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Microstructural Simulations of Dynamic Recrystallization

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Abstract

A Monte Carlo model for the simulation of static recrystallization and grain growth has been adapted for dynamic recrystallization by adding recrystallization nuclei **and** stored energy continuously with time. The results of the simulations have shown that many of the essential features of dynamic recrystallization are reproduced. The stored energy of the system, which may be interpreted as the flow stress, goes through a maximum and then decays, monotonically under some conditions and otherwise in an oscillatory manner. The principal parameters that were varied were the rate of adding stored energy, ΔH, and the rate of adding nuclei, ΔN. As ΔH increases, for fixed ΔN, the oscillations decay more rapidly and the asymptotic stored energy rises. As ΔN increases, again the oscillations decay more rapidly but the asymptotic stored energy decreases. The mean grain size of the system also oscillates in a similar manner to the stored energy but 90° out of phase. Necklacing of the prior grain structure by new grains is observed for low ΔH and high ΔN; it is however, not an invariable feature of grain refinement i.e. cases where the dynamic grain size is smaller than the initial grain size. All these results were obtained without the addition of special parameters to the model such as a critical strain for the initiation of recrystallization.

Introduction

When crystalline materials are plastically deformed at low temperatures the dislocation density stored within the material increases. On subsequent heating to elevated temperatures, the dislocation density may decrease by either recovery or recrystallization. Recovery is the organization of the dislocations into low-energy patterns (e.g. dislocation cells) and the concomitant mutual annihilation of dislocation. Recrystallization, on the other hand, occurs when a relatively dislocation-free region or nucleus forms and grows out into the highly dislocated surrounding material. This recrystallized region or nucleus is separated from the adjacent dislocated material by a high angle grain boundary which acts as a sink for matrix dislocations. The growth of the recrystallized grain is driven by the reduction of energy associated with the decrease in dislocation density that occurs as a result of the motion of the grain boundary. While recovery and recrystallization are competing processes, they are not entirely separable. When a material is plastically deformed at elevated temperatures (e.g. at greater than 1/2 of the melting temperature) the accumulation of dislocations occurs simultaneously with dislocation annihilation via recovery and/or recrystallization. Recovery predominates in high stacking fault energy materials while recrystallization is the dominant dislocation annihilation mechanism in low stacking fault energy materials. When the predominant annihilation mechanism is recrystallization, this process is known as dynamic recrystallization. The term "dynamic" indicates that recrystallization goes on continually in response to the continuous addition of dislocations during the deformation.

The elevated temperature flow behavior of a material often provides a signature of the presence of dynamic recrystallization since the flow stress is proportional to the square root of the dislocation density. At low strain rates and high temperature the flow curves often show an initial peak followed by a decaying oscillatory profile. At higher strain rates and/or lower temperatures the flow curves are relatively flat (or monotonically decrease) following the initial peak. Experimental studies by Sakai[1] and co-workers have shown that the single peak behavior has been associated with grain refinement while the oscillatory behavior has been associated with increases in grain size. Luton and Sellars[2] have analyzed the dynamic recrystallization process in terms of the incubation strain for the onset of recrystallization, ε_c, and the strain or time required for completion of the recrystallization process, ε_x. When $\varepsilon_c > \varepsilon_x$, one recrystallization cycle has been completed before the next begins and an oscillatory flow curve is predicted. On the other hand, when $\varepsilon_c < \varepsilon_x$, a second wave of recrystallization starts before the first recrystallization wave is completed and hence the oscillatory behavior of the flow curve is suppressed. More recent theories have refined this basic idea[3,4,5]. A rather complete review of the experimental and theoretical aspects of dynamic recrystallization has recently been provided by Sakai and Jonas[1].

The observed correlations between grain size and flow behavior indicates a complete understanding of dynamic recrystallization must account for the evolution of the microstructure. The objective of the present work is to develop a simple model for dynamic recrystallization by extension of the simulation procedures developed to account for microstructural evolution in primary (static) recrystallization. The relationship between the flow stress, σ, and the dislocation density, ρ, is given by

$$\sigma = M \alpha \mu b \sqrt{\rho} \tag{1}$$

where M is a Taylor factor, α is a geometrical constant of order 0.5, μ is the shear modulus, and b is the Burgers vector. This relationship permits a direct link to be made between the stored energy used in the simulations, which models the stored dislocations, and the flow stress of a material. The details of the simulation procedure are described in the following section. The dynamic recrystallization simulation method is then employed to study the effects of strain rate (i.e. dislocation storage rate - stored energy addition rate) and nucleation rate on the flow curves (i.e. stored energy vs. time), the grain size evolution and microstructure.

Simulation Procedure

The computer model employed in this work is based on the same Monte Carlo model developed previously for the simulation of grain growth[6,7]. An index S_i is associated with each site on a two-dimensional (2D) triangular lattice which represents the crystallographic orientation of the material in the vicinity of the site. A contiguous group of sites all with the same index are part of the same grain, while nearest neighbor sites with unlike indices must be separated by a grain boundary. Thus, for the case of isotropic grain boundary energy, the total energy of the system is

$$E = \frac{J}{2} \sum_{i}^{N} \sum_{j}^{m} (1 - \delta_{S_i S_j}) \tag{2}$$

where J scales the grain boundary energy, the first sum is over all of the sites in the model (N=40,000), the second sum is over the m=6 nearest neighbors of site i, and δ_{ab} is the Kronecker delta function. A zero temperature Monte Carlo method is employed which corresponds to choosing a lattice site at random, reorienting that site to a randomly chosen, different value of S and calculating the change in energy ΔE. If $\Delta E \leq 0$, the new orientation of the site is retained, while if $\Delta E > 0$, the old orientation of the site is returned. The continuous time method is employed to increase the efficiency of the Monte Carlo method. The unit of time in the present simulations is a Monte Carlo Step (MCS) which corresponds to N reorientation attempts.

The method employed to model dynamic recrystallization is similar to that employed for primary (static) recrystallization[8], where a stored energy is applied to each lattice site. For recrystallization,

$$E = \frac{J}{2} \sum_{i}^{N} \sum_{j}^{m} (1 - \delta_{S_i S_j}) + \sum_{i}^{N} H_i \tag{3}$$

where H_i is the stored energy at the i^{th} site. To model dynamic recrystallization, however, the model has been modified such that each grain has a unique orientation and the stored energy at a given site is a function of its orientation , S_i, and time. Nucleation of recrystallized grains is included in the present model by adding new grains to the model at randomly chosen positions. These new grains or nuclei are added periodically in time. Each new grain or recrystallization nucleus consists of three sites arranged in a triangle and is assigned a unique orientation number S_β with a stored energy of zero (i.e. $H_\beta = 0$). At regular intervals, however, the stored energy associated with every orientation number is incremented by a fixed amount amount, ΔH, such that grains that have been present in the structure for long times have a high H but newer grains have low H.

Simulations of Dynamic Recrystallization

Simulations were performed at a fixed nucleation rate (ΔN / MCS) of $\Delta N = 0.2$ (corresponding to 1 nucleus added every five MCS) and for stored energy increment rates (ΔH / MCS) of $\Delta H = 10^{-4}$, 2×10^{-4}, 5×10^{-4}, 10^{-3}, 2×10^{-3}, 5×10^{-3}, and 10^{-2}. Additional simulations were performed at $\Delta H=10^{-3}$ and for nucleation rates of $\Delta N = 0.1, 0.2, 0.5, 1, 2$, and 5. The starting microstructures were obtained from normal grain growth simulations. Dynamic recrystallization studies were also performed for initial grain sizes, R_o, of 12.6, 8.9, and 6.3 with $\Delta H=10^{-3}$ and $\Delta N = 1$. The data presented in the following section were obtained by averaging over five simulations under identical sets of initial and simulation conditions.

The mean stored energy per site present in the system is assumed to be related to the dislocation density of a deformed metal by Eq. (1). A linear increase of stored energy with time therefore represents a parabolic stress-strain relation for the constant strain rate case. Other work-hardening relationships can be incorporated into the model and will be the basis of further work on this topic. By associating a particular stored energy with each orientation number, it is possible, for example, to incorporate a work-hardening relationship where the hardening rate depends on the current flow stress which is closer to current opinion in constitutive relations. It should be noted that the quoted nucleation rates are actually the rate at which nuclei are introduced into the system. Since the nuclei are surrounded by grain boundaries, there is a grain boundary interfacial tension which tends to make these nuclei shrink away. Consequently, at low stored energies the nuclei survival rate depends on the availability of prior grain boundaries (i.e. heterogeneous nucleation)[9]. Hence the actual nucleation rate is less than or equal to the quoted nucleation rate. The present model makes no assumptions about a critical strain being required to start or complete the nucleation process (e.g. the start of nucleation).

Results

The behavior of the flow curve during high temperature, constant strain rate experiments often provides the first indication of dynamic recrystallization. Since the flow stress is simply related to the stored energy (as described above), the stored energy versus time (strain) plot determined during the simulation should show the same general features as the experimental flow curves. The stored energy is plotted as a function of time in Fig. 2a for a grain growth microstructure with initial mean grain size $R_0 \sim 3.5$, a fixed nucleation rate of 0.2 nuclei per MCS ($\Delta N = 0.2$) and for a range of energy (dislocation) storage rates in the range of $10^{-4} \leq \Delta H \leq 10^{-2}$, corresponding to a constant strain rate simulated dynamic recrystallization experiment.

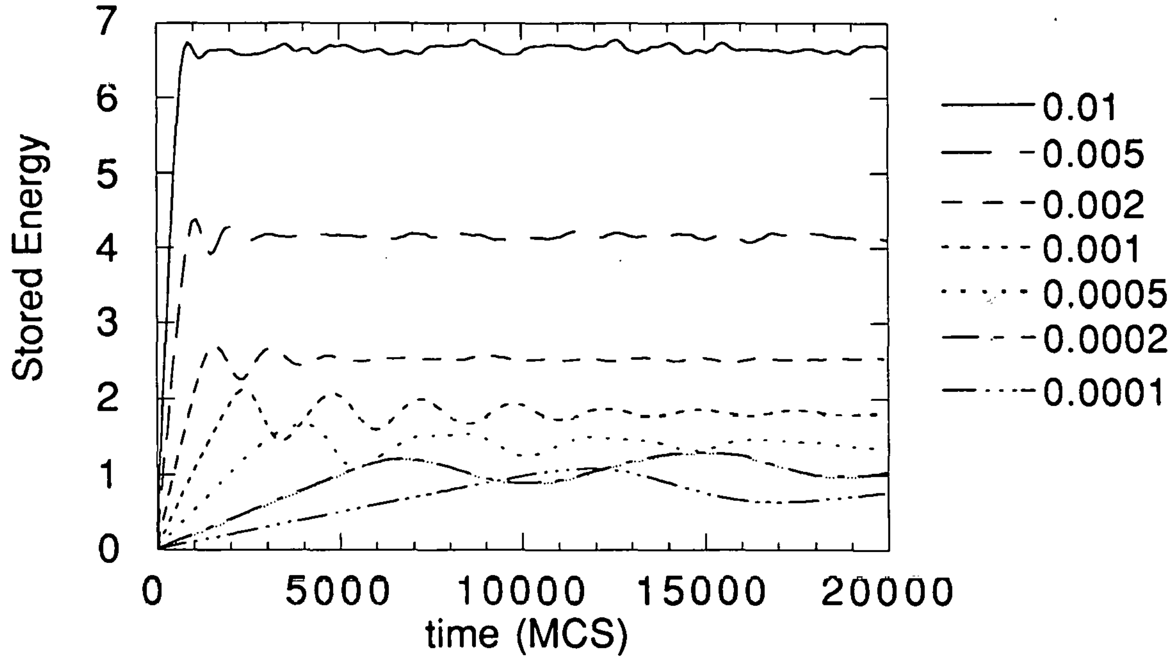

Fig. 1. Plot of stored energy versus time for constant ΔN (=0.2 per MCS): values of ΔH noted on graph.

The main features of these curves may be described as follows: (i) the stored energy (flow stress) rises with increasing time, peaks at a high value and saturates at a lower, constant value at long times, (ii) the initial rate at which the stored energy rises increases with increasing storage rate ΔH, (iii) the asymptotic (long time) value of the stored energy increases with increasing storage rate, (iv) oscillations in the stored energy versus time plots occur at all values of the storage rate, (v) the oscillations decay to the constant, asymptotic value of the stored energy, more quickly with increasing storage rate, and (vi) the period of the oscillations decreases with increasing storage rate. In order to aid in the comparison of this figure with experimental data (Fig. 1), it is useful to note that the rate at which dislocations (and hence energy) are added and stored in the material increases monotonically with strain rate but decreases with increasing temperature due to recovery.

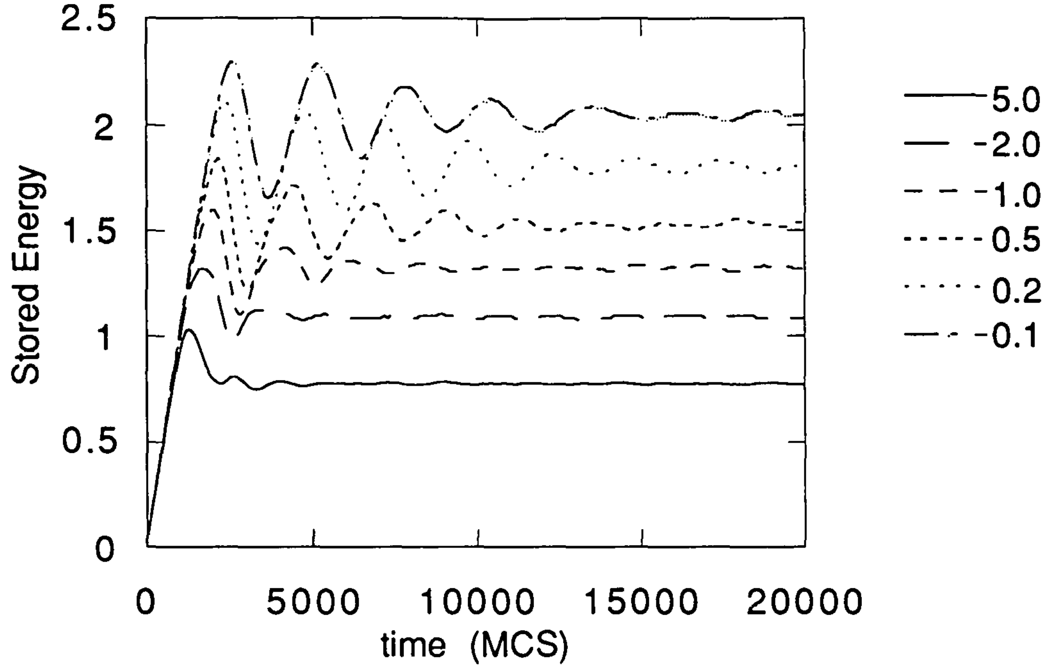

Fig. 2. Plot of stored energy versus time for fixed ΔH (=0.001 per MCS); values of ΔN noted on graph.

Variations in the rate at which potential nuclei are added to the system (in random locations) is expected to have a pronounced effect on the flow curves through their effect on the recrystallization rate of the material. The simulated analog of the flow curves (i.e. stored energy versus time) is shown in Fig. 2 for a range of nucleation rates (ΔN) in the range of $0.1 \leq \Delta N \leq 5$, for an initial grain size of $R_0=3.5$, and for $\Delta H=10^{-3}$. The main features of these curves may be described as follows: (i) as in Fig. 1, the stored energy (flow stress) rises with increasing time, peaks at a high value and saturates at a lower, constant value at long times, (ii) the initial rate at which the stored energy rises is independent of the nucleation rate, (iii) the asymptotic (long time) value of the stored energy increases with decreasing nucleation rate, (iv) oscillations in the stored energy versus time plots occur at all values of the nucleation rate, (v) the oscillations decay to the constant, asymptotic value of the stored energy, more quickly with increasing nucleation rate, (vi) the period of the oscillations decreases with increasing nucleation rate, and (vii) the amplitude of the oscillations increase with decreasing nucleation rate.

For the entire set of data represented in Figs. 1 & 2, the first maximum in the stored energy versus time plots always represents the absolute maximum stored energy in the system at any time during the dynamic recrystallization simulation. As indicated above, the peak height increased with increasing storage rate and decreasing nucleation rate. Figure 2 indicates that the flow curves show oscillations for all of the energy storage rates and nucleation rates considered. For very small energy storage rates or large nucleation rates, these oscillations are quite strongly damped with only a very few oscillations visible. The periods of the oscillations were determined as two times the time span between the first peak and subsequent minimum in the stored energy. The oscillation period decays with the energy storage rate (ΔH) as $\exp(-0.62\ \Delta H)$. At fixed energy storage rate, the oscillation period decays with increasing nucleation rate (ΔN) for small nucleation rates and then increases at larger value values of the nucleation rate. The observed minimum in the oscillation period with nucleation rate occurs for $0.5 \leq \Delta N \leq 1$.

Another parameter of interest is the mean grain size which also oscillates in a similar fashion to the stored energy. Figs. 3 shows the mean grain size <R> plotted as a function of time for various nucleation rates. Examination of Fig. 3 shows that a short transient in the time dependence of the grain size exists, followed by a period of oscillating grain size, and then, at long times, the mean grain size becomes time independent. As in the stored energy versus time plots (Figs. 1 and 2), the oscillations in the grain size are observed at low nucleation rates but not at high nucleation rates.

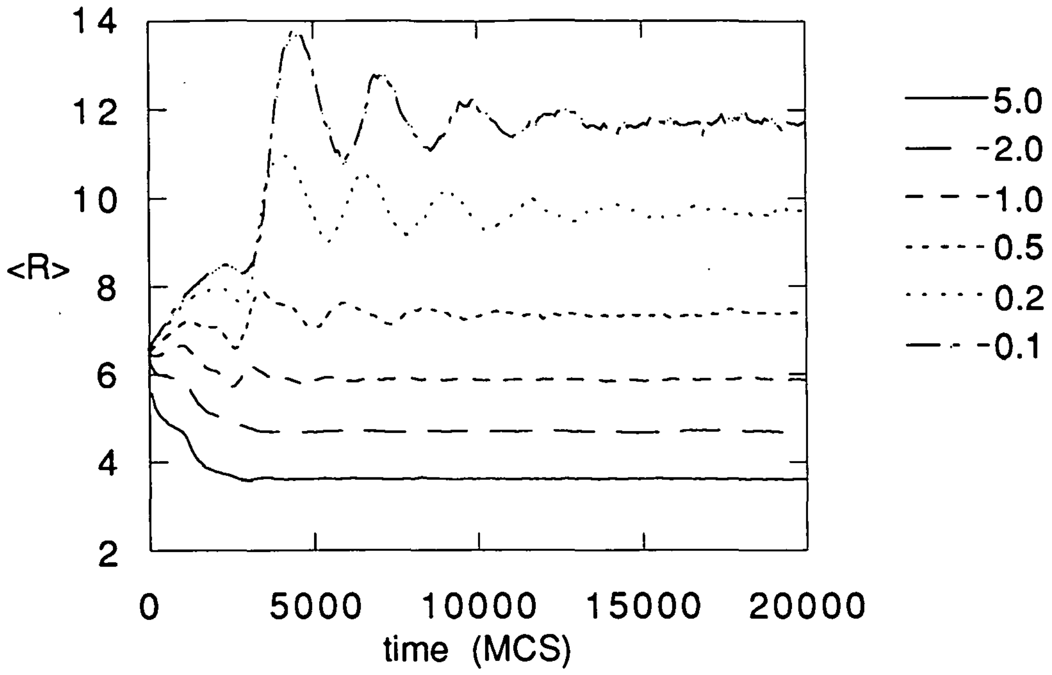

Figure 3. Plot of mean grain size versus time for fixed ΔH (=0.001 per MCS) and various values of ΔN as noted on the graph.

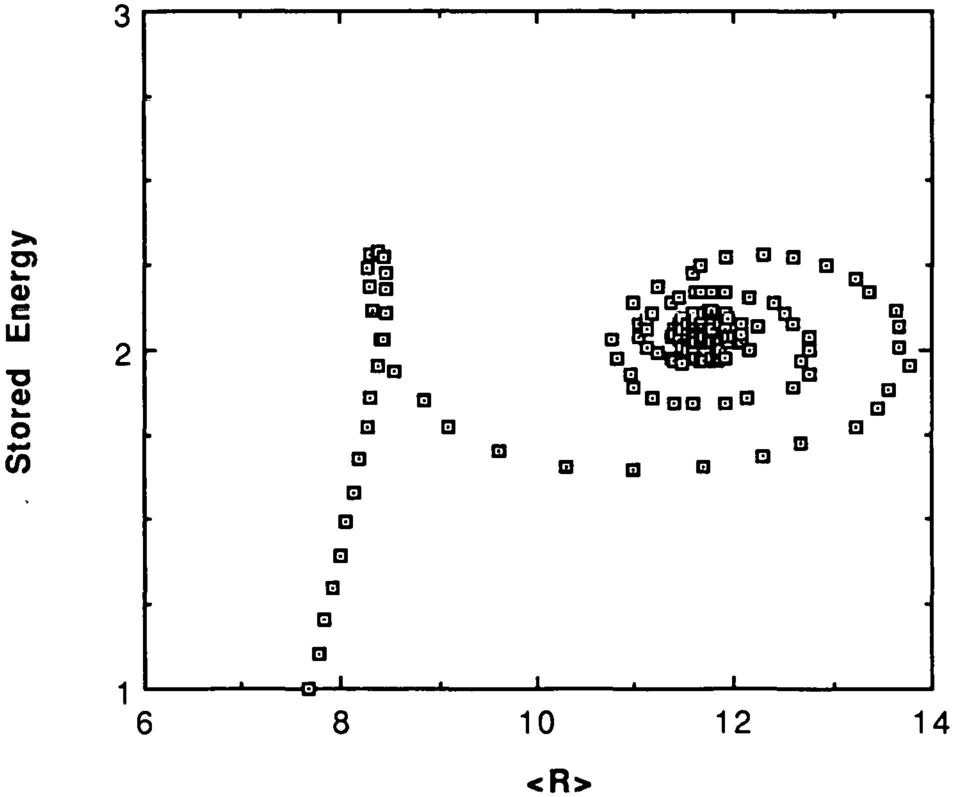

Figure. 4. Lissajous figure of stored energy versus mean grain radius for conditions of ΔH=0.001 and ΔN=0.1 per MCS

Comparison of Figs. 2 and 3 shows that the oscillations in grain size occur with the same period as do the oscillations in the stored energy. It is interesting to note, however, that the oscillations in grain size and stored energy appear to be out of phase by approximately $\pi/2$ (i.e. a quarter of a period). This is shown most clearly in a Lissajous figure where the mean grain size is plotted versus mean stored energy (both as a function of time), Fig. 4, for the case where $\Delta N=0.1$ and $\Delta H=10^{-3}$. After an initial transient, the data describe a spiral that converges on a point as the oscillations damp out. If <R> and H were in phase, the plot would be a straight line. The initial transient behavior observed in the time dependence of the grain size (before the onset of the regular oscillations) does not occur in the stored energy versus time plots. Although the transients observed are indeed distinct from the later oscillatory behavior, hints of the oscillations are observed in the transient regime. Additionally, the temporal extent of the transient regime is nearly equal to the grain size oscillation period observed at slightly later times.

Figure 5 shows a microstructure at short times for a very coarse initial grain size, a nucleation rate of 5 per MCS and an energy addition rate of 10^{-3}. Although nuclei are inserted into the model in a spatially random fashion, clearly only those nuclei that are contact with the prior grain boundaries survive and grow at the low stored energies present at short times. The nucleation rate is high enough that the prior grain boundaries are completely coated with new grains. This microstructure shows clearly that "necklacing" does occur in this model under a restricted set of initial conditions. Other cases of grain refinement during dynamic recrystallization do not show necklacing.

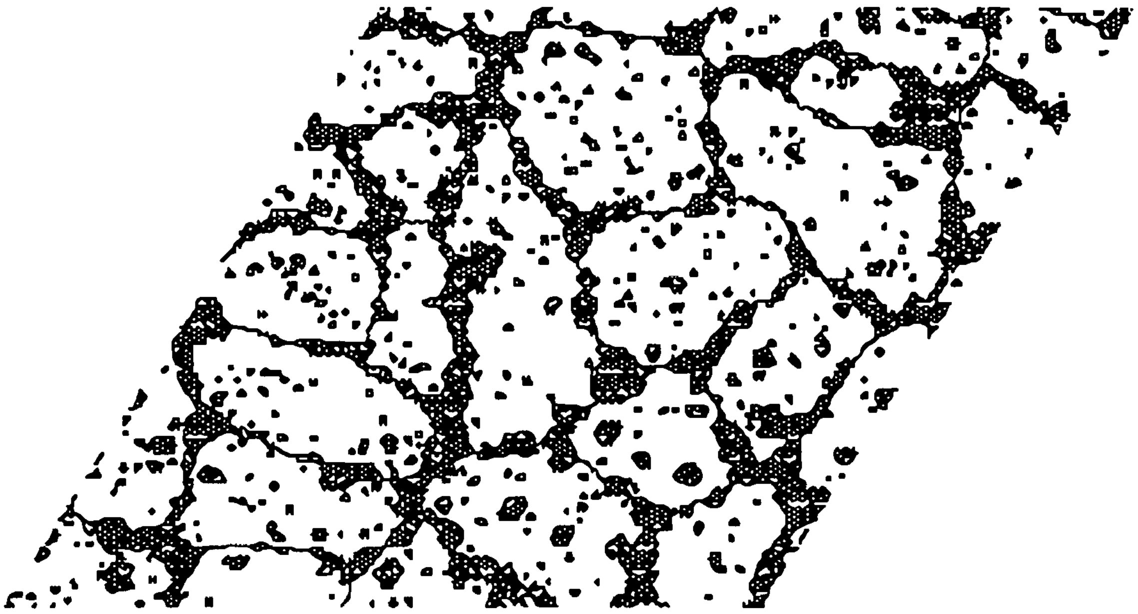

Figure 5. Microstructure at 2000 MCS for $\Delta H=0.001$ and $\Delta N=5$ per MCS, showing necklacing of the prior (coarse) grain structure by new grains.

Discussion

Oscillations in flow curves are one of the commonly referred to hallmarks of dynamic recrystallization (see Fig. 1). Inspection of the stored energy versus time plots (Figs. 1 and 2) demonstrates that the simulations reproduce this basic, experimentally observed feature of dynamic recrystallization. Close examination of these curves show that oscillations in the stored energy (flow stress) occur for all energy storage rates and for all nucleation rates. Such oscillations are most pronounced at high energy storage rates and/or low nucleation rates. Both of these conditions lead to large grain sizes. This is consistent with the observations of Sakai and Jonas[1] who associated oscillations in the flow curves with a coarsening of grain size. Nonetheless, the simulations clearly show that such oscillations do occur independent of whether the final grain size is larger or smaller than the initial grain size. The rate at which the oscillations decay does indeed seem to be correlated with final grain size (i.e. a slow decay for large grain sizes and fast decay for small grain sizes). In other words, the stored energy oscillations are underdamped at large asymptotic grain sizes but become more severely damped (or overdamped) in the limit of small grain sizes. Comparisons of Figs. 1 and 2 show that the degree of damping is not simply determined by the final grain size. The simulations with the largest energy storage rates (e.g. $\Delta H=0.01$, $\Delta N=0.2$) are significantly more strongly damped than those simulations with higher nucleation rate and smaller stored energy (e.g. $\Delta H=0.001$, $\Delta N=5.0$), although the latter situation results in a much finer final grain size.

While at long times the microstructure is completely specified by the dynamic recrystallization parameters, ΔH and ΔN, we have not identified a single composite parameter which describes both of the main microstructural features, asymptotic grain size and asymptotic stored energy. The asymptotic grain size is plotted as a function of the asymptotic stored energy in Fig. 6 for the entire range of ΔH and ΔN simulated. This figure shows very different behavior when the nucleation rate is varied at fixed storage rate compared with varying the storage rate at fixed nucleation rate. Specifically, as the storage rate is increased the ratio of grain size to stored energy decreases while the converse applies to variations in the nucleation rate. Varying the energy storage rate effects the asymptotic stored energy than the asymptotic grain size; conversely, varying the nucleation rate affects the asymptotic grain size more than the asymptotic stored energy. This result is consistent with the experimentally determined effect of increasing strain rate on the ratio of steady state stress to dynamic recrystallized grain size. Clearly, it is possible to create different dynamical recrystallization samples with the same asymptotic grain size but with completely different stored energies (and vice versa), depending on the nucleation rate and energy storage rate. The experimental data quoted by Sandstrom and Lagneborg[5] suggests that for Fe and Ni, at least, the expected behavior lies between the extremes defined by Fig. 6. That is to say, it is reasonable to suppose that as the strain rate is increased, for example, both the storage rate <u>and</u> the nucleation rate will increase. Similarly as the temperature is decreased, both the storage rate and the nucleation rate should increase. Such a coupled variation would lead to a single line in Fig. 6, whose slope would be intermediate between the -0.4 for varying ΔH and the 2.5 for varying ΔN.

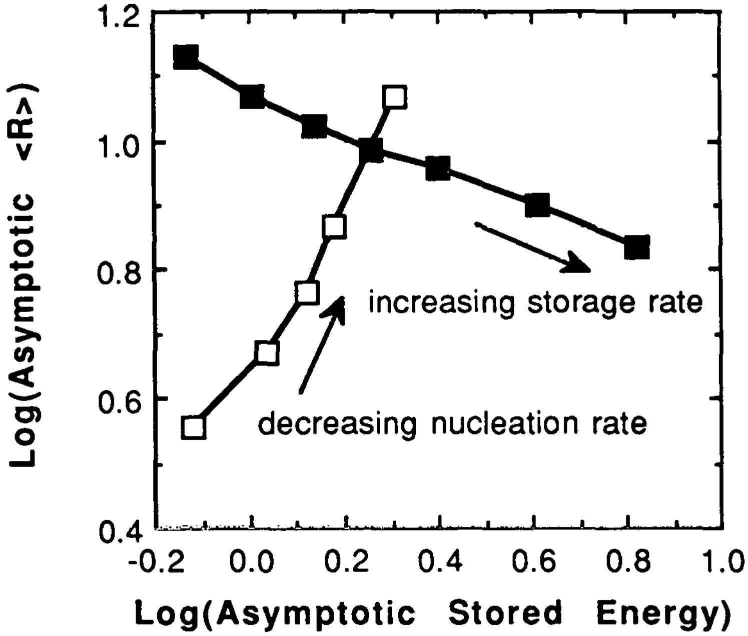

Figure 6. Plot of logarithmn(asymptotic mean grain size) versus logarithmn(asymptotic stored energy).

Conclusions

- A comparatively simple model of recrystallization has been shown to be capable of simulating many of the essential features of dynamic recrystallization, notably the oscillations in flow stress, as represented by the stored energy of the system.
- The oscillations in stored energy (flow stress) have been shown to have associated osciallations in the mean grain size. These oscillations occur out of phase with those in the stored energy.
- The variation in asymptotic stored energy and asymptotic grain size is dependent on which parameter is varied. Comparison with experimental data suggests that in real life, variations in nucleation rate and dislocation storage rate are not independent.

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