A R C H I V E S O F M E T A L L U R G Y A N D M A T E R I A L S
Volume 50 2005 Issue 1

J. SZPUNAR*, H. LI* J.-T. PARK**

MODELING OF TEXTURE AND MICROSTRUCTURE TRANSFORMATION OF METALS DURING ANNEALING[1)]

MODELOWANIE TANSFORMACJI TEKSTURY I MIKROSTRUKTURY METALI PODCZAS WYŻARZANIA

In this article, we would like to outline examples of research of our group on recrystallization and grain growth textures. Rules that govern the transformation of texture and structure of metals during annealing are complex and not well defined. For this reason, the computer simulation of the transformation of the microstructure and texture received much attention in recent years. Computer models allow to introduce more realistic microstructural conditions that control the transformation of texture and microstructure.
Keywords: texture, microstructure, annealing, simulation, modeling, stored energy, grain growth, recrystallization.

W pracy przedstawiono przykłady badań tekstury rekrystalizacji i wzrostu ziaren. Prawa dzialające podczs wyżarzania są złożone i trudne do zdefiniowania. Z tej przyczyny dużym zainteresowaniem cieszy się w ostatnich latach komputerowa symulacja transformacji tekstury i struktury. Modele komputerowe pozwalają na wprowadzenie bardziej realistycznych warunków mikrostrukturalnych kontrolujących transformację tekstury i struktury metali.

The processes of nucleation, recrystallization, grain growth and abnormal grain growth are governed by factors such as the crystal structure, the phase composition, the elastic stored energy that depends on the metal's thermo-mechanical history, and on the various microstructural defects that affect the mobility of grain boundaries. At various stages of the annealing, different processes take place; the nucleation may depend on the previous treatment of materials, phase composition or precipitate distribution. If

* DEPARTMENT OF MINING, METALS AND MATERIALS ENG., MC GILL UNIVERSITY, MONTREAL, CANADA, H3A 2B2
** ELECTRICAL STEEL RESEARCH GROUP, TECHNICAL RESEARCH LABORATORIES POSCO, GEODONG-DONG, NAM-GU, POHANG-SHI, GYEONGBUK, 790-785 SOUTH KOREA, POHANG P.O. BOX 36
1) invited lecture

the metal was cold rolled, the location of the nucleation sites and the orientation of the nuclei will depend on the distribution and the magnitude of the stored elastic energy and structure of local microstructural inhomogeneities. The stored energy as a function of grain orientation can be at present estimated based on measurement of the broadening of X- ray [1] or neutron diffraction [2] or approximated using the quality of EBSD diffraction patterns [3]. Such stored energy data were used in computer programs [4, 5] and allow rather realistic analysis of the transformation of microstructure, the prediction of the nucleation sites, and the orientations of generated nuclei. However, there is no unique model that will allow making a decision as to where the nuclei are formed and what orientation they have. In some cases, like in the case of recrystallization of aluminum alloy, we have argued that the rate of changes of elastic stored energy is the most important [5, 6] while in the case of LC steels and IF steels the maximum value and the gradient of stored deformation energy decides the nucleation site [7]. In general, it is very difficult to propose a general rule as to what the orientation of the nuclei should be. However, in some cases, it was possible to link the orientation of the nuclei to the orientation of the neighbor grains assuming that most of the nuclei are formed at the grain boundaries of deformed grains [7] and that the orientation of the nuclei is influenced by the elastic energy stored in two neighbor grains.

Recrystallization is the next step after nucleation and during this step the nuclei grow and consume the deformed matrix lowering the elastic energy stored in deformed grains. In this stage it is very important to know what elastic energy is stored in grains of different orientations[3], to model the driving force of recrystallization and to assign appropriate mobility to grain boundaries.

The high mobility of high energy grain boundaries is a fundamental assumption in all our simulation of recrystallization and grain growth. [8–13] in aluminum and steels. However in the case of LC and IF steels the nucleation decides what the recrystallization texture will be while the development of Cube texture in aluminum is a result of competition at the level of both the nucleation and growth. In addition, our results presented in [7] indicated that the Cube textured grains in aluminum do not have the highest stored energy but nucleate at the faster rate.

Finally, the explanation of abnormal grain growth and development of texture in grain oriented Fe-Si steel is a particularly important example of the simulation of texture transformation during annealing. The most important finding is the observation that the Goss grains are surrounded by a very high percentage of high energy grain boundaries [10, 12, and 13]. The diffusion along such grain boundaries is much faster than in bulk and along other grain boundaries and therefore the precipitate coarsen at the fast rate around the Goss grains. As a result the Goss grain will grow while grains of other orientations are prevented from growing because their grain boundaries are pinned by precipitates [14]. This is a very sensitive and well balanced process and the success of the abnormal growth of Goss grains depends on the rate of precipitation coarsening and texture developed before the final high temperature annealing.

All these complex transformations of texture and microstructure during annealing cannot be predicted by analytical rules and models. The rules of textural transformation

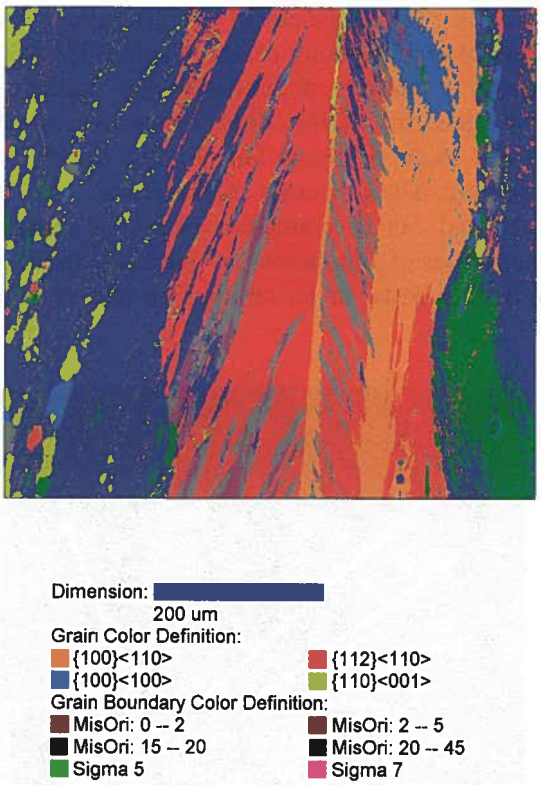

Fig. 1. Grain map of deformed 2%Si steel

during annealing in materials that have, at the microscopic level, inhomogeneous and complex structure are too complex and depend on the thermo-mechanical history of the materials. For these reasons the simulation of various aspects of the annealing processes received much attention in recent years. Notable achievement in this area was first reported by Anderson et al. [15] in simulating grain growth phenomena within the framework of the Q-state Potts model. Simulation of texture development during nucleation and grain growth were initiated by Tavernier and Szpunar [16, 17] within the same model by introducing the concept of maps of stored energy of deformation to propose the criteria of texture nucleation and assuming that certain nuclei which achieved a critical size could grow. A grain growth model was based on the assumption that the difference in the mobility of boundaries having different energy may influence the development of texture. This simple model was developed further by Hinz and Szpunar [4] and was used with different modification in the simulation of different annealing processes in metals.

Texture measurements by X-ray or neutron diffraction are used at present to verify the kinetics of transformation at various stages of annealing and to allow statistical

verification of the models. Computer generated microstructures, however may not offer a realistic representation of inhomogenity of the structure before annealing.

Considerable progress in this area of simulation was made by L i et al. [18] using the microstructure determined from OIM (EBSP) measurements which represents not only orientation, size and shape of grains but also the distribution of elastic energy stored in this microstructure. The processes of nucleation, recrystallization and grain growth can be followed and can be compared with OIM experiments. Such an approach opens new possibilities of simulations of microstructural transformation during annealing and should help in better understanding the nucleation and recrystallization processes.

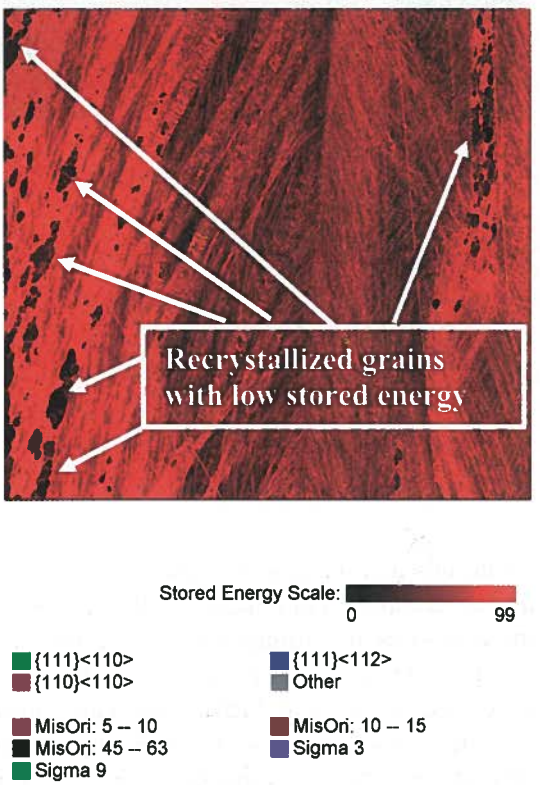

Fig. 2. Stored energy distribution deformed 2%Si steel

An example of such simulation is shown in Figs. 1–3. Fig. 1 shows the deformed microstructure of 2% Si steel specimen after 75% cold rolling reduction. The measurement was done by Philips XL-30 FEG with TSL orientation imaging system. Grains in blue have {111}< 112 > orientation; grains in green have {111}< 110 > orientations; grains in red have {112}<110> orientation; and grains in dark yellow are Goss grains that are already recrystallized. The deformation stored energy distribution can be estimated from the image quality of OIM measurement. The image quality (IQ)

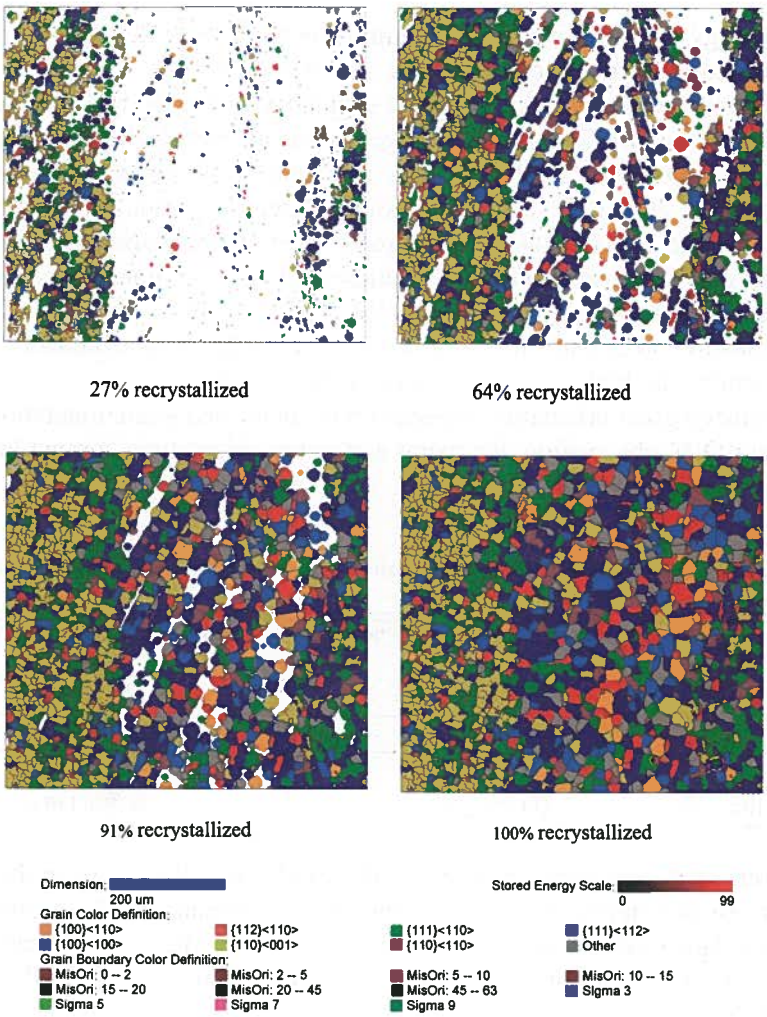

Fig. 3. Illustration of different simulation stages 2%Si steel

represents the distortion of crystallographic structure of the grain. Lower IQ value is assumed to indicate that the grain experienced more severe distortion and therefore has the higher stored energy. The stored energy can also be estimated by calculation of the dislocation density when the dislocation density is associated with the low angle grain boundary with misorientation less than 2 degree. Both of the IQ values and dislocation calculation give the similar results on stored energy distribution. Fig. 2 shows the stored energy distribution estimated from IQ values. Red color indicates high stored energy locations and black color indicates low stored energy locations. It is very important to see that the darkest regions represent the grains that are already recrystallized which can be confirmed by comparing the corresponding locations on Fig. 1. This result is considered as the experimental verification of the proposed methodology to evaluate

the stored energy, because recrystallized grains have zero stored energy and therefore should represent the darkest regions on the stored energy map.

Fig. 3 shows the four different stages of simulation where the recrystallized volume is 27%, 64%, 91 and 100%. At the early stage of recrystallization, Goss grains, indicated by dark yellow color, have small grain size and form in cluster inside the shear band, which usually has 20° or 35° angle with rolling direction. Then, γ fiber components, marked by blue and green colors, and also some other components start to form and the size of these grains increases. For this simulation, the assumptions of recrystallization mechanism are briefly defined as follows [19]:

1. The nucleation takes place first in area having the highest stored energy. The shear band contains the highest stored energy in this simulation.
2. Recrystallized grain orientation depends on the deformed grain orientation. According to our OIM observation, the major and minor orientations formed in deformed grains are shown in Table 1.

TABLE

Major and minor orientations of the recrystallized nuclei of 2%Si steel observed by OIM

Deformed matrix	Major orientations of recrystallized nuclei	Minor orientations of recrystallized nuclei
Shear band	{110}<001>	{001}<100>
{111}<112>	{111}<110>	{111}<112>
{111}<110>	{111}<112>	{111}<110>
{112}<110>	{111}<112>	{112}<110>

However, as it was mentioned above, the mechanism that governs the recrystallization process is complicated and depends on the material and deformation history. There is no unique mechanism that can be used to describe the recrystallization process in all cases. Therefore, a software is being developed that will eventually allow user to define their own mechanism and rules for recrystallization.

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Received: 24 January 2005.