Monte Carlo Simulation of Recrystallization

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A Monte Carlo computer simulation technique, in which a continuum system is modeled employing a discrete lattice, has been applied to the problem of recrystallization. Primary recrystallization is modeled under conditions where the degree of stored energy is varied and nucleation occurs homogeneously (without regard for position in the microstructure). The nucleation rate is chosen as site saturated. Temporal evolution of the simulated microstructures is analyzed to provide the time dependence of the recrystallized volume fraction and grain sizes. The recrystallized volume fraction shows sigmoidal variations with time. The data are approximately fit by the Johnson-Mehl-Avrami equation with the expected exponents, however significant deviations are observed for both small and large recrystallized volume fractions. Under constant rate nucleation conditions, the propensity for irregular grain shapes is decreased and the density of two sided grains increases.

***Index Terms*—Monte Carlo simulation, Recrystallization.**

I. Introduction

In the last decade, several microstructural models have been developed for simulating the temporal evolution of recrystallization microstructures, as well as for predicting the recrystallization kinetics. These models can be grouped as cellular models [1-3], computer Avrami models [4-5], and models based on the Monte Carlo (MC) [6-9], and Cellular Automaton (CA) [10] techniques.

Simulation of recrystallization has advanced significantly in the last time and this activity has prompted a resurgence of interest in the understanding of this phenomenon. Recrystallization is of fundamental importance at all levels of metallurgy, from grain size control in commercial metal alloys to understanding the kinetics of grain boundary motion. A key concept in the microstructural understanding of recrystallization is that nucleation of recrystallization is invariably a heterogeneous process and is therefore dependent on the deformed state of the precursor. Also, the development of misorientation (other than prior grain boundaries) depends on the micromechanics of dislocation slip, the heterogeneities of which have been the subject of some elegant computer simulation. These simulations, however, lead up to recrystallization and there has been a significant effort to address the microstructural evolution that occurs during the process.

In earlier papers [11, 12] this simulation has been applied to the simple process of grain growth. Grain growth refers to the increase in grain size which occurs upon annealing a polycrystalline aggregate after primary recrystallization is complete. The driving force for growth is the reduction in the energy associated with a decrease in grain boundary area. Through computer modelling in which the rate theory concept of boundary migration is simulated, we have shown that all of the characteristic features of normal grain growth (topology, kinetics and size distribution) can be properly reproduced.

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The grain growth problem involves a driving force which is localized in the sense that excess energy is found at the grain boundaries where atoms lack ideal coordination. Microstructural evolution is dominated by the tendency of boundaries to move toward their centre of curvature in response to the interface energy. Another driving force which is equally important in microstructural development is that associated with excess energy which is distributed in grain interiors. Examples of this type of energy include the stored energy from cold work, residual stresses, and surface energy in two-dimensional materials. Microstructural evolution with this type of driving force is dominated by the tendency of boundaries to move in response to differences in the volumetric energy.

In this paper, we concentrate on homogeneous nucleation in which nucleation is treated as constant rate. No specific assumptions have been made as to the particular mechanism of nucleation. We study recrystallization in which both stored energy and grain boundary energy have been included. The purpose of the study is to establish the relationship between growth and microstructure, and hence the operative variables are nucleation rate and amount of stored energy.

II. Simulation Procedure

In thermo-mechanical processing the volumetric energies introduced by working and the concomitant grain boundary motion together dictate the final microstructure. Depending on the details of how the energy is stored (e.g. dislocations, twins, stress) and released, phenomena as diverse as static recrystallization, dynamic recrystallization and super plasticity are observed. As a first attempt to directly correlate microstructural development with volumetric energy induced boundary migration, we have considered the simplest example of this, which is primary recrystallization.

Primary recrystallization is the process in which a deformed material is transformed into a strain free structure. This occurs by the nucleation of strain free regions (nuclei) which grow

and eventually replace the original deformed matrix. One of the most obvious experimental features of primary recrystallization is the sigmoidal time dependence of the recrystallized volume fraction, *F*. This type of dependence can often be described by a single mathematical relationship derived by Johnson , Mehl and Avrami [4, 5]

$$F = 1 - e^{\left(-At^{p}\right)} \quad (1)$$

where *A* and p are constants and t is elapsed time. Experimental data are often fit to equation (1). Theoretical values for *A* and p depend on the assumptions for the nucleation rate per unit volume and volume at time. For the case of site-saturated, homogeneous nucleation, p is 3 in three dimensions and 2 in two dimensions. For constant nucleation rate, p is 4 in three dimensions and 3 in two dimensions.

In order to incorporate the complexity of grain boundary into this work, the microstructure is mapped onto a discrete lattice. Each lattice site is assigned a number between 1 and Q corresponding to the orientation of the grain in which it is embedded. In the present model, a grain boundary segment is defined to lie between two sites of unlike orientation. The grain boundary energy is specified by defining an interaction between nearest neighbor lattice sites. The grain boundary energy is specified by associating a positive energy with grain boundary sites and zero energy for sites in the grain interior, according to

$$E_{i,1} = -J\sum_{nn}(\delta_{S_i S_j} - 1) \quad (2)$$

where S_i is one of the Q orientations on site y ($1 \leq S_i \leq Q$) and δ_{ab} is the Kronecker delta. The sum is taken over all nearest neighbor sites. Thus, nearest neighbor pairs contribute J to the system energy when they are of unlike orientation and zero otherwise.

In order to incorporate the energy stored within the grain an additional term is added to equation (2) such that unrecrystallized regions have a positive energy as described by

$$E_{i,2} = -H\sum_{i}\theta(Q_u - S_i) \quad (3)$$

where $\theta(x)= 1$ for $x \geq 20$ and 0 for $x < 0$. *H* is a positive constant which sets the magnitude of the stored energy and Q_u is the number of distinct orientations of unrecrystallized grains. In the present simulations Q_u is chosen to the 48. The recrystallized nuclei are given orientations with $S_i > Q_u$, such that S_i for a given recrystallized nucleus are shared by no other grains or nuclei. The total site energy is thus defined as $E_i = E_{i,1} + E_{i,2}$.

The kinetics of boundary motion are simulated employing a Monte Carlo technique in which a lattice site is selected at random and its orientation is randomly changed to one of the other grain orientations. The change in energy associated with the change in orientation is evaluated. If the change in energy is less than or equal to zero, the re-orientation is accepted. However, if the change in energy is greater than zero, the re-orientation is accepted with a probability $P = \exp(-\Delta E/kT)$

Time, in these simulations, is related to the number of re-orientation attempts. N re-orientation attempts is arbitrarily used as the unit of time and is referred to as 1 Monte Carlo Step (MCS), where N is the number of lattice sites (40.000). The conversion from MCS to real time has an implicit activation energy factor, exp(-W/RT), which corresponds to the atomic jump frequency. Since the quoted times are normalized by the jump frequency, the only effect of choosing $T \cong 0$ (as done in the present simulations) is to restrict the accepted re-orientation attempts to those which lower the energy of the system. Reorientation of a site at a grain boundary corresponds to boundary migration. The boundary velocity determined in this manner yields kinetics that are formally equivalent to the rate theory model. The efficiency of the Monte Carlo algorithm has been greatly enhanced by employing the continuous time simulation method.

We have used one type of nucleation: constant nucleation rate. In this case, a fixed number of nuclei are randomly placed on the lattice after each Monte Carlo step. If a new nucleus is placed in a grain which already has been recrystallized, that nucleus is removed. In this way, the total nucleation rate (i.e. number of nuclei successfully added per MCS divided by the *total* number of sites) is reduced. During the evolution of the microstructure an unrecrystallized site can change orientations to either another unrecrystallized orientation (grain growth) or to a recrystallized orientation (recrystallization). Spontaneous nucleation is suppressed by only allowing the reorientation of unrecrystallized sites to recrystallized orientations when the unrecrystallized site is adjacent to a recrystallized neighbouring site. Recrystallized orientations are allowed to reorient to other recrystallized orientations. This allows for the possibility of grain growth competition between recrystallized grains. For very small values of *H/J* recrystallized grains can also reorient to unrecrystallized orientations.

In classical homogeneous nucleation theory the minimum radius of a spherical nucleus which will grow is $2\gamma/\Delta G$, where γ is the surface energy per unit area and ΔG is the difference between the energy stored in the nucleus and that stored in the surrounding matrix (normalized per unit volume). In the present simulations, the minimum nucleus radius which will grow but cannot shrink, without regard to location in the microstructure is proportional to *J/H,* where the proportionality constant depends on nucleus shape. While the critical nucleus size in a continuum system is a continuous function of *J/H,* on a discrete lattice at $T = 0$ the critical size changes discontinuously. On the triangular lattice the critical nucleus size is one site for $H/J > 4$, three sites for $4 > H/J > 2$ and essentially infinite for $2 > H/J > 0$. For $H/J < 2$, the nucleation can only be heterogeneous. For metallic systems undergoing recrystallization, the ratio *H/J* is in the range 0.01-0.1. However, larger values than these are required in the discrete lattice model to vary between heterogeneous to homogeneous nucleation and growth behaviour. The present simulation were all performed at T = 0 in order to minimize the demand for computer resources so that a large number of simulations could be run and because the available temperature range is limited (for Q = 48 the system disorders at $kT/J = 0.74$).

III. Results

Figs. 1–3 present microstructures simulated with the increasing nucleation and H/J = 1, 2 and 3, respectively. These figures indicate strong influence of H/J value on the recrystallized grain size and its distribution. The degree of stored energy H/J is strictly connected with the cold plastic deformation before the recrystallization. Higher value of H/J corresponds to bigger deformation.

FIG. 1 HERE

FIG. 2 HERE

FIG. 3 HERE

The initial lattice for the recrystallization simulation was created by the Monte Carlo grain growth simulation and then deformed. Frequency of the nucleation occurring at the grain corners, grains boundaries and grain interior was investigated and we have observed that in the simulation nucleation at the grain interior is zero or very low at H/J = 1. The nucleus will grow only on the grain boundary or in the junction of three boundaries. It is considered to be heterogeneous nucleation. For H/J = 2 and 3 the critical nuclei can grow when placed anywhere in the lattice. Nucleation on the grain interior becomes dominant. This can be referred to as homogeneous nucleation. The basic nucleation were simulated by increasing nucleation rate $N_r = n(i-1)/10$ new nuclei were placed on the lattice every 10 MCS until N_r = 100, n = 10, i = 1, 11, 21, . . ., 101 MCS.

As can be seen, after recrystallization is complete, the microstructure exhibits a relatively uniform grain size. The final mean grain area is found to be inversely proportional to the initial nuclei concentration.

FIG. 4 HERE

The recrystallized volume fraction F is plotted vs time in Fig. 4 for *H/J=1. F* is found to be a sigmoidal function of time, in agreement with experimental observations. The simulations show no incubation period for recrystallization. This is consistent with site saturated nucleation at time zero. However, in the case that the experimentally detectable recrystallized grain size is finite, an apparent incubation period will exist. All the recrystallized volume fraction curves (Fig. 5) can be superimposed upon one another through appropriate scaling. The scaling function may be derived from equation (1). The Avrami exponent p is given by

$$p = \frac{\partial \log\left[\log\left(\frac{1}{1-F}\right)\right]}{\partial \log t} \tag{4}$$

where *F vs. t* is measured from the simulation. Such a determination is made in Fig. 5. It is observed that curvature is present, particularly at very short and very long times. While deviation from linearity in the long time behaviour may be attributed to insufficient statistics, the deviation at short times is apparently real. It is possible that the deviation at early times is due to deviation from the linear relationship between recrystallized grain radius and time at small grain sizes. However, since the Johnson, Mehl and Avrami analysis is approximate, it is also possible that some of these deviations are a consequence of limitations of the model. Theoretically, the curves in Fig. 5 are expected to show slopes to two.

FIG. 5 HERE

The recrystallized grain morphology which is observed has some features in common with those found for site saturated nucleation. Many grains have an elongated shape, which is a consequence of constraints of random nucleation and growth. However, the propensity toward irregular grain shapes appears to be somewhat decreased, with an overall trend towards more compact forms. The microstructures of the site saturated nucleation simulations also show topological differences compared with the constant nucleation rate simulations. In site saturated nucleation, where all recrystallized grains are nucleated at the same time, these conditions are never met and consequently no appreciate different in sided grains are observed.

Prior to complete recrystallization, the microstructure developed under constant nucleation rate condition appears to be more homogeneous than for site saturated nucleation. This more uniform distribution need be attributed to continued nucleation of recrystallized grains in the unrecrystallized materials. Consequently pockets of unrecrystallized material are noticeably absent. Since new grains are constantly formed in the unrecrystallized material, the distribution of final grain sizes is much broader than under site saturated conditions.

IV. Conclusion

Static recrystallization kinetics is simulated by the Monte Carlo technique. In the simulation the degree of stored energy H/J and the nucleation models are varied. The performed Monte Carlo simulations of the primary static recrystallization confirm correctness of the models concerning the curves of the recrystallized volume fraction F. The sigmoidal time dependence of recrystallized volume fraction observed in the simulation is often emphasized in the literature and the Avrami exponent p = 2 is properly reproduced by the simulations.

The dependence of the recrystallized grain size on the degree of stored energy H/J also remains in agreement with theoretical works of other authors.

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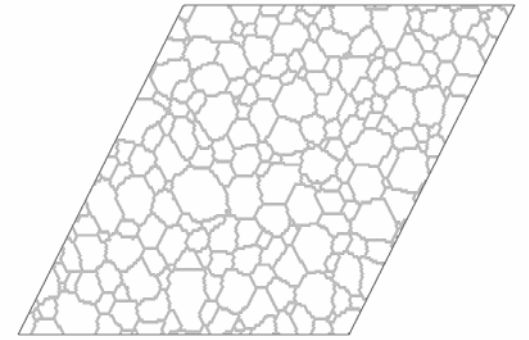

Fig. 1. Microstructure simulated under decreasing nucleation rate and degree of stored energy H/J=1.

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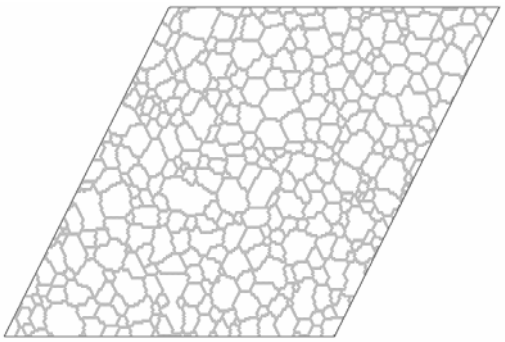

Fig. 2. Microstructure simulated under decreasing nucleation rate and degree of stored energy H/J=2.

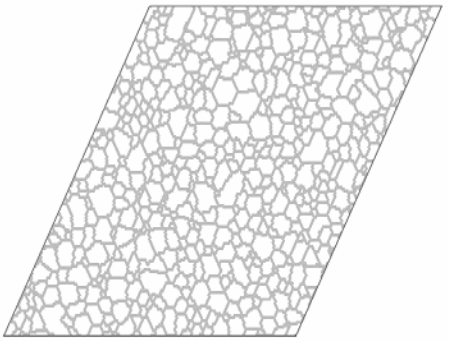

Fig. 3. Microstructure simulated under decreasing nucleation rate and degree of stored energy H/J=3.

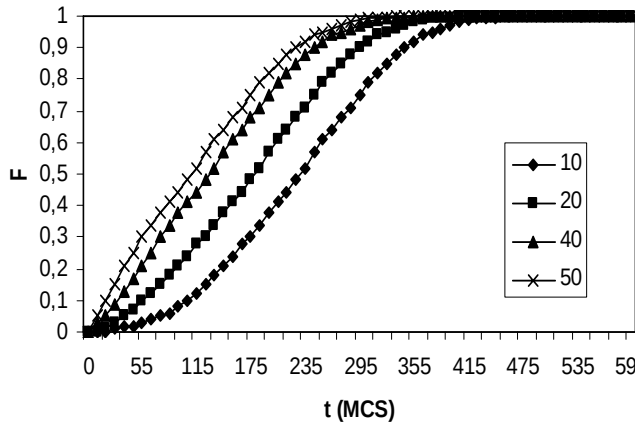

Fig. 4. The recrystallized area fraction, F, vs time for site saturate nucleation conditions with $H/J = 1$. *Curves* correspond to 10, 20, 40 and 5 nuclei.

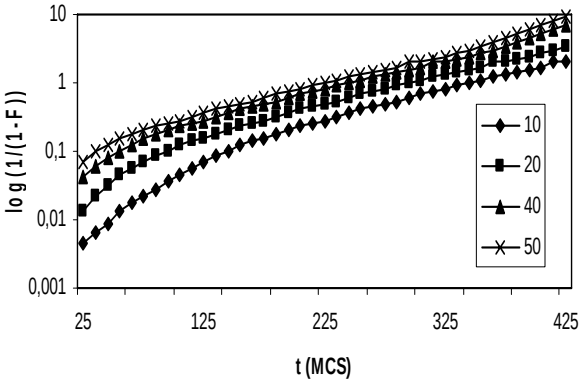

Fig. 5. The Avrami plots for the degree of stored energy $H/J = 1$ and for 10, 20, 40 and 50 nuclei.