation procedure (the 75% cold rolled sample) and for the validation of simulation results (the fully recrystallized sample). For the nucleation stage, 700 nuclei are chosen from the matrix pixels with higher KAM valuess.

Microstructure and texture that are obtained from our simulation, at the end of recrystallization, are shown on (Fig.2a) and (Fig.2b), respectively. Texture is characterized by a fiber γ more pronounced than α fiber with an ODF maximum on {111}<112> component. This evolution is in agreement with the experimental trend.



(a) (b)

Figure 2: Simulation results at the end of recrystallization: (a) microstructure, (b)φ_2=45° ODF section showing texture.

Conclusion

In this paper, a Monte Carlo model was proposed to simulate primary recrystallization in an IF steel where nuclei were inserted among pixels of higher KAM values. When simulation and experimental textures are compared, it was

found that in both case there is reinforcement of γ fiber at expense of α fiber. Therefore, our model gives satisfactory results to describe primary recrystallization in IF steels and the KAM can be considered as good parameter to detect nuclei which could develop during recrystallization.

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