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Title: Mesoscopic Simulations of Recrystallization

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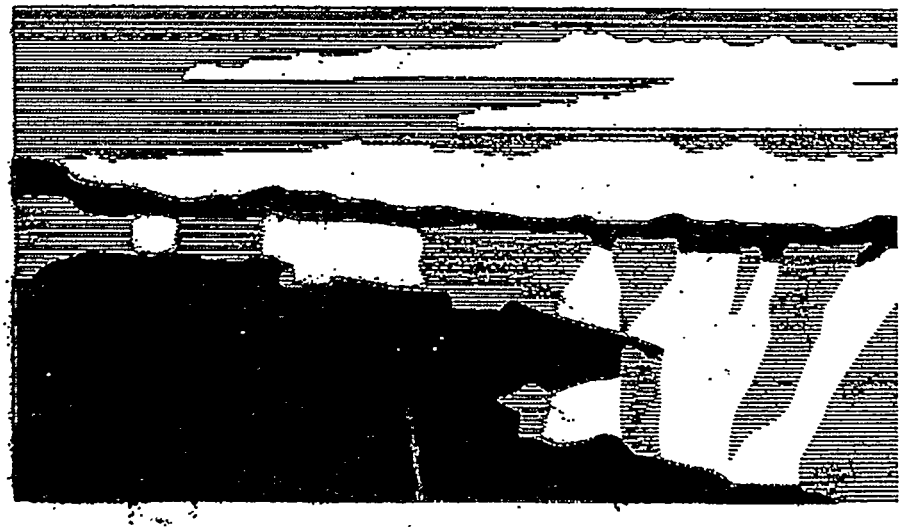

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MESOSCOPIC SIMULATIONS OF RECRYSTALLIZATION

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1. Abstract

The application of computer simulation to grain growth and recrystallization was strongly stimulated in the early 80s by the the realization that Monte Carlo models could be applied to problems of grain structure evolution. By extension of the Ising model for domain modeling of magnetic domains to the Potts model (with generalized spin numbers) it was then possible to represent discretely grains (domains) by regions of similarly oriented sets of material (lattice) points. In parallel with this fascinating development, there also occured notable work on analytical models, especially by Abbruzzese and Bunge, which has been particularly useful for understanding the variation of texture (crystallographic preferred orientation) during grain growth processes. Geometric models of recrystallization, worked on most recently and productively by Nes et al., have been useful in connection with grain size prediction as a result of recrystallization. Also, mesh-based models have been developed to a high degree by Kawasaki, Fradkov and others, and, rather recently, by Humphreys to model not just grain growth but also the nucleation process in recrystallization. These models have the strength that they deal with the essential features of grains, i.e. the nodes, but have some limitations when second phases must be considered. These various approaches to modeling of recrystallization processes will be reviewed, with a special emphasis on practical approaches to implementing the Potts model. This model has been remarkably successful in modeling such diverse phenomena as dynamic recrystallization, secondary recrystallization (abnormal grain growth), particle-inhibited recrystallization, and grain structure evolution in soldering and welding. In summary, the application of mesoscopic simulation to the phenomenon of recrystallization has yielded much new insight into some longstanding deficiencies in our understanding. There is an obvious need, however, to continue the effort and incorporate more of the known microstructural complexity into the simulations.

2. Introduction

The aim of this article is provide both a summary of the available techniques for the computer simulation of recrystallization, and an overview of what has been accomplished in this area. The description of the simulation techniques will focus primarily on the Monte Carlo method because most of the literature has used that method and because it currently appears to be the most versatile method. The application of computer simulation to recrystallization has yielded much new insight into some long-standing deficiencies in our understanding of the process. If this article encourages even a few researchers to employ computer simulation, the authors will consider this and the associated workshop to have been a success.

3. Background

The simulation of recrystallization has advanced significantly in the last decade 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 precursor deformed state. For example, the long-lived and lively debate over Oriented Nucleation versus Oriented Growth as to the origin of the cube texture component during recrystallization in fcc metals has been significantly affected by computer simulation of texture development during deformation. 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. One issue, for example, has been that of grain size morphologies and distributions. Mahin et al.[1, 2] and later Saetre et al.[3] examined the effect on microstructure of different nucleation and growth kinetics. The kinetics of recrystallization have remained a challenge and Rollett et al.[4], later Marthinsen et al.[5], have examined how heterogeneities in nucleation and growth can affect the apparent exponent (n in the equation above) when the standard analysis is applied. The effect of variable grain boundary mobilities has been examined for grain growth by Novikov[6], Holm[7], Abbruzzese[8], Rollett[9] and others and many of the conclusions would appear to apply equally well to recrystallization. The initial growth of a recrystallization nucleus, for example, may well correspond to the abnormal grain growth of a subgrain.

4. Simulation Methods

The application of computer simulation to grain growth and recrystallization was strongly stimulated in the early 1980s by the realization that Monte Carlo models could be applied to problems of grain structure evolution. By extension of the Ising model for domain modeling of magnetic domains to the Potts model (with generalized spin numbers) it was then possible to represent discretely grains (domains) by regions of

similarly oriented sets of material (lattice) points. In parallel with this fascinating development, there also occurred notable work on analytical models, especially by Abbruzzese[8], which has been particularly useful for understanding the variation of texture (crystallographic preferred orientation) during grain growth processes. Geometric models of recrystallization, worked on most recently and productively by Furu[10], have been useful in connection with grain size prediction as a result of recrystallization. Also, mesh-based models have been developed to a high degree by Fradkov[11, 12] and others, and, rather recently, by Humphreys[13] to model not just grain growth but also the nucleation process in recrystallization. These models have the strength that they deal with the essential features of grains, i.e. the nodes, but have some limitations when second phases must be considered.

We review three methods of mesoscopic simulation for recrystallization. The first, geometrical, method addresses the final microstructural state and cannot be used to investigate microstructural evolution. The second method, cellular automata, discretizes the microstructure and has also been successfully applied to recrystallization. Physically based rules are used to determine the propagation of a transformation (e.g. recrystallization, solidification) from one cell to its neighbor. It has not, however, been used for as wide a range of metallurgical phenomena as has the Monte Carlo method. This latter relies on the Potts model to both discretize the structure and simulate boundary motion via an energy minimization procedure.

4.1. GEOMETRICAL

For investigations in which the details of how boundaries move and interact are unimportant, it is sufficient to construct geometrical models. Rules are chosen for the selection of nucleation sites (in a continuum space); this allows for the clustering of sites if so desired. Then a rule is chosen for the intersection of the grains (e.g. perpendicular bisectors between pairs of points), and the space is tesselated. The result, for the case where the growth rates of the grains are isotropic and constant, is the Voronoi polygon structure. The simplest nucleation conditions are those of site saturation. If the growth of each individual grain is tracked, however, considerable variations in microstructure can be obtained by varying the nucleation conditions[14]. Simple rules can be used to exclude previously recrystallized material from nucleation during continuous nucleation thereby achieving the decrease in effective nucleation rate that is observed. The microstructures obtained from such purely geometrical models suffer from the disadvantage of not allowing for grain growth during the recrystallization process. Grain shapes are non-compact in many cases, in contrast to typical experimentally observed structures. Grain size distributions from the models exhibit long tails towards small grain sizes.

4.2. CELLULAR AUTOMATA

The general modeling technique of cellular automata has been applied to recrystallization by Hesselbarth and others [15]. Automata exploit the quasi-deterministic characteristic of recrystallization in that the motion of a recrystallization front is irreversible. Therefore if one only seeks to describe the motion of the recrystallization fronts then the cellular automaton is very efficient. This method shares the characteristic with the Monte Carlo method to be described below that it discretizes the space by mapping

microstructure onto a lattice of cells. Nucleation is modeled by forcing individual cells to the recrystallized state. As in most simulations of recrystallization, nucleation is applied in a spatially random manner. This approach has also proved to be useful in simulating solidification in which undercooling of a melt provides the driving pressure for transformation.

One drawback of the method is that the growth morphology of the new grains is prescribed by the choice of the neighborhood of each cell. Hesselbarth et al. [15] model heterogeneous recrystallization by introducing a long range interaction between grains into the model. The result of this is grain shapes of (umimpeded) growing grains that are far from compact, and not physical in appearence.

The effect of heterogeneous stored energy has also been investigated with the cellular automaton approach[16]. For this case, the propagation rates for the recrystallization fronts were variable from one location to another. As with earlier Monte Carlo simulations[4], the results indicated marked deviations from the kinetics of homogeneous transformations, as indicated by a linear Kolmogorov-Johnson-Mehl-Avrami plot (see *kinetics* section below).

4.3. MONTE CARLO METHOD

The Monte Carlo also uses a discretized representation of microstructure; however, cell interactions are energetically controlled. A continuum microstructure is mapped onto a two-dimensional (2D) or three dimensional lattice (3D) lattice. Each lattice site is assigned a number, S_i, which corresponds to the orientation of the grain in which it is embedded. Lattice sites which are adjacent to sites having different grain orientations are regarded as being separated by a grain boundary, whilst a site surrounded by sites with the same orientation is in the grain interior. Each site contributes a bulk energy $H(S_i)$ to the system; in recrystallization modeling, $H(S_i)$ is the energy stored during deformation in the form of dislocations at site i. In addition, each unlike pair of nearest neighbors contributes a unit of grain boundary free energy J to the system. Summing bulk and surface energy contributions, the total energy of the system is calculated via the Hamiltonian

$$E = \frac{J}{2}\sum_{i}^{N}\left[H(S_i) + \sum_{j}^{z}(1-\delta_{S_i S_j}) \right] \tag{1}$$

where the sum on i is over all N sites in the system, the sum on j is over the z nearest neighbor sites of site i, and δ_{ij} is the Kronecker delta.

The evolution of the structure is modeled by picking a site and a new orientation at random from the set of allowable values. The change in total system energy ΔE for reorienting the site is computed, and the reorientation is implemented with transition probability, p, such that

$$A = \sum_{i=1}^{N} \Pi_i \tag{2}$$

where k is the Boltzman constant and T is the simulation temperature. It is important to note the difference between the meaning of temperature in the context of the Monte Carlo model and the physical parameter relevant to recrystallization. In the simulation, temperature governs the degree of disorder in the lattice, and above some critical temperature, dependent on the lattice type, the system disorders. Only second order effects are observed for variations in simulation temperature [17] on the kinetics of grain growth. Because of this lack of effect, all simulations of recrystallization known to the authors have been performed at zero temperature. The consequence of this is simplify the transition probabilities as follows.

$$p(\Delta E) = \begin{cases} 1 & \text{if } \Delta E \le 0 \\ 0 & \text{if } \Delta E > 0 \end{cases} \tag{3}$$

N reorientation attempts is defined as one Monte Carlo Step (MCS). The number of Monte Carlo Steps is proportional to time.

Particles are introduced into the simulation as sites which have an orientation different from any of the grains and which can not be reoriented during the course of the simulation. This assumption results in an equality of the particle-matrix interfacial energy and the grain boundary energy, which is reasonable for particles that are incoherent with respect to the matrix. Also, the particles cannot move through the lattice which means that grain boundary drag of particles is not permitted[18].

In static recrystallization simulations, the stored energy per site is assumed to be positive for initially unrecrystallized material and zero for recrystallized material. When dynamic recrystallization is simulated, however, the stored energy at each point is a function of both time and position.

4.4. CONTINUOUS TIME METHOD *or* N-FOLD WAY

The Monte Carlo method would be very inefficient if it were applied in its basic form to large data sets because of the sparseness of the problem to be worked. Once much coarsening has occurred in grain growth, or recrystallization is nearly complete, most sites in the lattice are surrounded by sites of the same orientation, i.e. they are in the bulk of a grain. Therefore the probability of their changing orientation is nil and expending computational effort there is wasted. The crucial contribution of Bortz et al.[19] was to propose a method (for the Ising model) for eliminating the need to compute unsuccessful changes in orientation. The key feature of the algorithm is that the time step after each orientation change is calculated as

$$\Delta t = -\frac{(Q-1)\tau}{A} \ln \Gamma \tag{4}$$

where Γ is a random number over the range [0,1], τ is 1 MCS, and A is the system activity. The system activity is defined as the sum of the transition probabilities for all possible reorientations at each site,

$$A = \sum_{i=1}^{N} \Pi_i \tag{5}$$

where Π_i is the activity of site i, defined as

$$\Pi_i = \sum_{j=1}^{Q} \pi_{ij} \tag{6}$$

where π_{ij} is the probability of reorienting site i to orientation $S_j \in [1,Q]$. The derivation of Eq. 4 is obtained by considering the probability in the conventional Monte Carlo scheme [19] of whether or not a successful reorientation has occurred in a certain time interval. This leads to a differential equation which is integrated to give Eq. 4. Sahni et al. [20] and Holm [21] extended the continuous time method to the Monte Carlo Potts model with Q different grain orientations in the system. Eq. 4 then becomes:

$$\Delta t = -\frac{(Q-1)\tau}{A} \ln \Gamma \tag{7}$$

To perform a simulation using the continuous time method, each site is visited in proportion to its activity Π_i; at zero temperature, bulk sites have $\Pi_i = 0$ so are never selected. One of the allowed reorientations is chosen with probability proportional to π_{ij} and is performed. Time is then incremented according to Eq. (7). Since the system activity A decreases as the number of energetically favorable reorientations decreases (i.e. as the system coarsens), the time increment increases as the simulation progresses.

The great advantage of the continuous time method is that it greatly speeds up the computation of microstructural evolution in sparse systems. For 2D grain growth, for example, Holm found that the conventional Monte Carlo method was more efficient only when the mean grain radius was less than 3 and efficiency increased monotonically as the simulation progressed [21]. Even at high fractions of the critical temperature, the continuous time method was more efficient for long simulation times.

The fact that recrystallization introduces new grains means that is not practicable to work with a fixed list of orientation values as can be done in grain growth, wherein the maximum numbers of grains occurs at time zero. Therefore it is convenient to introduce each new grain with a unique orientation value. The computational efficiency of the continuous time method is unaffected by this characteristic of recrystallization simulations.

4.5. LATTICES

Implicit so far in the discussion has been the connectivity of the points that represent the discretized microstructure. It turns out that the lattice can have a strong effect on the results of the simulation. A survey of lattice types for both two and three dimensions is available in the thesis by Holm[21]. The grain boundary energy per unit length is anisotropic with respect to the boundary orientation in the lattice. This anisotropy can be characterized by a Wulff shape which is directly related to the coordination number and symmetry of the lattice. Tables 1 and 2 list the lattice types with their geometries and the anisotropy of the Wulff plot. The number in parentheses after the lattice type

denotes the number of shells of neighbors, such that square(1,2) means a square lattice with first and second nearest neighbors. The lattice type cubic (2*) denotes a simple cubic lattice with first, second, third nearest neighbors and neighboring points located at [222].

TABLE 1. Listing of 2D lattice types with geometries and anisotropies.

Lattice Type	Wulff Shape	Coordination Number	Anisotropy	Grain Growth
Square (1)	square	4	1.414	inhibited
Triangular	hexagon	6	1.154	normal
Square (1,2)	octagon	8	1.116	normal
Triangular (1,2)	dodecagon	18	1.057	normal

TABLE 2. Listing of 3D lattice types with geometries.

Lattice Type	Wulff Shape	Coordination Number	Grain Growth
Cubic (1)	cube	6	inhibited
Cubic (1,2)	18-hedron	18	inhibited
Cubic (1,2,3)	26-hedron	26	normal
Cubic (2*)	98-hedron	124	normal
fcc (1)	rhomboid dodecahedron	12	inhibited
fcc (1,2)	18-hedron	18	inhibited
hcp (1)	trapezoidal dodecahedron	12	inhibited

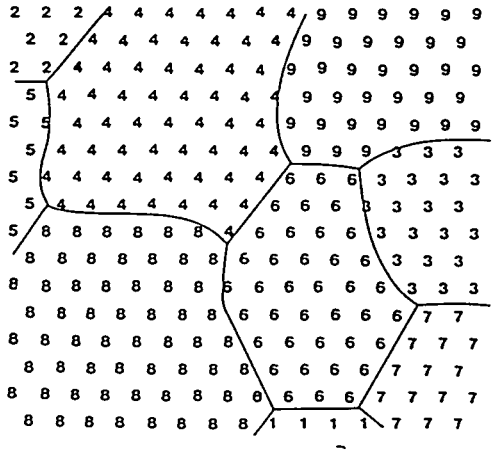

Figure 1. Diagram of the triangular 2D lattice, showing orientation numbers at each site, and boundaries drawn between sites with dissimilar orientations.

The characteristic of many lattices that has been ignored by several authors is the tendency towards self-pinning (for grain growth) in simulations performed at zero temperature. The last column in each table shows which lattices can sustain grain growth without self pinning and are therefore suitable for studies of microstructural evolution. For example, in three dimensions, both of the close packed lattices, face centered cubic and hexagonal, can not sustain coarsening to long times. The reason for this is a combination of high lattice anisotropy tending to favor grain facets that lie on

high symmetry planes, and a tendency for kinks or steps in boundaries to anneal out with time. If the microstructural features that allow boundaries to move are lost, then it is not surprising that self pinning occurs. Finite temperature can be used, however, to maintain a population of kinks and steps thereby allowing grain growth to proceed.

If the grain boundary energy J is uniform for all boundary segments in a recrystallization simulation, these authors have concluded that the triangular lattice is suitable for the simulation of recrystallization in two dimensions, and that the cubic(1,2,3) lattice is suitable in three dimensions. For other types of simulations, careful examination for lattice effects must be made even for these lattices. Figure 1 shows a 2D triangular lattice with boundaries drawn between regions of uniform orientation.

4.6. NUCLEATION

Nucleation of recrystallized grains is modeled by adding small embryos to the material at random positions at the beginning of the simulation (i.e. site saturated nucleation). The stored energy is set to zero at each site belonging to the embryo. Continuous nucleation is simulated by adding embryos at regular intervals during the simulation. In both cases the effective nucleation rate decreases with time because, at long times, most the available space has been recrystallized and has zero stored energy; embryos placed in recrystallized material will shrink and vanish. Dynamic recrystallization is modeled by adding stored energy to each lattice point continuously. This means that it is not possible to distinguish between recrystallized and unrecrystallized material after the first cycle of recrystallization is complete. The process of work hardening starts anew with each new grain which means that the stored energy at any given point is related to the length of time that has elapsed since the nucleation event associated with that grain.

Embryos have orientations that differ from those of all other grains and particles as discussed above. If the bulk stored energy H is too small, the embryos are sub-critical and shrink away. The value of H required for embryo growth depends on its surroundings. Above some critical H/J, an isolated embryo is super-critical and can grow as a new grain nucleus. Below that H/J, the embryo must be adjacent to an existing grain boundary in order to become a nucleus; its growth then occurs preferentially along the prior grain boundaries. In the 2D triangular lattice, homogeneous nucleation cannot occur for $H/J < 2$. Embryos of two lattice sites can grow when $2 \leq H/J < 4$. Single-site embryos can grow when $H/J \geq 4$.

4.7. INITIALIZATION OF RECRYSTALLIZATION SIMULATIONS

Monte Carlo recrystallization simulations are typically initialized by performing grain growth simulations [22, 23] for a period of 10^3 MCS after which the microstructure contains approximately 1000 grains with a mean grain area of approximately 40 sites. At this point, single site "particles" are randomly placed within the microstructure to obtain a certain area fraction. The stored energy is initialized to the desired value for each site.

4.8. RELATIONSHIP OF PHYSICAL GRAIN SIZE TO SIMULATION GRAIN SIZE

Most computer simulations require significant amounts of computer time so it common practice to minimize the size of the lattice that is used. Therefore it is useful to analyze the relationship between grain size in the Monte Carlo recrystallization model, and physical grain sizes [24].

Assume that the ratio of stored energy to grain boundary energy per unit volume can be equated in the model and in real materials.

The physical process has the following characteristic driving pressures P. From the stored dislocation content, P^{store} = 10 MPa, typically. For grain growth driven by grain boundary curvature, $P^{grgr} = \gamma/\langle r \rangle$, where γ is the grain boundary energy per unit area, and $\langle r \rangle$ is the mean grain radius.

In the 2D triangular lattice, the stored energy per unit area is given by $P^{store} = H/[3\ s^2 \sin(60°)]$ where s is the unit boundary length on the lattice. The stored energy due to boundary curvature is

$$P^{grgr} = \frac{\gamma^{model}}{< r >^{model}} = \frac{J}{s < r >^{model}} \tag{8}$$

The initial grain size in the Monte Carlo simulations is typically about 6s. Thus, for the model

$$\frac{P^{store}}{P^{grgr}} = \frac{H < r >^{model}}{3sJ \sin 60°} = 2.5\frac{H}{J} \tag{9}$$

Using a typical value for the grain boundary energy, $\gamma = 0.5\ J.m^{-2}$, for physical systems

$$\frac{P^{store}}{P^{grgr}} = 20 < r > \mu m^{-1} \tag{10}$$

Equating the energy densities for the model and physical systems and rearranging gives

$$\langle r \rangle = 0.125\ H/J\ \mu m \tag{11}$$

Then for a typical simulation with H/J = 2, we can estimate $\langle r \rangle = 0.25\ \mu m$, which is a small but not unphysical grain size. Clearly, however, it would be preferable to simulate recrystallization with lattices with linear dimensions an order of magnitude larger than is currently typical.

4.9. KINETICS

The kinetics of recrystallization can be measured by the fraction of the structure that has been transformed. A more useful analysis for comparison with theory is given by converting the data to a Kolmogorov-Johnson-Mehl-Avrami (KJMA) plot. The standard analysis for the kinetics of phase transformations has been given in many other places and will not be derived here. The central concept for accounting for impingement

between neighboring grains is that of extended volume for transforming grains to grow into; a differential relation is then deduced between the increment of transformed volume that would have been obtained in the absence of impingement and the actual volume increment. For the simplest case of spatially random nucleation, the relationship is simply

$$dV_{actual} = (1\text{-}V)\, dV_{extended} \tag{12}$$

where V is the volume fraction transformed or recrystallized. The extended volume increment is given an appropriate definition of the temporal and spatial dependence of the growth of new grains. Integration then leads to a the form

$$V = 1 - \exp(-B\, t^n) \tag{13}$$

where the constants B and n contain information about nucleation rate and growth. For the purposes of plotting kinetic data, it is convenient to use the logarithmic form of the equation:

$$\ln\left\{\ln\frac{1}{1-V}\right\} = n.\ln\{t\} + B \tag{14}$$

Many authors plot their data in this form with the aim of extracting activation energies where temperature was a variable, and microstructural information from the slope (the exponent n). For example, for site saturated nulceation conditions and two dimensional growth, n=2: for continuous nucleation and three dimensional growth, n=4. As Vandermeer[25] has pointed out, however, nucleation conditions may both the form of $dV_{extended}$ and the differential relationship.

A characteristic of the Monte Carlo model of recrystallization is that a finite recrystallized volume is introduced at the beginning of simulations when site saturated nucleation conditions apply. This becomes apparent in a KJMA plot as a curvature at early times. A simple correction may be made for the finite initial fraction transformed by adding a constant to the measure of time. The correction is of course heuristic because it depends on the results themselves.

The growth rate of recrystallized grains in the Monte Carlo model is also not linearly related to the stored energy density. As with nucleation, each integer increment of H/J leads to a discrete change in which sites can change orientation with a neutral or negative change in system energy.

5. Results of Simulation of Recrystallization

The section provides a review a number of areas in which useful results have been obtained from recrystallization simulation.

5.1. ABNORMAL GRAIN GROWTH

The early stages of recrystallization are labeled as nucleation even though no new phase appears in the material. At the level of the dislocation structure, however, the existing

heterogeneities of the deformed structure coarsen in the process known as polygonization. The heterogeneities exist at several length scales from cells to shear bands to prior grain boundaries. Many observations have been made which suggest that individual subgrains acquire a growth rate advantage over their neighbors and become identifiable as new grains. This growth advantage can result from a difference in mobility between the boundary of the new grain and the boundaries in the surrounding material. This process of competitive growth has been observed in the Monte Carlo model in both 2D [9] and 3D [26] simulations. By altering the rate at which sites are sampled for reorientation, the mobility of specific grain boundaries can be varied. Small ratios in mobility between one grain and another lead to marked abnormal grain growth behavior, which may correspond to the early growth of new grains in recrystallization.

5.2. STATIC RECRYSTALLIZATION

A key observation in grain growth is that an isolated grain will shrink and eventually vanish in response to tendency to minimize grain boundary area. When an isolated grain can eliminate stored energy by growing, however, it does so, provided that the grain is not smaller than a critical size. In a polycrystalline structure with $0<H/J<1$, any recrystallized grain will grow at the expense of its neighbors because of the bias imposed on the unit step of the grain growth process. That is to say, the motion of kinks along a boundary is reversible when the change in energy associated with a step is zero, as is often the case for the 2D triangular lattice; however, such energy neutral steps become irreversible when biased by the elimination of stored energy at each step. Clearly, the Monte Carlo simulation of the motion of recrystallization fronts is much closer to a deterministic model than for grain growth.

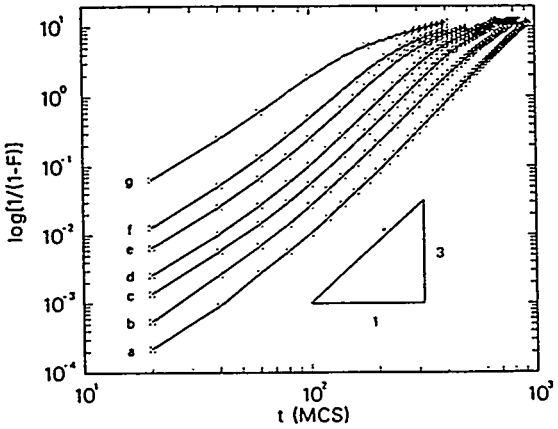

Figure 2. KJMA plot of the kinetics of recrystallization under homogeneous nucleation conditions. Continuous nucleation at various rates was applied with H/J=5. Curves a-g correspond to 0.2, 0.5, 1, 2, 10 and 50 nuclei/MCS, respectively.

The kinetics of recrystallization have been found to reproduce those anticipated from theoretical analysis very closely. For example, in 2D simulations [27] site

saturated nucleation conditions with a high enough stored energy density (H/J>2), a KJMA plot of the fraction recrystallized versus time show a slope of 2 at long times; continuous nucleation gives a slope of 3, as shown in Fig. 2 above. Both results are as predicted from classical KJMA analysis. For low stored energy densities (H/J<2), nucleation is heterogeneous in the sense that embryos must be adjacent to existing boundaries in order to survive and grow, as shown in Fig. 3 below. In this case the kinetics show significant deviations from the classical KJMA pattern[28]. The key observation here is that the growth of new grains at low stored energies is highly dependent on the prior structure. For H/J≤1, the recrystallization front grows out from a triple point and is concave with respect to the unrecrystallized side. The net effect is that growth is very slow in early stages of recrystallization.

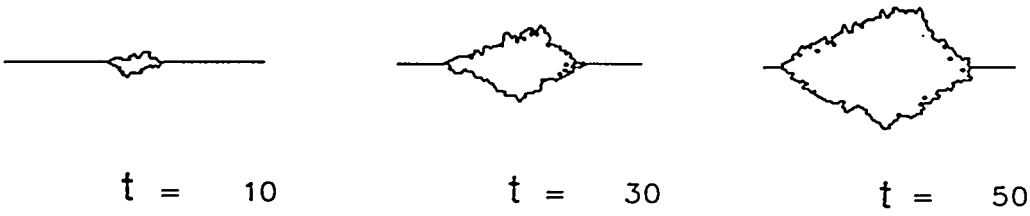

Figure 3. Illustration of the growth mode of new grains at 1<H/J≤2. Note that the most rapid growth direction is parallel to the prior boundary.

5.3. RECRYSTALLIZATION IN THE PRESENCE OF PARTICLES

Recrystallization with inert particles present is easily modeled by assigning sites orientation values that cannot be changed, as described above. Although only the effect of single site particles have been studied [24] to date (whereas particle shape and size has been examined for grain growth), the results appear to be general, at least for small particles. Large particles in physical systems have the effect of stimulating nucleation, an effect that has not been addressed by microstructural simulations.

During recrystallization simulation with sufficient stored energy ($H/J \geq 3$ in the triangular lattice) the recrystallization front can readily bypass particles regardless of particle size or area fraction. Under these circumstances the recrystallization growth kinetics are unaffected by particles. The overall kinetics are accelerated slightly, however, by heterogeneous nucleation on particles.

At intermediate stored energies ($1 \leq H/J \leq 3$) nearly all recrystallization boundaries can move past single-site particles. Boundaries with a very high particle density will stop moving. However, the irreversible propagation of grain boundary kinks allows most boundaries to achieve a configuration from which two kinks can join to move past single-site particles. The presence of prior grain boundaries further enhances recrystallized boundary motion. In these systems, boundaries intersect particles at random, and recrystallization kinetics are substantially unaffected by particles, as shown in Fig. 4, where a single recrystallized grain shows unrestricted

growth for H/J = 1. Larger particles may inhibit recrystallization in this stored energy regmine, however, since two boundary kinks cannot join directly.

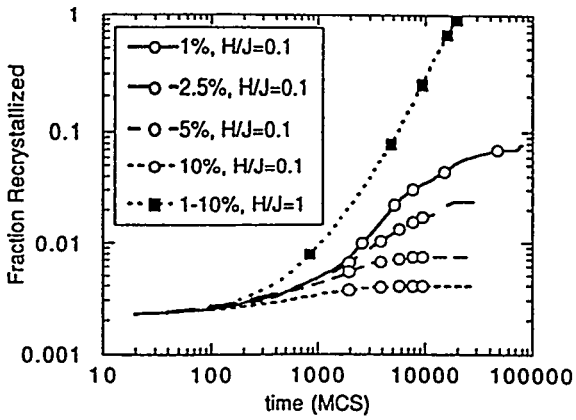

Figure 4. Plot of the fraction recrystallized versus time for two different stored energies, various area fractions of particles and a single nucleus.

At low stored energies (H/J < 1) grain boundary energy governs boundary motion, and the recrystallization front is strongly pinned by particles which leads to a much higher than random density of particles on the recrystallization front. In these circumstances recrystallization is strongly inhibited which usually results in incomplete recrystallization, as shown in Fig. 4. When only small particle fractions are present, however, recrystallization may go to completion because pinning does not occur until after the transformation is complete.

In addition, prior grain boundaries may still enhance motion of recrystallized grain boundaries, so that the recrystallized grains can grow (at low particle fractions) much larger than the deformed matrix grains. This is sufficient to drive the recrystallizing grains past some particles, but only if the matrix grain size is much smaller than the interparticle spacing. In other words, recrystallization at low stored energy and at very low particle fractions is similar to abnormal grain growth.

Grain boundaries undergoing curvature driven growth (both in the deformed state and after complete recrystallization) rapidly acquire a higher than random density of particles which then inhibits grain growth. If the recrystallized grain size is smaller than the normal grain growth particle pinned grain size, grain growth continues until pinning occurs and the microstructure is a normal grain growth microstructure. However, when the recrystallized grain size is large compared to the normal grain growth particle pinned grain size, particle pinning occurs almost immediately following the completion of recrystallization thus preserving the non-compact grain shapes and sharply peaked grain size distribution that are characteristic of randomly distributed nuclei. The following figure illustrates the point that the density of particles on boundaries is higher for ordinary boundaries than for recrystallization fronts. The latter intersect with particles at near random values.

Analysis of recrystallization in particle containing materials suggests that there are two limiting values of particle drag; a low (Zener) value with a random density of particles and a much higher value if particles have become highly correlated with the

recrystallization front (as in grain growth). The simulation results show both these behaviors, depending on the H/J ratio. The figure below plots the density of particles on boundaries for two types of boundaries; recrystallization fronts have a lower, near random density of particles; general boundaries exhibit a higher than random density, suggesting that they are more strongly pinned. Experimental studies appear to show only the lower particle drag (Zener) as studied by Ashby et al.[29].

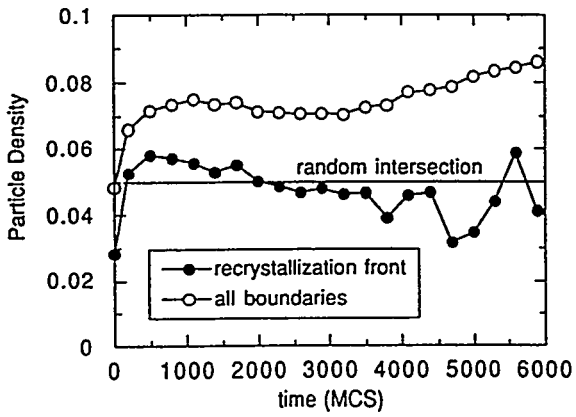

Figure 5. Plot of the fraction of particles on boundaries for H/J=1.01, with a particle area fraction of 5% and 1000 nuclei (site saturation conditions). The solid symbols represent results for recrystallization fronts, which intersect particles on a near random basis. General boundaries have a higher than random density of particles.

5.4. DYNAMIC RECRYSTALLIZATION

As described in the methods section, dynamic recrystallization has been successfully modeled with the Monte Carlo model[30]. In its simplest form, stored energy at each point of the lattice is increased at a fixed rate and embryonic new grains are continually added at a constant rate. The basic result is that temporal oscillations are observed both in the grain size and in the stored energy which is analogous to the flow stress, as shown in Fig. 6 below. These oscillations are observed over almost the entire range of recrystallization parameters examined (energy storage rate, nucleation rate, initial grain size) and damp out over time periods that decrease with increasing storage rate and increasing nucleation rate. The oscillations in both grain size and stored energy have the same period but are out of phase by approximately one quarter of a period. Examination of the simulated dynamic recrystallization microstructures which were formed under the same conditions but with different initial grain sizes shows that the evolution of the microstructure may be divided into three distinct stages: an initial microstructure dependent transient stage, an initial microstructure independent transient stage, and a

steady state stage. While necklacing was observed in these simulations under some circumstances, it is apparent that it is not a necessary condition for grain refinement in dynamic recrystallization. This phenomenon is associated with refinement of the relatively coarse initial microstructure and overdamped oscillations in the flow stress. Therefore, even when there are no obvious oscillations in the flow curve and no necklacing is observed, dynamic recrystallization cannot be precluded.

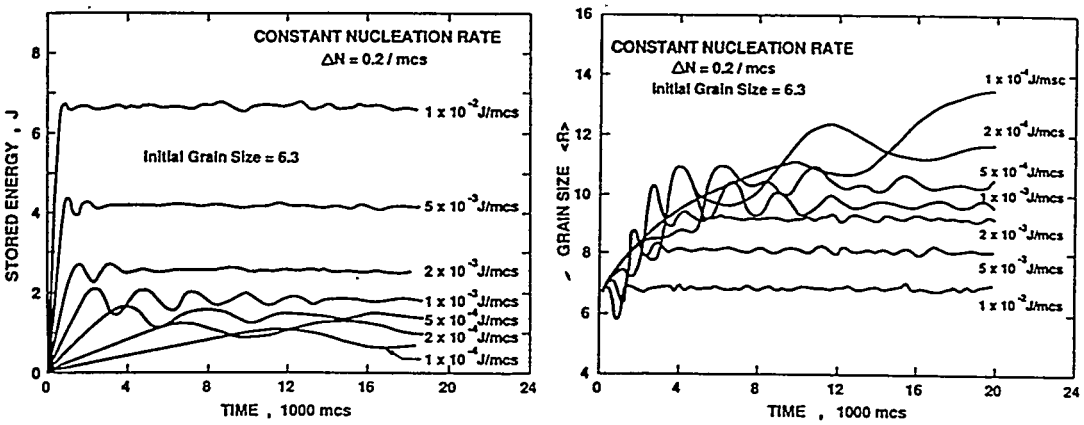

Figure 6. Plot of a) the variation of the stored energy (as representative of the flow stress) and b) of the mean grain size as a function of time.

It should be noted that the geological community had applied the Monte Carlo model to dynamic recrystallization but had only examined the microstructural aspects. Jessel[31] published a description of an adaptation of the Monte Carlo model for the simulation of deformation of quarzite. Although the model is similar to the combined grain growth and recrystallization model described above, the Jessel work used only differences in stored energy between sites to evaluate transition probabilities for orientation changes. Also, the only results given were for microstructural evolution, with no attempt to investigate stress-strain relationships. The simulations were used to investigate the development of texture (*fabric* in geological terms), based on the Taylor model (strain compatibility enforced on all grains) with some degree of success.

Peczak and coworkers have investigated several aspects of the correspondence between this type of simulation and have added several refinements to the model, see for example [32], in order to allow detailed comparisons with experimental data. They have modified the nucleation process such that the probability of an embryo appearing in a region of high stored energy is higher than for low stored energies. This has the consequence that the effective nucleation rate increases with time as stored energy is added to the system and is also position dependent during the simulation. They have also modified the rate of stored energy addition from the original constant addition rate to correspond to a Voce-type equation (i.e. an exponential work hardening curve) with a saturation (asymptotic) flow stress given by a Zener-Holloman parameter. By making these modifications they have been able to reproduce many of the characteristics of the phenomenon of dynamic recrystallization. For example, the transition from multiple

peaks to a single peak in the flow curve occurs when the ratio of the initial to the steady state grain size drops below 2.3. The relationship between the steady state grain size and flow stress in the model shows grain size decreasing with increasing stress as expected; the slope is ~1, Fig. 7, which is close to the experimental value of 0.7 [33].

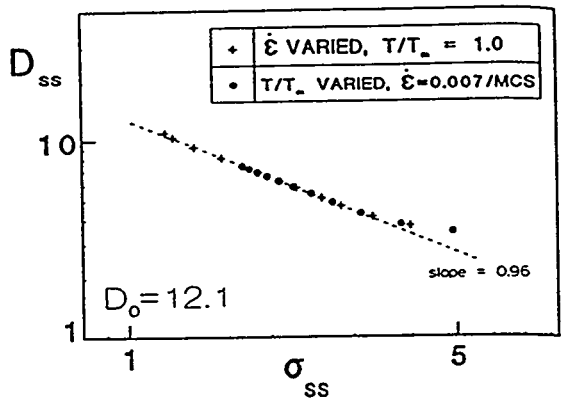

Figure 7. Plot of asymptotic grain size, D_{ss}, versus asymptotic stress, σ_{ss}, for a variety of simulation conditions, from Peczak[32]. Slope of -0.96 is close to experimental observations.

6. Summary

The principal methods for modeling the phenomenon of recrystallization have been reviewed. In view of the frequency with which the Monte Carlo model has been used in the literature, that method has been reviewed in more depth. The characteristics of the various lattice types, the Hamiltonians for the system energy, the transition probabilities, and the continuous time method were briefly treated. Key results from the simulation literature have been reviewed and summarized.

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