ABNORMAL GRAIN GROWTH - THE ORIGIN OF RECRYSTALLIZATION NUCLEI?

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ABSTRACT

The origin of recrystallization nuclei is reviewed with particular emphasis on materials in which well-developed cells are present in the deformed state. Nucleation is discussed in terms of coarsening of the subgrain network that develops on annealing and an analogy is made with abnormal grain growth. The results of a theoretical analysis of abnormal growth are summarized. The Monte Carlo model for grain growth is adapted for variable grain boundary energy and mobility in order to investigate the behavior of individual grains with special properties. The simulation results show that both energy and mobility affect abnormal growth as expected from the theoretical analysis. The results are discussed in terms of the stability that subgrain networks may exhibit depending on their mean misorientation.

INTRODUCTION

The simplest view of nucleation in recrystallization is that a small volume of material recovers, i.e. the dislocations stored during plastic deformation are eliminated, and that the volume element also possesses a mobile (high angle) boundary segment that then proceeds to migrate, see, e.g. [1]. Continued migration of the boundary of the new grain further eliminates stored energy of deformation and recrystallization is thus accomplished. An alternative view of nucleation takes account of the organization of the dislocations that make up the deformed structure into cells, whose walls contain most of the dislocations. The cell structure possesses a range of cell sizes and crystallographic orientations such that cell boundaries exhibit a range of energies and mobilities. Although recovery within the cells may still be significant, nucleation of recrystallization is simply abnormal grain growth of the cell or subgrain structure whereby a small fraction of the original subgrains acquire such a large size advantage that they act as recrystallizing grains, e.g. [2, 3]. That this is possible is not hard to understand when one considers the low mobility of grain boundaries associated with small misorientations, i.e. less than about 10°, and the great increase in mobility that occurs as the misorientation increases. The variation in mobility with misorientation is conjectural, however, as

few experimental data are available. Fridman et al. investigated migration rates in high purity aluminum, but only down to a minimum misorientation of 10° [4]. Viswanathan and Bauer measured migration rates in copper [5] for boundaries with misorientations of 2°, 5°, 9°, 18° and 32° about an [001] axis; Sun and Bauer measured the migration rates of tilt boundaries in NaCl [6]. We have extracted approximate mobilities for illustrative purposes by dividing the quoted values of migration rate at a particular temperature and dividing by the stated values of grain boundary energy, which themselves are assumed to follow the Read-Shockley relation. These mobilities, normalized to the value at the largest misorientation, have been plotted in Figure 1, together with assumed analytical forms for the variation in energy and mobility. The variation of energy with misorientation is simply the Read-Shockley relation, which has been substantiated experimentally [7], and the mobility variation is an assumed sigmoidal form; see Eqs. 5 and 6 below for further discussion. Note that the higher activation energies observed for migration at low misorientations means that decreasing the temperature will tend to increase the dynamic range of grain boundary mobility. Given these substantial variations in energy and mobility then, it is of some interest to explore the conditions under which abnormal or *discontinuous* coarsening of grain structures can occur.

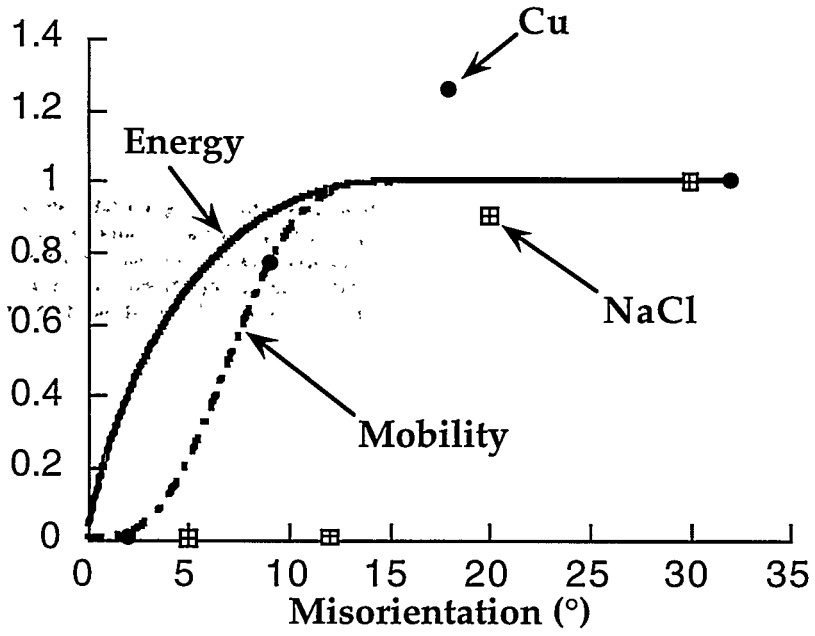

Fig. 1. Sketch of variation of boundary energy and mobility with misorientation. The energy is assumed to follow the Read-Shockley equation (Eq. 5), and mobility a sigmoidal variation with misorientation (Eq. 6). Experimental mobilities are plotted (squares) for work by Sun and Bauer [6] on NaCl (at ~750K, from their Fig. 6), and (solid circles) for work by Viswanathan and Bauer [5] on Cu (at ~973K, from their Fig. 8).

Nucleation in cell-forming materials has been studied on a number of occasions by thin foil electron microscopy, e.g. Bailey's observations of small recrystallized grains in copper and nickel [8]. Although some authors have emphasized subgrain coalescence [2] as a means of attaining a size advantage, we prefer to emphasize the importance of relative growth rate as influenced by grain boundary energy and mobility. A major gap in our ability to describe subgrain coarsening quantitatively is the lack of experimental data on boundary mobility at small and intermediate misorientations. The advent of orientation imaging microscopy shows promise, however, as a means of determining properties that are dependent on grain boundary character [9].

Rollett and Mullins [10] recently extended the analysis of relative growth rates originally examined by Thompson et al. [11] to account for both boundary energy and mobility on the growth of an isolated grain with special boundary properties. Their main result was an equation relating relative growth rate ($d\rho/dt$) to relative size and other parameters:

$$\frac{d\rho}{dt} = \frac{M\gamma}{2\langle r\rangle^2} G(\rho,\mu,\Gamma) \tag{1}$$

where

$$G(\rho,\mu,\Gamma) = \left\{\mu\Gamma\left(a + (a-2)\frac{1}{\rho}\right) - \frac{\rho}{4}\right\} \qquad \text{and} \qquad a(\Gamma) = (6/\pi)\sin^{-1}(1/2\Gamma). \tag{1a}$$

The relative grain size ρ=R/<r>, where R is the size of the isolated grain and <r> is the mean grain size in the matrix. M and γ are the mobility and energy, respectively, of the matrix grain boundaries. The ratio of boundary energy and mobility for the isolated grain to the matrix values are given by Γ and μ, respectively. By setting $G(\rho,\mu,\Gamma)$ to zero in order to find the lower and upper values of relative size, between which abnormal growth is predicted, the map shown in Fig. 2 is obtained.

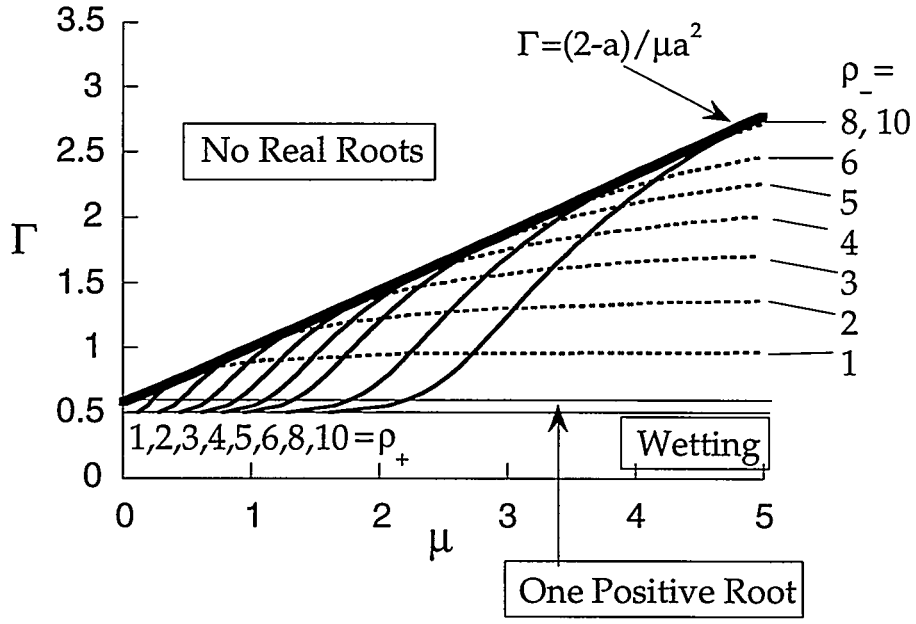

Figure 2. The μ, Γ plane with regions of stable ρ delineated. For $\Gamma<0.5$, wetting occurs; for $0.5\leq\Gamma\leq1/\sqrt{3}$, only one positive root exists; in the lower right triangle ($\Gamma>1/\sqrt{3}$) two positive roots exist. Contours of constant ρ_+ (solid curves) and ρ_- (dotted curves) have been drawn; the difference between the ρ_+ and ρ_- values at any point in the two root region defines the range of relative sizes over which abnormal growth can occur. If abnormal growth occurs, the relative size is predicted to converge on the upper root, ρ_+.

This map has four regions of interest. For energy ratios below 0.5, wetting of the matrix by the central grain occurs. For high enough values of energy ratio in the upper left region, no abnormal growth occurs. For values of energy ratio above 0.5 and high enough mobility ratios, abnormal growth can occur: the range of relative sizes over which this can occur is indicated by the contours of upper limit (solid lines) and lower limit (dashed lines). For $\Gamma<1/\sqrt{3}$, no lower limit exists, which

corresponds to the circumstance in which even three-sided grains can grow. Note that even when the isolated grain has a high boundary energy, provided that its boundary is mobile enough and that it possesses a size advantage, it can grow abnormally.

This paper presents some results of simulation of abnormal growth with the Potts model in which the combined effects of variable boundary energy and mobility were investigated. The results show that abnormal grain growth is constrained by higher grain boundary energies, and promoted by high mobilities. The results of the simulations are then related to the theoretical analysis briefly reviewed above.

MONTE CARLO (POTTS) MODEL

The Monte Carlo model that is commonly applied to grain growth problems has been described in theoretical and computational detail [12, 13]. We will give only the pertinent details for this particular implementation of the Potts model. Each element i in a square lattice of N elements was assigned an index $S_i \leq 100$ corresponding to its membership in grain S_i. The total system energy is given by

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

where the inner sum is taken over the n first and second nearest neighbors of element i, δ is the Kronecker delta function, and J is the energy of a unit of boundary between elements of indices S_i and S_j. To evolve the structure, an element and a new index were chosen at random. The element was reoriented to the new index with probability

$$P\left(S_i, S_j, \Delta E, T\right) = \begin{cases} \dfrac{J\left(S_i, S_j\right)}{J_{max}} \dfrac{M\left(S_i, S_j\right)}{M_{max}} & \Delta E \leq 0 \\ \dfrac{J\left(S_i, S_j\right)}{J_{max}} \dfrac{M\left(S_i, S_j\right)}{M_{max}} exp\left(-\Delta E / kT\right) & \Delta E > 0 \end{cases} \tag{3}$$

where ΔE is the energy change for the reorientation, M is the boundary mobility between elements of indices S_i and S_j, J_{max} and M_{max} are the maximum boundary energy and mobility respectively, k is the Boltzmann constant, and T is the lattice temperature. After each reorientation attempt, the time is incremented by 1/N Monte Carlo Steps (MCS), and a new reorientation is selected.

An efficient algorithm which avoids the wasted effort of computing unsuccessful reorientation attempts was utilized in these simulations [12]; this is particularly necessary for simulation at finite lattice temperatures in which even elements in grain interiors have a finite probability of reorientation, as in these simulations. A finite temperature was used in order to ensure that small differences in boundary energy did not lead to irreversible motion of boundary segments. At zero lattice temperature, the central grain shrinks monotonically if assigned a boundary energy higher than that of the matrix.

Simulations were performed with uniform boundary properties in order to obtain an initial, normal microstructure with a mean grain area of about 10 lattice elements. A large, circular grain of type A was then inserted near the center of this structure. The central grain was assigned a special orientation number (S=1). The interface of the special grain with the matrix grains of type B was assigned values of energy J_{AB} and mobility M_{AB} that varied from the otherwise uniform properties in the matrix, J_{BB} and M_{BB}. The energy ratio Γ and the mobility ratio μ are defined so that

$$\Gamma=J_{AB}/J_{BB} \quad \text{and} \quad \mu=M_{AB}/M_{BB}. \tag{4}$$

The larger energy and mobility values (whether AB or BB type) were assigned the value of one. This form of the Potts model is similar to that used to that used previously to model abnormal grain growth with variable boundary mobility[14].

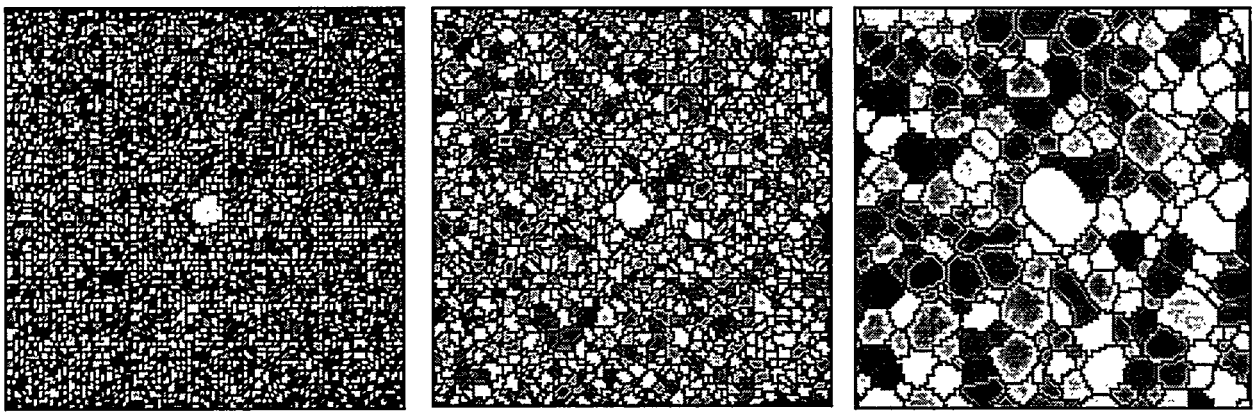

Fig. 3. Evolution of an abnormal grain with boundary mobility twice that of the matrix boundaries (μ=2) and energy 30% higher (Γ=1.3).

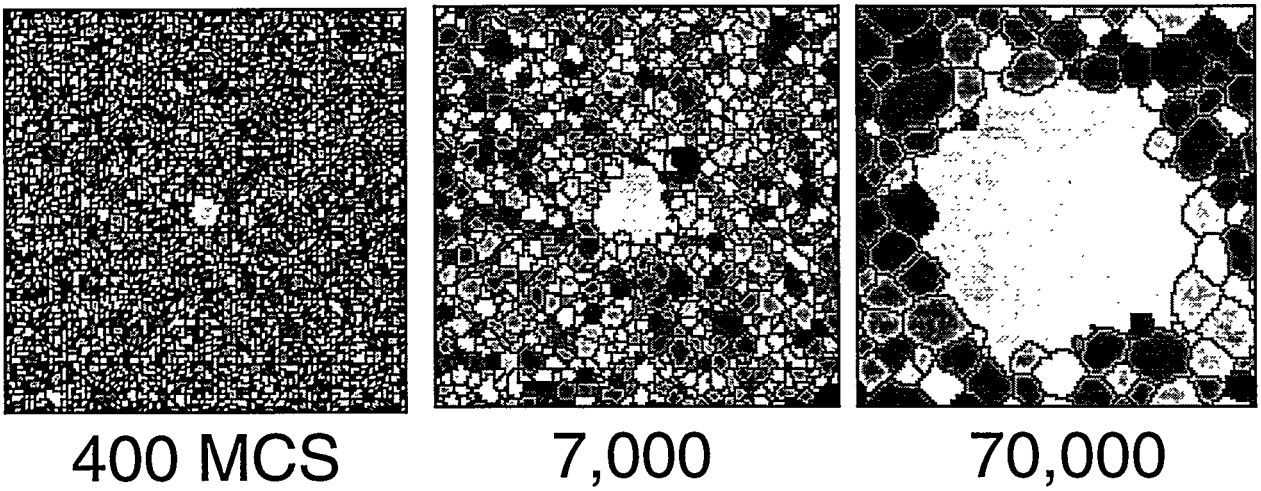

Fig. 4. Evolution of an abnormal grain with boundary mobility twice that of the matrix boundaries (μ=2) and energy 40% lower (Γ=0.6).

SIMULATION RESULTS

We show first the results of simulations of abnormal grain growth with a series of snapshots of the microstructures. The first series, Fig. 3, shows the evolution of an initially large grain with both a mobility advantage, μ=2, and boundary energy disadvantage, Γ=1.3. This grain does not grow more quickly than its surrounding grains, and abnormal grain growth does not occur.

By contrast the second series, Fig. 4, shows how an initially abnormal grain with both mobility and energy advantages, μ=2 and Γ=0.6, grows in an obviously abnormal fashion. Moreover the interboundary angles at the triple points around the edge of the grain are clearly perturbed from the

value of $2\pi/3$ applicable to uniform boundary energy; this demonstrates that the model is capable of reproducing the expected variation in grain morphology.

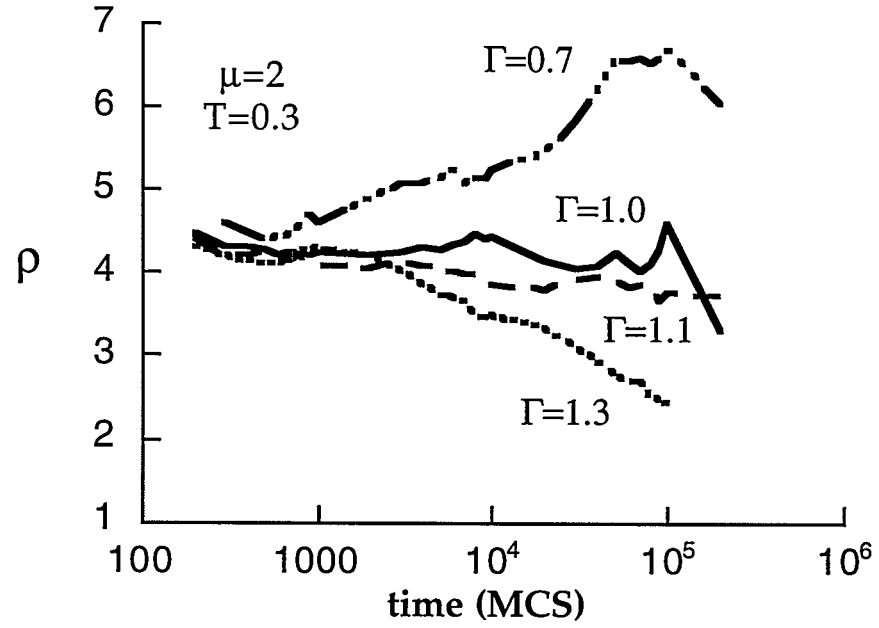

Fig. 5. Variation in relative grain size with time for simulations of abnormal grain growth in which the boundary of the central grain has twice the mobility of the matrix boundaries (μ=2); for each simulation the ratio of the central grain boundary energy to the matrix boundary energy, Γ, is noted on the plot.

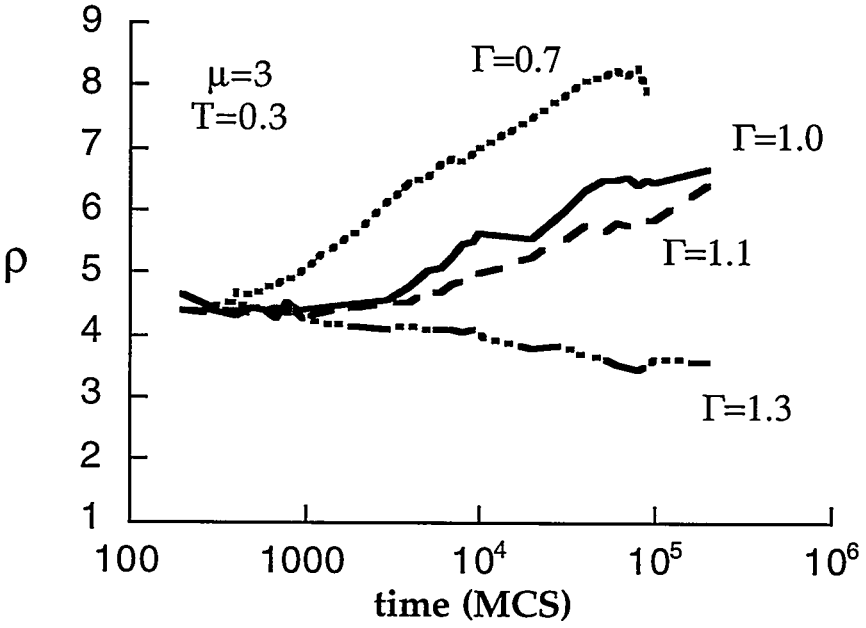

Fig. 6. Variation in relative size with time for simulations of abnormal grain growth in which the boundary of the central grain has three times the mobility of the matrix boundaries (μ=3) and boundary energy ratios as noted on the plot. The decrease in relative size at long times for the lowest energy ratio (Γ=0.7) is a consequence of limited lattice size in the simulation.

Of more importance is the variation in *relative* size (ρ) of the central grain as a function of time and boundary properties; $\rho = R_A / \langle r \rangle$ where R_A is the radius of the central grain, and $\langle r \rangle$ is the mean radius in the matrix. Figure 5 shows the variation of relative size for a fixed mobility ratio and various ratios of boundary energy. The results show that the central grain grows abnormally, i.e. maintains its size advantage over the matrix, for the smaller energy ratios but tends to rejoin the general size distribution for higher energy ratios.

Figure 6 shows that same information for a higher mobility ratio, $\mu=3$. In this case the central grain grows abnormally for boundary energy ratios less than $\Gamma=1.3$. These results are important because they qualify the previous result that suggested that small advantages in mobility will lead to abnormal grain growth [14]: instead, higher grain boundary energies appear to constrain abnormal grain growth. We shall see below how to set limits to abnormal grain growth.

Another important issue is the influence of initial conditions. Although the same matrix microstructure was used for all simulations, different initial sizes for the central grain were tested. Figure 7 shows how the relative size appears to converge on a single asymptotic value at long times.

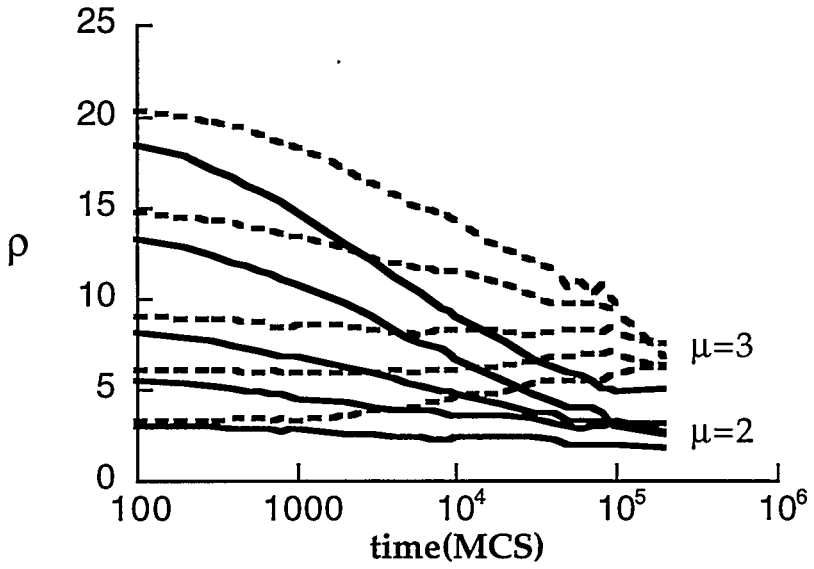

Fig. 7. Variation in relative size with time for simulations of abnormal grain growth in which the boundary of the central grain has either twice ($\mu=2$, solid lines) or three times ($\mu=3$, dashed lines) the mobility of the matrix boundaries. The relative size appears to converge towards an asymptotic value for each value of the mobility ratio.

When a recrystallizing grain grows, the misorientation across its boundary changes with each new grain that it contacts. Therefore it is unlikely that the boundary properties remain constant during growth, as is the case for the simulations presented here. In the case of subgrain coarsening, an orientation gradient across a set of subgrains can allow a growing grain to accumulate a large misorientation. The growing grain then encounters both small and large misorientation boundaries in the matrix. For secondary recrystallization it is possible to imagine that a growing grain could include a large fraction of special boundaries if the matrix contains a very small number of texture components, with some of which the growing grain has a special misorientation. Therefore several simulations of abnormal growth were performed where the central grain possessed various fractions of special boundary segments. Boundaries between matrix grains were energetically isotropic (with J=1) and had uniform mobility (M=0.5). Boundaries between the central grain and normal matrix

grains (those of index $S_i > icut$) possessed the same properties as the matrix boundaries. However, boundaries between the central grain and certain special grains (those with index $S_i \leq icut$) were of higher mobility and lower energy so that for those boundaries $\mu=2$ and $\Gamma=0.8$. The choice of $\mu=2$ and $\Gamma=0.8$ is one for which abnormal growth of the central grain occurs unambiguously when all central grain/matrix boundaries are special.

Table 1. Assignment of special boundary properties.

	S_i=1	S_i=2..icut	S_i=icut..100
S_j=1	n/a	M=1, J=0.8	M=0.5, J=1.0
S_j=2..icut	M=1, J=0.8	M=0.5, J=1.0	M=0.5, J=1.0
S_j=icut..100	M=0.5, J=1.0	M=0.5, J=1.0	M=0.5, J=1.0

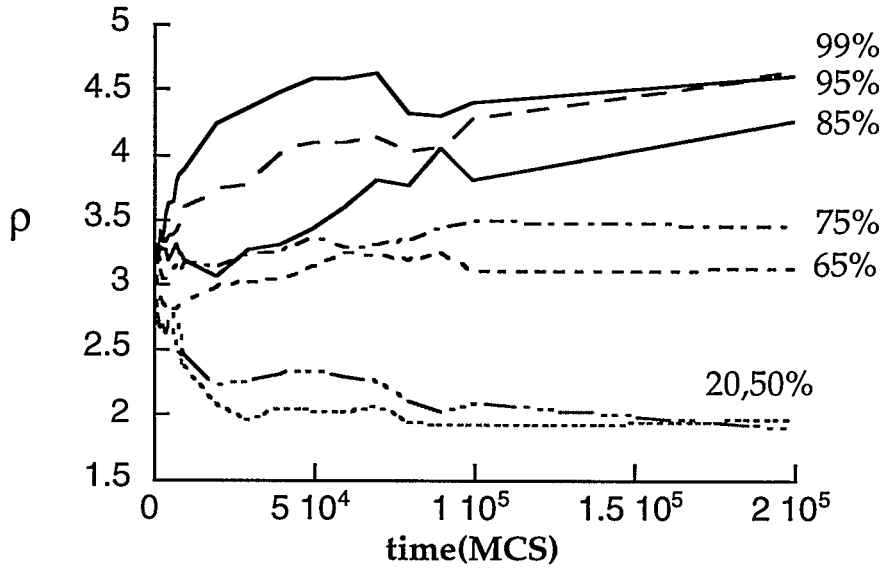

Fig. 8. Growth of the central grain for simulations of abnormal grain growth in which a fraction of the central grain/matrix boundaries has special properties. The results suggest a transition from normal to abnormal growth when the grain has between 60% and 80% special boundaries.

The results of varying the fraction of special boundaries are shown in Figure 8. For a high fraction of special boundaries, the central grain grows abnormally, as expected, and conversely, for a fraction below 50%, only normal coarsening is observed. Between fractions of 80% and 60%, a transition appears to occur between abnormal and normal coarsening. The results of the simulations were confirmed by examining the microstructures at long times for the various fractions of special boundaries.

DISCUSSION

The results of the simulations are in good agreement with the predictions of the theoretical approach summarized in the introduction. For a given mobility ratio, high boundary energies decrease the range of relative grain size over which abnormal grain growth occurs. Low values of boundary energy expand the incidence range for abnormal grain growth. The relative grain size increases or decreases towards a stable value (upper root in Fig. 2), depending on its initial value. The fraction of

special boundaries surrounding an initially large grain must be quite high in order to sustain abnormal growth. This may be relevant to recrystallization because it is a common observation that recrystallizing grains grow to sizes many times the original subgrain size and then stop, e.g. [15, 16].

Having established the sensitivity of abnormal grain growth to the properties of the grain boundaries, it is interesting to examine the consequences for coarsening of subgrain networks. Extending the analysis of Humphreys et al. [17], we consider the expected variation in energy and mobility ratio with mean misorientation in a network. The generally accepted form for energy as a function of misorientation is that of Read-Shockley [18]:

$$\frac{\gamma(\theta)}{\gamma_{HAGB}} = \begin{cases} \dfrac{\theta}{\theta_{HAGB}}\left(1-\ln\dfrac{\theta}{\theta_{HAGB}}\right) & \theta < \theta_{HAGB} \\ 1 & \theta \geq \theta_{HAGB} \end{cases}, \quad \theta_{HAGB}=15° \tag{5}$$

where θ is the misorientation angle, γ is the boundary energy, γ_{HAGB} is the energy of a high-angle boundary (i.e. the limiting case), and θ_{HAGB} is the misorientation cut-off between low- and high-angle boundaries. The mobility is assumed to take a sigmoidal form with θ:

$$\frac{M(\theta)}{M_{HAGB}} = M_{min} + (1 - M_{min})\left[1 - exp\left(-k\theta^3\right)\right] \tag{6}$$

where M_{HAGB} is the limiting high-angle boundary mobility, and k=0.002 and $M_{min}=10^{-3}$ are scaling parameters.

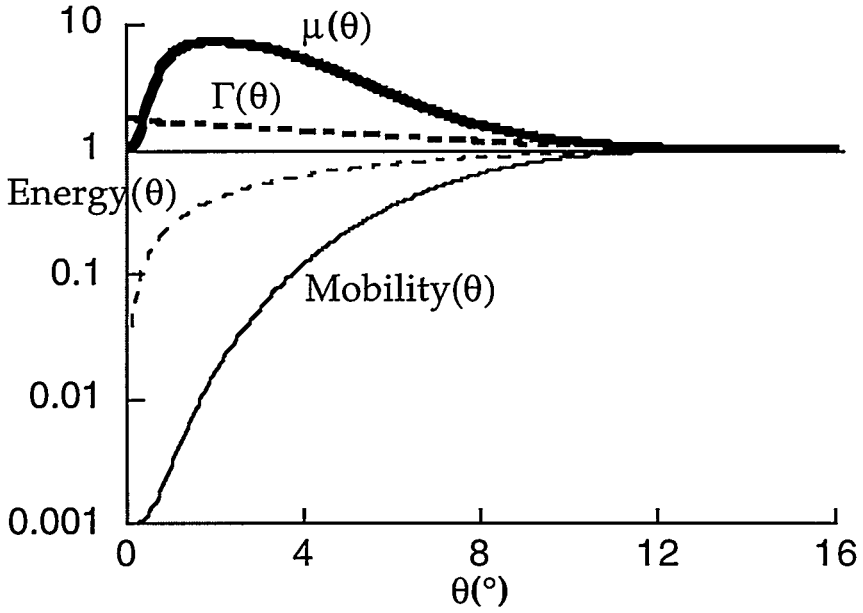

Fig. 9. Variation in boundary energy and mobility with misorientation θ according to Eqs. 5 and 6, normalized to the values for high angle boundaries. Also plotted is the variation in energy ratio Γ and mobility ratio μ with mean misorientation θ based on the assumption that the maximum misorientation is twice the mean misorientation.

In a network of subgrains, there will be a spread in size and orientation. While most normal subgrains have a relatively low misorientation with their neighbors, a few special subgrains have larger misorientations. If we assume that the largest special misorientation observed scales with the

normal, mean misorientation, the ratio of maximum to mean boundary energy, Γ, will depend on the mean misorientation. In Fig. 9, we plot Γ as a function of mean misorientation θ, where we assume that the maximum misorientation observed is twice the mean misorientation. Γ decreases continuously towards unity as the mean misorientation increases. Similarly, we estimate the maximum to mean mobility ratio, μ, again assuming that the maximum misorientation observed is twice the mean misorientation. Note that the maximum in mobility ratio (μ) is a consequence of the (assumed) sigmoidal variation; the position of the maximum will vary with the assumptions made about the distribution of misorientation.

The variation in mobility and energy ratios with misorientation can then be plotted on the Γ-μ plane as shown in Fig. 10 (c.f. Fig. 2) to illustrate the potential for abnormal grain growth. The contour for a relative grain size ρ=3, typically the largest relative size observed in a normal microstructure, is included to show how the Γ-μ trajectory falls below this line for moderate misorientations, indicating that grains at the upper end of a typical size distribution could have the properties for abnormal growth. Although the Γ decreases monotonically with misorientation, μ goes through a maximum. Hence a subgrain network may be initially stable at low mean misorientations but as the mean misorientation increases during coarsening, it can reach a point at which it is likely to undergo abnormal grain growth. As the mean misorientation increases towards high angle values, however, the stability increases. Even if certain grains grow abnormally, they are unlikely to grow to relative sizes that are much larger than the mean size.

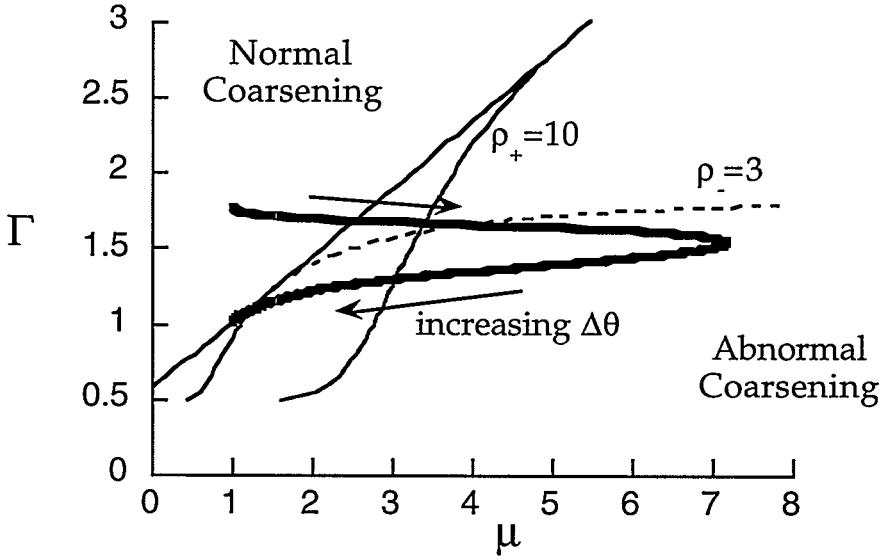

Fig. 10. Plot of the trajectory (heavy line) through Γ,μ space for the variation in mobility and energy ratios shown in Fig. 9. The theoretical analysis predicts that abnormal behavior is unlikely for mean misorientations that are either very small (upper left point on heavy line) or close to high angle boundaries (lower left point). At moderate misorientations where the mobility increases rapidly with misorientation, the analysis predicts that abnormal growth can occur over a large range of relative size. Grains with boundaries having (Γ,μ) below the dashed line for ρ_-=3 are likely to grow abnormally if they are at least three times larger than the mean size.

SUMMARY

An analysis of abnormal grain growth has been reviewed. The results of Monte Carlo simulations of abnormal grain growth are in good agreement with the analysis. When the boundary of an abnormal grain has a higher mobility and a lower energy than boundaries of normal grains, abnormal growth is

more likely. the upper limit on relative grain size depends on the boundary energy and mobility ratios; the relative size of abnormal grains will converge to this limit. A certain fraction of the boundary of the abnormal grain must possess special properties in order for abnormal growth to occur; the simulation results suggest that a threshold may exist for this fraction and that, below this threshold, no abnormal behavior occurs. Finally, the impact of the results on the stability of subgrain networks is discussed based on our current understanding of the properties of low angle grain boundaries.

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