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Microstructural Evolution in Grain Growth

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The grain switching and the disappearance of grains in grain growth were analysed by the Surface Evolver method that models the process of boundary motion by curvature to minimize the boundary energy.

Key words: grain growth, simulation, grain switching, distribution

1. INTRODUCTION

The microstructural tailoring of alloys and ceramics is a key technology to control and improve the properties. The grain boundary of polycrystalline solids forms complex three-dimensional network structures. The grain boundary moves toward minimizing grain boundary energy at elevated temperatures, then the motion changes the topology of the grain boundary network. The motion of boundary changes the size and shape of grains. The small grains shrink and disappear, and the mean size of the remaining grains increases. The grain boundary network reaches to a steady structure that is geometrically similar in a statistical sense. In normal grain growth, the distribution function of grain size $F(R/\langle R\rangle)$ maintains the self-similar shape where $\langle R\rangle$ is the mean grain size.[1-6] The state of a grain is classified according to its number of faces, f, which is equivalent to the number of nearest-neighbor grains.[6] The distribution function of the number of faces $P(f)$ maintains a steady shape in normal grain growth also. As a grain changes its size, it varies the topological state f as shown in Fig.1. The elemental processes of topological change are grain switching (T1 process) and disappearance of grain (T2 process).[1] Grain switching is a process to make or lose contact with other grains, namely creation and elimination of a face of the grain.[5]

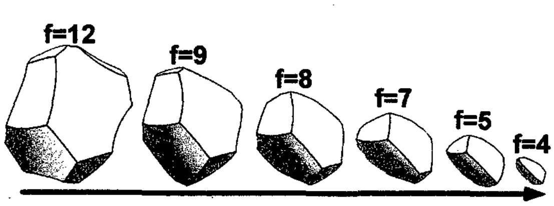

Fig. 1. Topological evolution of a grain in the 3D simulation.

In the normal grain growth, the mean grain size increases with time as follows:

$$\langle R(t)\rangle^2 - \langle R(0)\rangle^2 = 2\beta M\gamma t, \quad (1)$$

where t is time, M is the grain-boundary mobility, γ is the free energy of grain boundaries and β is Mullins' structural kinetic parameter.[3,4] This parabolic law of "grain growth" expresses the concept in *the statistics of survived grains*

On the other hand, all grains except one shrink and disappear ultimately after very long time because the state of minimal energy is a single crystal. An alternative formulation of the "grain growth" process is available by considering the statistics of disappearing grains. Every grain except one starts shrink and disappear sooner or later. A grain has a life span.

In this paper, we formulate the grain growth by the statistics of grain switching and by the statistics of disappearing grains.

2. NUMERICAL SIMULATION

Brakke's[7] Surface Evolver program was used to simulate the grain growth in three dimensions. The surface of grains, including both internal interface and surface, is represented as a set of triangular finite element, facets, as shown in Fig. 2. The grain boundary has a energy that is proportional to its area. The program causes the grain boundary to evolve towards minimal energy. The simulation of ideal grain growth was conducted by assuming isotropic boundary energy and mobility.

Even though the simulation was started from an idealized structure in which uniform grains were packed arbitrarily, the boundary network approached a steady structure after the incubation period and the transition period.[8] In the following discussions, the origin of time is the beginning of the normal grain growth period that is characterized by the steady structure.

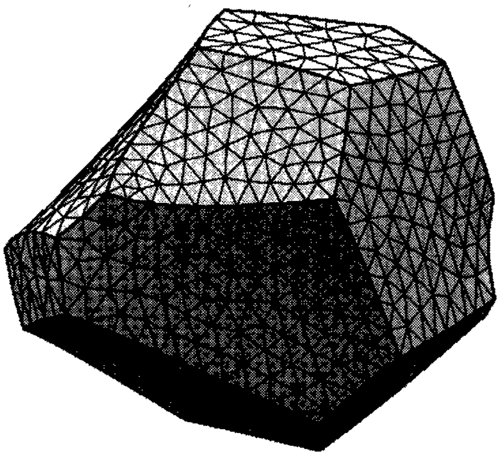

Fig. 2. Example of triangular mesh of a grain

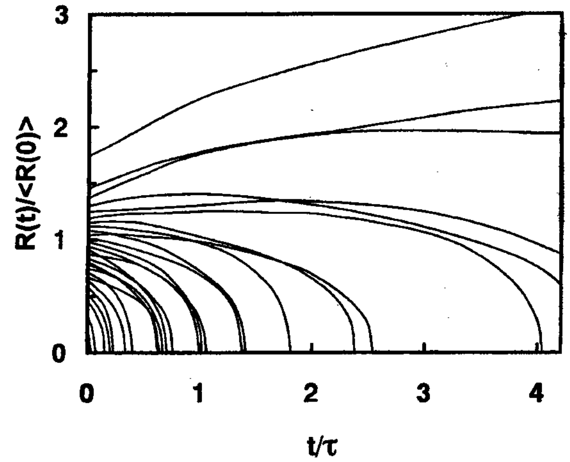

Fig. 3 Variation in the individual grain size with time in normal grain growth. The curves for some selected grains are shown.

3. LIFE SPAN OF GRAINS

The sizes of several grains are plotted as a function of time in Fig. 3 where the characteristic time τ is defined as the time where the number of grains decreases to half the initial value. Although the sizes of large grains increased monotonically, all grains shrink and disappear after a very long time. The time to disappearance of grain is the life span t_d of the grain. The larger grains had longer lives generally, but the trajectories of individual grains in grain size-time space crossed in some cases. The life span against initial grain size is plotted in Fig. 4. The life span of a small grain is short. The points plotted on the right-hand side indicate the surviving grains at the end of simulation. The probability of survival is high for grains with large initial grain sizes. The scatter in life spans was large for larger grains.

Although the life span of a grain cannot be determined by its initial grain size, the mean life span can be predicted from the distribution function of the initial grain size. If we assume that the smallest grains disappear one by one, the number of grains that have disappeared at t is related to the largest grain size of the grains that have disappeared. The mean life span of grains with the initial size R is,[9]

$$\bar{t}_d = \frac{\tau}{(2^{2/3}-1)}\left\{\left[1-\tilde{F}\left(R/\langle R(0)\rangle\right)\right]^{-2/3}-1\right\} \qquad (2)$$

where the cumulative distribution function of grain sizes is

$$\tilde{F}\left(R/\langle R\rangle\right)=\int_0^R F\left(R/\langle R\rangle\right)dR \qquad (3)$$

The distribution function $F(R/\langle R\rangle)$ of grain sizes and the cumulative distribution function in our simulation are shown in Fig. 5. The gray curve in Fig. 4 is the theoretical prediction of equation (2). The observed life spans scattered around the mean life span predicted from the initial distribution function of grain sizes because the curves in Fig. 3 cross each other. However, the theoretical curve represents the statistical features of the simulation results very well.

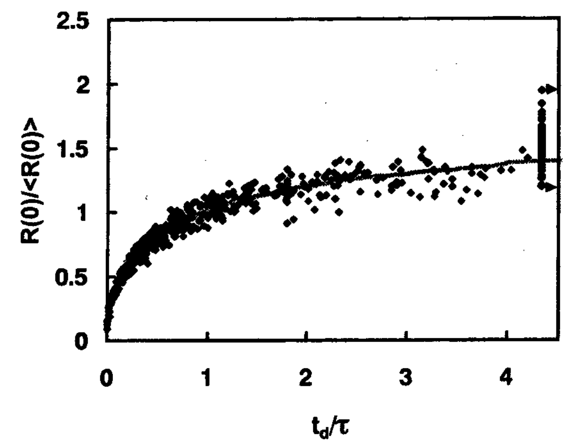

Fig. 4 Plot of life span against initial grain size.

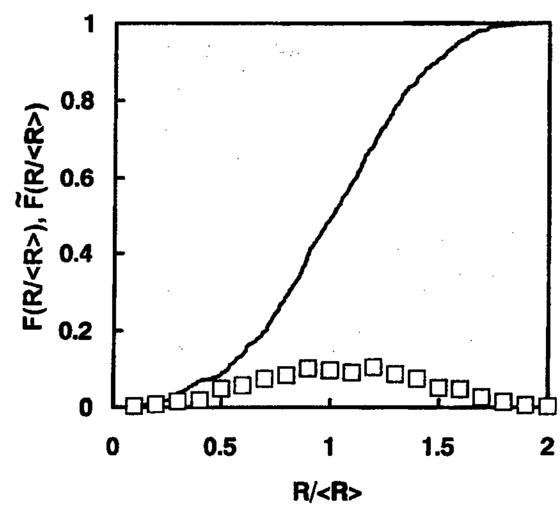

Fig. 5 The distribution function (□) and the cumulative distribution function (solid line) in normal grain grain growth.

4. THREE-DIMENSIONAL MODELS OF GRAIN SWITCHING

The topological transformations of grains occur by grain switching. Rhines and Craig[5] discussed the grain switching in 3D for the first time. In this section we illustrate the elemental processes of grain switching in 3D by using the aggregate of grains as a model.

When the interface between grain A and grain B is encircled with n grains, the interface has n edges. In most cases, a face of grain becomes triangular before it vanishes. If the volumes of grain A and grain B are smaller than those of three encircling grains, the grains A and B shrink as shown in Fig. 6. (upper part). The small triangular interface between A and B vanishes as a result of boundary motion, and then the initially contacted grains A and B separate with each other [(2) → (4)]. We shall call this process as face-*elimination* switching. On the other hand, if the volumes of grain A and grain B are larger than those of three encircling grains, the reversal process proceeds [(4) → (3) → (2)]. The new triangle is created after the coalescence of two vertices. This is face-creation switching.

The interface of grain E, which encircles grains A and B, shows that the interface *a* and *b* loses their common edge and the interface *c* and *d* grain a common edge in face-elimination switching as shown in Fig. 6 (lower part). This change of pattern is similar to that in two-dimensional neighbor switching.

5. TOPOLOGICAL PATH OF ONE GRAIN

In their pioneering paper, Kurtz and Carpay[6] constructed a model of grain growth by considering the transfer rate of a grain between classes divided according to f. The transition of a grain from the state f to $f-1$ occurs by loss of its neighbor grain through face-elimination switching or disappearance of the neighbor. The transition to $f+1$ occurs by the formation of contact with a new grain through a face-creation switching.

Figure 7 shows an example how the grains undergo variation of f with time. Small grain (a) lost its faces as it shrank monotonously. In this way the shrinking small grains lose their faces by face-elimination switching.

Grain (b), which had 16 faces at first, increased both its size and f at the beginning and then started shrinking and losing faces. It disappeared when it became a small tetrahedron (f = 4). The number of faces of grain (c), which had 23 faces at first, fluctuated up and down. The face-creation switching occurred frequently when the grain continued growing. The number of faces decreased occasionally as the neighbor grains disappeared.

All processes in grain growth were analyzed by studying the change of f for all grains in a similar way. The statistical analysis of grain switching will be described in the following sections.

6. TOPOLOGICAL DYNAMICS

We formulate here the process of transition between different states, including the creation and elimination of faces by grain switching in 3D. The total number of disappeared grain at time t is

$$\Delta N = N(0) - N(t) \quad (4)$$

where $N(t)$ is the number of grains. We assume that the

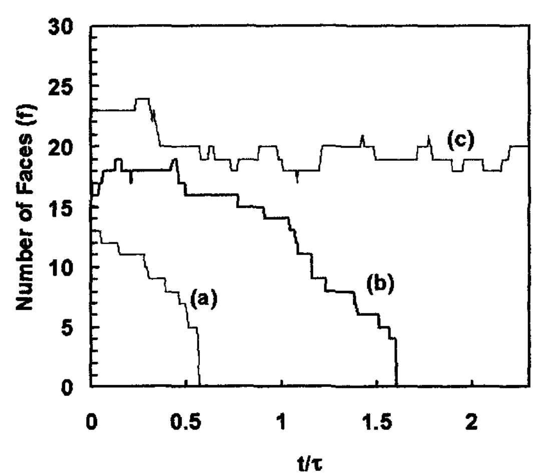

Fig. 7 Variation of individual grain's f with time.

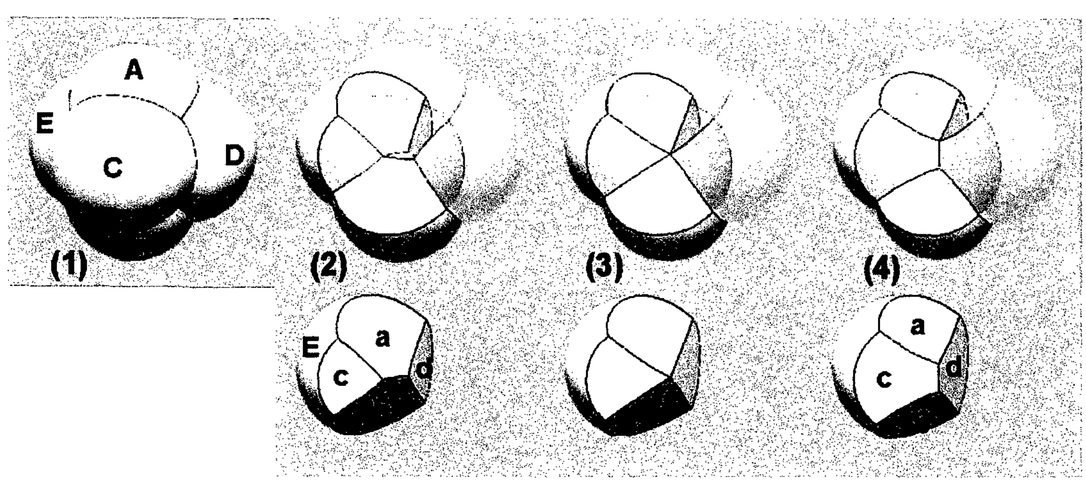

Fig. 6 Five-grain model of grain switching in 3D: (1) surface of five grains; (2) initial stage; (4) final stage. The upper figures show the internal interface. The interfaces among the encircling grains (C, D, E) are shown also. The lower figures show the interfacial patterns of encircling grain E. The faces a, b, c, and d show the interfaces to grains A, B, C and D, respectively.

distribution function of the number of faces $P(f)$ is time-invariant in normal grain growth. The change in the number of f-faced grain is,

$$\Delta N(f) = N(0)P(f) - N(t)P(f) = \Delta N\, P(f) \quad (5)$$

The number of f-faced grain varies by transition between topological states. The number of f-faced grains which undergo face-elimination switching is $\Delta N^{-}(f)$, the number of f-faced grains which undergo face-creation switching is $\Delta N^{+}(f)$, and the number of f-faced grains which disappear is $\Delta N^{*}(f)$. The change in the number of f-faced grains is determined by the difference in the current of grains arriving at and leaving from state f.

$$\Delta N(f) = \Delta N^{-}(f) + \Delta N^{+}(f) + \Delta N^{*}(f) - \Delta N^{-}(f+1) - \Delta N^{+}(f-1) \quad (6)$$

After substitution of Eq. (5) into Eq. (6), Eq. (6) is normalized by ΔN. The equation (6) becomes

$$P(f) = n^{-}(f) + n^{+}(f) + n^{*}(f) - n^{-}(f+1) - n^{+}(f-1) \quad (7)$$

where $n^{-}(f)$, $n^{+}(f)$, $n^{*}(f)$ are the normalized numbers. For example, $n^{-}(f)$ is the number of f-faced grains which undergo face-elimination switching when one grain disappears. The distribution of topological state $P(f)$ is determined by the number of f-faced grains which undergo switching and disappearance.

By analysis of the variation of f for all the grains in 3D simulation, $n^{-}(f)$, $n^{+}(f)$, and $n^{*}(f)$ are plotted as functions of f in Fig. 8.[10] The distribution function $P(f)$ was calculated by substituting the values of $n^{-}(f)$, $n^{+}(f)$, and $n^{*}(f)$ in Fig. 8 into Eq. (7). This distribution function from the dynamic analysis was compared with the statistical distribution function of the steady structure in Fig. 5. Since the statistical distribution function of the steady structure fluctuated slightly with time, it was averaged over time. The agreement between both distribution functions was fairly good.

7. CONCLUSION

The grain boundary motion in three-dimensional grain growth was simulated by the Surface Evolver program. In the normal grain growth, in which the network structure maintained the steady-state structure statistically, the mean life span of grains could be predicted from the distribution function $F(R/\langle R\rangle)$ of grain sizes in the steady state structure. The individual grain increased or decreased its number of faces, f, many times as the grain grew or shrank. The normalized number of transitions from f to $f+1$, that from f to $f-1$, and that of disappearance of grain were determined by the analysis of the simulation results. The observed distribution function $P(f)$ in normal grain growth agreed with the distribution function which was predicted from the balance in topological transformations.

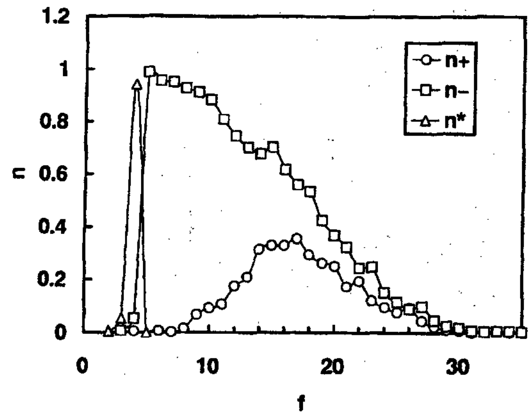

Fig. 8 Normalized number of face-creation switching (n^{+}), face-elimination switching (n^{-}), and grain disappearance (n^{*}) as a function of f.

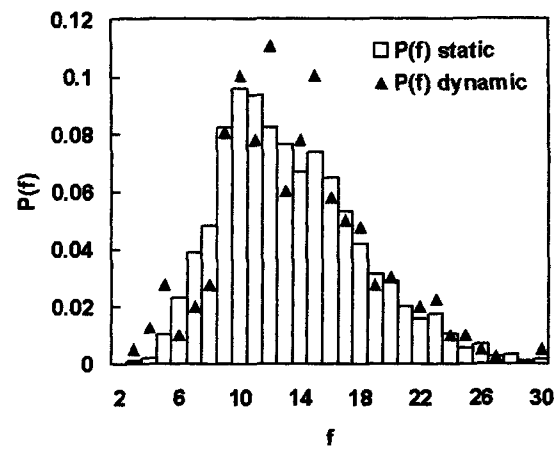

Fig. 9 Distribution function of the number of faces in the steady structure (static) and that from the dynamic analysis.

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