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MICROSTRUCTURAL DYNAMIC STUDY OF GRAIN GROWTH

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1. INTRODUCTION

The complete prediction of microstructural development in polycrystalline solids as a function of time and temperature is a major objective in materials science, but has not yet been possible primarily due to the complexity of the grain interactions. The evolution of the polycrystalline structure depends upon the precise specification of the coordinates of the grain boundary network, the crystallographic orientations of the grains, and the postulated microscopic mechanisms by which elements of the boundaries are assumed to move. Therefore, a general analytical solution to this multivariate problem has not yet been developed. Recently, we have been able to successfully incorporate these aspects of the grain interactions, and have developed a computer model which predicts the main features of the microstructure from first principles [1,2]. The polycrystal is mapped onto a discrete lattice by dividing the material into small area (2d) or volume (3d) elements, and placing the centers of these elements on lattice points. Interactions and dynamics are then defined for the individual elements which are analogous to those postulated in continuous systems. This discrete model preserves the topological features of real materials, and can be studied by computer simulation using Monte Carlo techniques. In this paper we report the application of the Monte Carlo method to the metallurgical phenomenon of grain growth with isothermal annealing. Extension of the model to treat primary recrystallization is presented elsewhere [3,4].

Grain growth is the term used to describe the increase in average grain size which occurs upon annealing a polycrystalline aggregate after primary recrystallization is complete. Normal grain growth is a steady state kinetic process characterized by time invariance of the normalized grain size distribution function, $F(R/\bar{R})$, and the topological distribution function, $P(N_e)$, where R is the grain radius and N_e is the number of grain edges as measured from polished sections [5]. In the long time limit the mean grain size $\bar{R}$ increases with time as [6]

$$\bar{R} = \alpha t^n \quad (1)$$

where α is a temperature dependent constant and n is the growth exponent. While scatter in the value for n exists, n has a maximum value of 0.5 and a mean value of approximately 0.4 [6].

Most of the existing grain growth theories [5,7-9] implicitly assume that grains can be described as spherical, and that growth occurs in an average environment. This, however, ignores the fact that adjacent grains share common boundaries, resulting in a microstructure that is topologically connected. These theories [5,7-9] predict long time growth kinetics of the form of Eq. (1) with $n = 1/2$. Since experimental studies of grain growth yield an exponent, n , less than 1/2, the discrepancy may be a consequence of neglecting topological constraints, and the detailed environment.

To examine this possibility, Monte Carlo studies have been made of grain growth in both two dimensions (2d) and three dimensions (3d).

II. SIMULATION PROCEDURE

In order to incorporate the complexity of grain boundary topology, the microstructure is mapped onto a discrete lattice (Fig. 1). Each lattice site is assigned a number between 1 and Q corresponding to the orientation of the grain in which it is embedded. Q is chosen large enough so that grains of like orientation impinge infrequently, typically $Q = 48$ or 64 . Since the speed of the computer algorithm decreases with increasing Q , larger values of Q are not routinely employed. However, for $Q \geq 36$, the results are insensitive to the magnitude of Q . In the present model, a grain boundary segment is defined to lie between two sites of unlike orientation.

The grain boundary energy is specified by defining an interaction between lattice sites within a given distance (usually nearest neighbor in two-dimensions (2d) and up to the third nearest neighbors in three-dimensions (3d)),

$$E_i = -J \sum_j (\delta_{S_i S_j} - 1). \quad (2)$$

Here S_i is the orientation of site i ($1 \leq S_i \leq Q$), δ_{AB} is the Kronecker delta and the sum is taken over all sites within a specified distance. J is a position constant which sets the scale of the grain boundary energy.

The kinetics of boundary motion are simulated via a Monte Carlo technique in which a site is selected at random and re-oriented to a randomly chosen orientation between 1 and Q . If the change in energy associated with the re-orientation, ΔE , is less than or equal to zero the

Figure 1 - Sample microstructure mapped onto a triangular lattice. The integers denote orientations and the lines represent grain boundaries.

Figure 2 - Evolution of an initially spherical grain of initial radius $R_0 = 30$ (in units of lattice sites) in an infinite matrix on a simple cubic lattice for $t = 0, 200, 400$ and 600 MCS.

re-orientation is accepted. However, if the re-orientation attempt results in $\Delta E > 0$, the re-orientation is accepted with probability $\exp(-\Delta E/k_B T)$, where $k_B T$ is the thermal energy. A unit segment of grain boundary, therefore, moves with a velocity, $v_i = C[1 - \exp(-\Delta E_i/k_B T)]$, where C is a constant proportional to the boundary mobility. This description of the

local boundary velocity is formally equivalent to that derived from classical reaction rate theory. Time, in these simulations, is proportional to the number of re-orientation attempts. N re-orientation attempts is used as the unit of time and is referred to as 1 Monte Carlo Step (MCS), where N is the number of lattice sites. The conversion from MCS to real time has an implicit activation energy factor, $\exp(-W/k_B T)$, which corresponds to the atomic jump frequency. Since the quoted times are normalized by the jump frequency, the only effect of choosing $T \neq 0$ (as in these simulations) is to restrict the accepted re-orientation attempts to those with $\Delta E < 0$. Re-orientation of a site at a grain boundary corresponds to boundary migration.

III. RESULTS

Extensive simulations have been performed in both 2d and 3d. Most studies in 2d were carried out on a triangular lattice of size 200×200 . The results in 3d were obtained employing a simple cubic lattice of size $60 \times 60 \times 60$ or $100 \times 100 \times 100$.

A. Morphology

As a demonstration of the isotropy of the model, the shape of a circular grain (2d) or spherical grain (3d) was monitored as a function of time. The position of the grain boundary is plotted in approximately 200 MCS increments in Fig. 2 for the great circle of a shrinking spherical grain. In both 2d and 3d, the embedded grain remains nearly circular or spherical as it shrinks. This demonstrates that the product of the driving force and the boundary mobility is isotropic.

For the simulations of polycrystalline grain growth, the microstructure is initialized by randomly assigning an orientation between 1 and 0 to each lattice site. The temporal evolution of a polycrystalline microstructure is shown in Fig. 3 for growth on a 2d triangular lattice and in Fig. 4 for a (100) planar section on the 3d simple cubic lattice with first, second and third nearest neighbor interactions. Steps are clearly visible in the micrographs in Fig. 4 due to the small size of the simulated volume (100^3 lattice sites). These steps are less visible in Fig. 3 for the 200^2 system. In spite of these steps, good correspondence to planar grain morphologies in isotropic polycrystalline metals and ceramics is obtained. In both 2d and 3d, grain boundaries tend to intersect at 120° when examined on a scale larger than a unit step. Grains which are larger than the mean size (2d) or the mean size in cross-sections (3d) tend to have more than six sides and grow. Grains which are smaller than the mean size tend to have less than six sides and shrink.

B. Kinetics

Averaging the simulation data for the shrinking circular grain (2d) and shrinking spherical grain (3d) over 20 simulations shows that in both cases the radius decreases as the square root of time, $n = 1/2$ in Eq.(1). The kinetics obtained are in agreement with analytical treatments which are rigorous for these simple geometries. This demonstrates that the kinetic simulation technique employed is in accordance with the rate theory model.

The mean grain size was monitored as a function of time for the polycrystalline microstructures. In Fig. 5 the mean grain area for 2d and

Figure 3 - Temporal evolution of a two dimensional polycrystalline microstructure on a 200^2 triangular lattice for a pure, isotropic material. Grains with six edges have been shaded.

Figure 4 - Temporal evolution of the cross-section from the 3d microstructure for $Q = 48$ on a 100^3 simple cubic lattice.

Figure 5 - Log-log plot of the mean area A versus time for $Q = 48$ for the two dimensional grain growth simulations and for the cross-sectional area of the three dimensional simulations.

mean cross-sectional area for 3d is presented as a function of time. Averaging the simulation data over more than 40 simulations for each dimension show that the growth kinetics are $n = 0.41 \pm 0.03$ (2d) and $n = 0.37 \pm 0.02$ (3d) in Eq. (1). It is concluded from these results that the grain growth kinetics are independent of dimensionality (for $d \geq 2$). For comparison, the average grain growth exponent n derived from averaging the results for n from the literature for different metals and ceramics is 0.39 ± 0.07 [6].

C. Grain Size Distribution

The grain radius distribution was examined by plotting the frequency of occurrence versus the logarithm of the normalized grain radius determined from area in 2d and from area in cross-sections in 3d. These distributions were found to be time invariant when normalized by their respective means. Time averaged data are shown in Fig. 6. The size distribution functions are nearly identical between 2d and 3d. Comparison of the 3d model data with experimental data measured in our laboratory for pure Fe is presented in Fig. 7. Excellent agreement is obtained.

Figure 6 - Grain radius distribution as determined from cross-sections of the 3d lattice model (filled circles) and from the 2d lattice model (histogram).

Figure 7 - Grain radius distribution as determined from a cross-sectional area analysis of pure Fe (histogram) and from cross-sections of the three dimensional lattice model (filled circles).

Figure 8 - Distribution of the number of grain edges measured from cross-sections. The circles represent data from the 3d simulations. The triangles correspond to MgO (10), the squares to Al (11), and the diamonds to Sn (5). The curve is drawn through the simulation results.

Fig. 9 - Mean grain radius for each topological class versus number of edges N_e . The circles represent data from cross-sections of the 3d simulation. The triangles correspond to MgO (10) and the diamonds to Al (11). The squares represent the results obtained from the 2d simulation. The line is drawn through the 3d simulation results.

D. Topology

The grain topology was also examined by plotting frequency of occurrence versus the number of grain edges, N_e . Data in 3d were taken from cross-sections. It was found that these distributions are also time invariant. The topological distributions are nearly identical between 2d and 3d, similar to the grain size distribution functions. Comparison of the 3d topological data with experimental data for Al, Sn, and MgO is given in Fig. 8. The relationship between grain size and topology for the 3d model microstructure and the above materials is given in Fig. 9, where the mean grain size for each topological class (grains with the same number of edges) is plotted versus the number of grain edges. As before, the agreement between the simulation results and experiment is excellent.

IV. CONCLUSIONS

A simulation procedure for grain growth has been developed which accounts for local structure and topology. The simulated microstructures shown excellent agreement with those found in isotropic polycrystalline metals and ceramics. The grain size distribution, topological distribution, and the topology-grain relations are all in excellent agreement with experiment. Similarly, the kinetics found also reproduce the experimental results. It is suggested that the growth exponent, $n < 1/2$, is inherent to the grain growth process and is not due to impurities, preferred orientation, etc. as had been previously thought.

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