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Experimental verification of Monte Carlo recrystallization model

T.A. Walasek

Institute of Metal Working, Quality Engineering and Bioengineering
Technical University of Częstochowa
Al. Armii Krajowej 21, 42-200 Częstochowa, Poland

In the paper microstructures simulated by the Monte Carlo model of primary static recrystallization have been compared to the real microstructures. Both the computer simulations and the experimental tests have been performed in order to confirm the correctness of the nucleation models. The performed tests have shown satisfactory agreement of the deformed and recrystallized Armco iron microstructures and the ones from the simulation with the decreasing nucleation rate model.

1. INTRODUCTION

In metallic materials, according to Vandermeer [1], primary recrystallization is the microstructural change occurring during a post-deformation annealing heat treatment whereby new, strain-free grains emerge (become detectable) from within the plastically deformed microstructure (nucleation) and subsequently increase in size (growth) until the deformed volumes are consumed. The dominant driving force for this phenomenon is assumed to be stored energy of plastic deformation distributed in the interior of the deformed grains, in the form of point defects and dislocations.

The nucleation phenomenon in the recrystallization process is probably one of the least known due to the fact that it is extremely difficult to observe experimentally. It is assumed that the real nucleation does not occur during the recrystallization of cold worked metals [2] but the nuclei occur in the process of recovery by subgrain coalescence or by subgrain growth. It is known that deformed microstructure is highly heterogeneous and there are locations in the material of more favorable conditions to generate recrystallization nuclei. These locations have higher deformation energy stored in the form of dislocations and point defects structure.

2. SIMULATION TECHNIQUE

A number of applications of the Monte Carlo method were enumerated by Saito [3]. Maurice [4] compared eight network and Monte Carlo simulation techniques in terms of kinetics, size and side number distributions and obtained a very good similarity of distributions. A kind of relationship between the Monte Carlo time scale and the physical one, implicit in Network models, was revealed.

In the paper the Monte Carlo algorithm has been applied to model the primary recrystallization of variable nucleation rate.

The algorithm employed in the simulation of recrystallization is similar to that described by Anderson [5], Srolovitz [6] and Rollet [7]. The continuum microstructure is divided into a number of discrete points using a two dimensional *200x200* lattice. The crystallographic orientation of grains S_i, expressed by a number from *1* to *Q*, is assigned to each lattice site *ij*. A lattice site whose orientation is different from a neighbouring one is regarded part of a grain boundary. Otherwise the lattice site belongs to the grain interior. The grain boundary energy is specified by associating a positive energy with the elements of grain boundary as described by Srolovitz [6]:

$$E_i^1 = -J\sum_{nn}\left(\delta_{S_iS_j} - 1\right) \tag{1}$$

where $\delta_{S_iS_j}$ is the Kronecker delta, the sum is taken over nearest neighbouring sites and J is a positive constant that sets the scale of the grain boundary energy for the simulation.

The stored energy of the cold deformation is associated to the unrecrystallized sites according to Srolovitz [6]:

$$E_i^2 = H\sum_{(i)}\Theta\left(Q - S_i\right) \tag{2}$$

where: $\Theta(Q\text{-}S_i)=1$ for $Q\text{-}S_i \geq 0$, $\Theta(Q\text{-}S_i)=0$ for $Q\text{-}S_i < 0$, *H* is a positive constant which sets the magnitude of the stored energy, and *Q* is the number of all distinct orientation of unrecrystallized grains.

On the basis of classification given by Christian [8] four types of nucleation were simulated: *site saturated*, *constant nucleation rate*, *increasing nucleation rate*, *decreasing nucleation rate* – every *10 MCS*, *I-(n(i-1)/10)* nuclei were randomly placed on the lattice. In the paper: *I=200* , *n=10* and *i=1, 11, 21, ... MCS* were used. Every nucleation type was simulated using four degrees of stored energy *H/J=1*; *1.5*; *2* and *2.5*. [9, 10]

All the numerical simulations of the primary static recrystallization confirm correctness of the models considering the curves of the recrystallized volume fraction *F(t)*. The sigmoidal time dependence of recrystallized volume fraction is often emphasized in the literature and finds its justification in the experiment. The Avrami exponent *n=2* is properly reproduced by the simulations.

3. EXPERIMENTAL DATA

3.1 Stand and specimen preparation

In order to verify the model of the static recrystallization a number of experimental tests were carried out. The samples made of ARMCO iron were extruded to *10%*, *20%* and *30%* of deformation degree. Then the samples cut to *10x10x55 mm* dimensions were placed in the SMITWELD TCS 1405 thermal cycle simulator. The specimens were placed in the water cooled jaws, heated to the temperature *T=973K* and annealed for *t=300s*. Then microsections were made from the deformed and annealed specimens and they were observed under a metallographic microscope. The microstructures were measured with Joyce-Loebl image analyser.

3.2 Comparison of experimental and numerical data

Complete statistical tests were performed to verify the Monte Carlo simulation of primary recrystallization. T-Student test was used to compare the mean grain size obtained from all the simulations and from the experiment. Moreover, F-Fisher-Snedecor test was used to compare the variances of the grain size. The significance level of $\alpha=0.05$ for both T-Student and F-Fisher-Snedecor tests was taken. On the basis of the performed statistical tests it can be stated that the nucleation model fitting Armco iron recrystallization best is the decreasing nucleation rate model.

Distribution of the grain size for microstructure obtained from the described experiment for *10%* deformation compared with the microstructure from the Monte Carlo simulation of recrystallization for the decreasing nucleation rate and the degree of stored energy *H/J=1* was shown in figure 1. Both microstructures were tested with t-Student and F-Fisher-Snedecor tests showing a satisfactory agreement when significance level $\alpha=0.05$ was used.

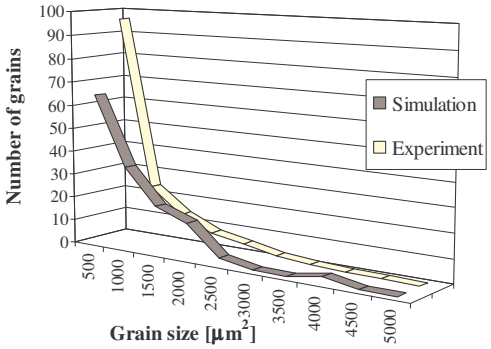

Figure 1. Histogram of the grain size for the specimen of Armco iron deformed *10%* and then recrystallized and the microstructure obtained from the simulation for decreasing nucleation rate and *H/J=1*.

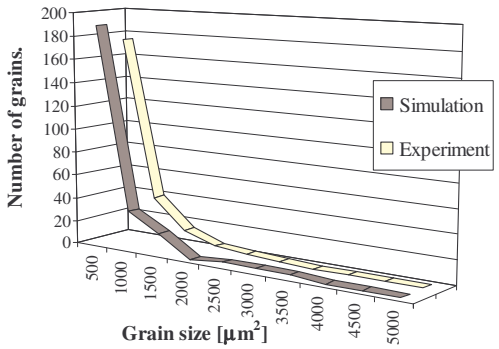

Figure 2. Histogram of the grain size for the specimen of Armco iron deformed *20%* and then recrystallized and the microstructure obtained from the simulation for decreasing nucleation rate and *H/J=1.5*.

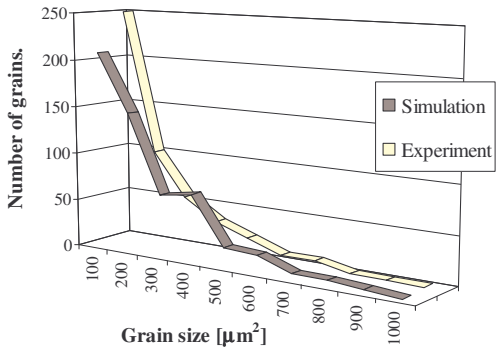

Figure 3. Concentrated histogram of the grain size ranging from *0-1000* μm^2 for the specimen of Armco iron deformed *30%* and then recrystallized and the microstructure obtained from the simulation for decreasing nucleation rate and *H/J=2*.

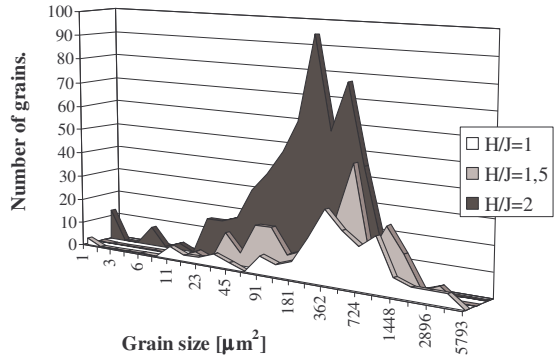

Figure 4. Histogram of the grain size distribution for the calculated microstructures for decreasing nucleation rate and the degree of stored energy *H/J=1, 1.5* and *2*.

Similarly, in figure 2, the grain size distribution of Armco iron deformed *20%* and then recrystallized was compared with the grain size distribution obtained from the decreasing nucleation rate model with *H/J=1.5*. Respectively figure 3 shows comparison of real material grain size distribution for deformation *30%* and the microstructure obtained from the simulation for the same model of nucleation and *H/J=2*.

The discussed dependence confirms correctness of the model as higher deformation introduces higher stored energy to the system and, as a result, higher degree of stored energy *H/J* used in the simulation. It was also observed in both the simulation and the experiment, that a higher degree of deformation as well as a higher degree of stored energy *H/J* results in finer grain microstructure (Fig.4).

4. SUMMARY

The microstructure evolution during the static recrystallization is simulated by the Monte Carlo technique. Different degrees of stored energy and the nucleation models are simulated. In a number of experimental tests the deformation degree varies to obtain different grain size distributions. The microstructures obtained from the simulation and these from the experiment are compared by statistical tests as far as the mean grain size and its variation are regarded. The dependence of the degree of stored energy *H/J* on the recrystallized grain size remains in agreement with theoretical and experimental works of other authors.[11, 12] Conformity of the structures modelled by the decreasing nucleation rate and the ones from the experiment has been stated as far as the mean grain size and its standard deviation are considered.

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