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Comparative Study on Primary Recrystallization of Metallic Materials Using Experimental and Numerical Simulations

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The phenomenon of primary recrystallization in metallic materials is a complex process that involves nucleation and growth of new grains from the deformed microstructure during post-deformation annealing heat treatment. In this study, we compare the experimental and numerical simulation results of primary recrystallization in metallic materials. The experimental tests were carried out on ARMCO iron samples extruded to 10, 20, and 30% of deformation degree and annealed at 973 K for 300 s. Microsections of the deformed and annealed specimens were analyzed using a metallographic microscope and Joyce–Loebl image analyzer. The numerical simulations were performed using a Monte Carlo algorithm to model the primary recrystallization of variable nucleation rate. On the basis of the classification given by Christian, four types of nucleation were simulated: site-saturated nucleation, constant nucleation rate, increasing nucleation rate, and decreasing nucleation rate, with different magnitudes of stored energy. Our results show that the decreasing nucleation rate model best fits the experimental data. The comparison between the experimental and numerical simulation results provides insights into the nucleation and growth of new grains during primary recrystallization in metallic materials.

topics: Monte Carlo, recrystallization, grain growth, numerical model

1. Introduction

The properties of alloys and metals subjected to plastic deformation and annealing depend significantly on the conditions of recrystallization. One of the ways to model grain growth and recrystallization at the microscopic scale is through Monte Carlo simulation [1–4]. This type of modelling process has several advantages. One of them is the ability to introduce multiple different and often competing driving forces at the fundamental level by defining the energy conditions and forces for each individual element. These relationships determine both the interrelations between elements and the external conditions. Another advantage is that simple assumptions can generate complex microstructures, and it is possible to observe the development of these microstructures at each stage. Additionally, the ability to generate structures consistent with any set of assumptions allows simulation of the nature of local energy conditions and dynamics. Theoretical hypotheses can be investigated by comparing microstructures obtained from simulations and those observed in experiments.

2. Modelling of the recrystallization

The Monte Carlo method was used for modelling recrystallization processes. The procedure used for modelling recrystallization has been described in detail in the author's previous works [5, 6]. A general description of the simulation is presented below. Recrystallization with variable nucleation rate was simulated as a function of free energy and the number of nuclei. The modelling procedure is based on a two-dimensional array. Each element in the array is assigned a grain orientation number (S_i) ranging from 1 to 48, representing the orientation of the grain in which the element is embedded, and a fixed value of grain boundary free energy and internal energy for that grain (E_i). Grain boundaries are determined by elements with different orientations. Potential nuclei are randomly placed in the deformed structure. Recrystallized grains have orientations given by numbers ranging from 49 to 64, distinguishing them from deformed grains. Energy values are also calculated for these grains. In each calculation step, a new number ranging from 1 to 64 is randomly assigned to each element in the array,

determining its new possible orientation. New values of grain boundary free energy and internal energy (E_i^*) are calculated for that element. If the change in energy due to reorientation satisfies the condition $E_i^* - E_i \leq 0$, the orientation S_i of that element is transposed to the new orientation. Otherwise, there is no modification of the orientation S_i. The change in orientation of an element located at the grain boundary to the orientation of the nearest neighbouring element indicates grain boundary motion. The orientations of recrystallized grains can change to other recrystallized grains in subsequent calculation steps.

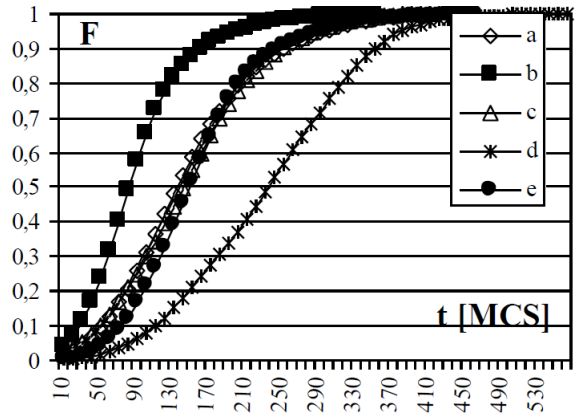

Fig. 1. Recrystallized volume fraction $F(t)$ for the degree of stored energy $H/J = 1$ and different models of nucleation: (a) decreasing nucleation rate I, (b) decreasing nucleation rate II, (c) site-saturated nucleation, (d) increasing nucleation rate, and (e) continuous nucleation rate.

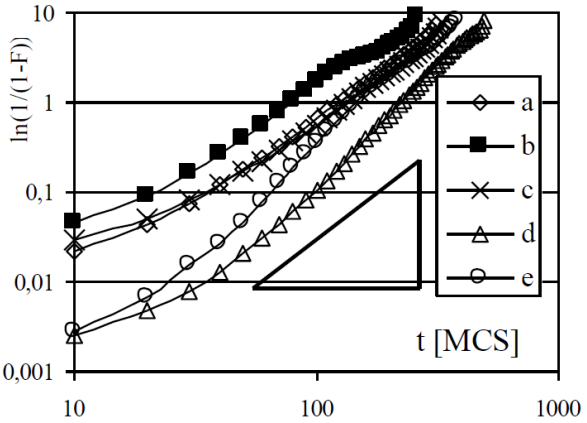

Fig. 2. The Avrami plots for the degree of stored energy $H/J = 1$ and different nucleation models: (a) decreasing nucleation rate I, (b) decreasing nucleation rate II, (c) site-saturated nucleation, (d) increasing nucleation rate, and (e) continuous nucleation rate.

3. Results

3.1. Computer simulation

As an initial structure for modelling recrystallization, the structure obtained from Monte Carlo grain growth simulation was adopted and then "deformed" to a specified degree of deformation. The number of different grain orientations was given as $Q = 48$ for grain growth and $Q + 16$ for recrystallization.

Extensive investigations were conducted for four types of nucleation:

- Variable nucleation with increasing nucleation rate, introducing I new nuclei into the structure every tenth step, until $I = 100$, where $n = 10$ and $i = 1, 11, 21, 31, \ldots, I_{\mathrm{MCS}}$.
- Variable nucleation with decreasing nucleation rate, introducing I new recrystallization nuclei into the structure at every tenth step; in the article, $I = 100$ (decreasing rate I) and $I = 200$ (decreasing rate II) were adopted.
- Continuous nucleation, introducing $I = 10$ nuclei randomly into the structure every ten steps of the Monte Carlo step (MCS).
- Saturation nucleation, introducing $I = 200$ nuclei randomly into the structure at $t = 0$.

For simulation purposes, a dimensionless value of the ratio of stored grain boundary energy to grain interior energy, denoted as H/J, was used to provide a simpler and more understandable description. The above studies were conducted under the same energy conditions, i.e., $H/J = 1$, 1.5, 2, and 2.5.

Figure 1 shows the relationship between the recrystallized volume fraction F and the time t expressed in Monte Carlo steps for four different nucleation rates and a degree of stored energy $H/J = 1$. The observed dependencies exhibit a sigmoidal shape, consistent with experimentally determined curves [7–9]. No incubation period was observed in the simulation since nucleation nuclei were introduced into the system at $t = 0$. It can be observed that the recrystallization kinetics depend significantly on the type of nucleation. The author's studies also indicate a strong dependence on the degree of stored energy H/J (see also [8]).

The most commonly used equation describing recrystallization is the relationship between the recrystallized volume fraction F and time t, known as the Johnson–Mehl–Avrami–Kolmogorov (JMAK) theory, i.e.,

$$F(t) = 1 - \exp(-kt^n), \tag{1}$$

where k and n are constants, and the constant n is referred to as the Avrami exponent. The graphical interpretation of the Avrami exponent is the slope of the Avrami line, which represents the relationship between $\log(-\ln(1-F))$ and $\log(t)$.

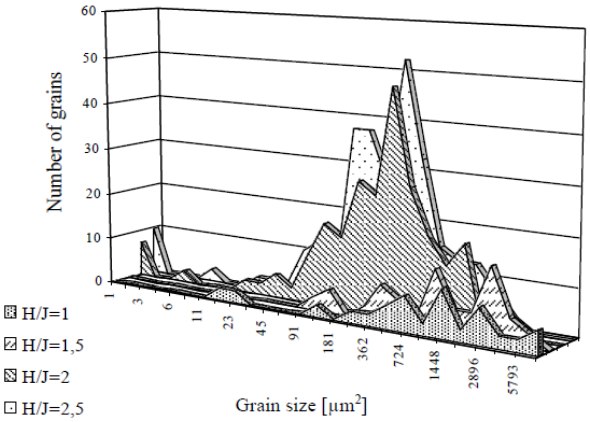

Fig. 3. Histogram of the grain size distribution for the calculated microstructures for saturated nucleation rate and the degree of stored energy $H/J = 1$, 1.5 and 2, and 2,5.

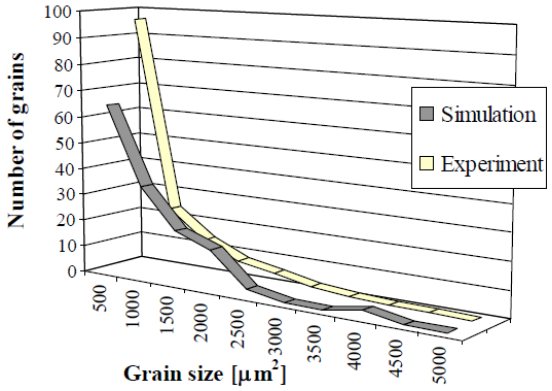

Fig. 4. Histogram of the grain size for the specimen of ARMCO iron deformed 10% and then recrystallized and the microstructure obtained from the simulation for decreasing nucleation rate and $H/J = 1$.

Figure 2 shows the graphical interpretation of the JMAK equation for the four types of nucleation and the degree of stored energy $H/J = 1$. The data plotted on the graph approximately follow parallel lines. The slopes of the Avrami lines are smaller in the initial period, which is attributed to the relatively large number of nuclei introduced into the system at $t = 0$. For all presented Avrami curves, the exponent n is approximately 2, consistent with the predictions of the classical JMAK theory.

Figure 3 presents the logarithmic scale distribution of grain sizes obtained from recrystallization simulations for saturation nucleation and different degrees of stored energy $H/J = 1$, 1.5, 2, and 2.5.

3.2. Experimental results

The experimental verification of the recrystallization model was conducted on ARMCO iron samples that were subjected to plastic deformation. The samples were drawn through a die, resulting in deformations of 10, 20, and 30%. Rectangular-shaped specimens with dimensions of $10 \times 10 \times 55$ mm^3 were prepared and mounted in the jaws of a TCS 1405 thermal cycle simulator manufactured by SMITWELD. The simulator jaws were water-cooled, allowing for controlled temperature conditions within the specimens. The recrystallization experiments were carried out at a constant temperature of $T = 973$ K and a holding time of $t = 300$ s. After cold deformation, the samples were rapidly heated to the desired temperature and held for the specified duration.

Figure 4 shows the comparison between the experimental microstructure and the simulated microstructure for a deformation of 30% and a recrystallization degree of $H/J = 1$. The simulated microstructure exhibits recrystallized grains with distinct boundaries, which align well with the experimental observations.

The comparison between the experimental and simulated microstructures confirms the capability of the recrystallization model to capture the essential features of the recrystallization process. The model successfully predicts the nucleation and growth of recrystallized grains, as well as the evolution of their size and distribution. The discrepancies between the simulated and experimental microstructures can be attributed to simplifications and assumptions made in the model, such as the isotropic nature of grain growth and the neglect of certain microstructural factors.

Further refinements of the model can be made by incorporating additional parameters and considering more complex mechanisms of recrystallization. The comparison between simulation and experimental results provides valuable insights into the recrystallization kinetics and helps to understand the underlying mechanisms governing the process.

4. Conclusions

In this study, a recrystallization model based on the Monte Carlo method was developed and experimentally verified. The model successfully simulates the nucleation and growth of recrystallized grains in deformed materials. By adjusting the energy parameters and the nucleation rate, the model can reproduce different recrystallization scenarios.

The simulated microstructures exhibit recrystallized grains with distinct boundaries, which aligns well with the experimental observations.

In conclusion, the developed recrystallization model based on the Monte Carlo method shows promise in simulating the recrystallization process

in deformed materials. It successfully predicts the nucleation and growth of recrystallized grains and provides valuable insights into the evolution of microstructures.

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