Model Calculation of Grain Growth in a Liquid Matrix

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Abstract

Growth behavior and kinetics of grains in a liquid matrix has been studied by computer simulation for various physical and processing conditions. The kinetics of growing and dissolving grains were considered to follow those of single crystals in a matrix. Depending on the shape of crystals, rounded or faceted, different kinetic equations were adopted for growing grains and an identical equation for dissolving grains. Effects of such critical parameters as step free energy, temperature, and liquid volume fraction were evaluated.

Keywords : Grain Growth, Abnormal Grain Growth, Stagnant Grain Growth, Simulation, Two-Phase System

1. Introduction

Grain growth in a liquid matrix is categorized into two types: normal grain growth (NGG) and abnormal grain growth (AGG). When NGG occurs, the microstructure changes in a uniform way to have a relatively narrow range of grain sizes and shapes, and the grain size distribution is independent of time and hence scales [1-3]. On the other hand, AGG is characterized as rapid growth of a few grains with the consumption of small matrix grains and hence development of a bimodal grain size distribution. With further annealing, however, the large abnormal grains impinge upon each other and grain size distribution reverts to a narrow and unimodal one [4]. In many recent investigations [5-9], it was observed that the grain growth type is closely related to the interface morphology. NGG was observed for rounded (atomically disordered and rough) interfaces and AGG or grain growth inhibition for angular (atomically ordered and faceted) interfaces.

In the present investigation, model calculations for the growth of grains in a liquid matrix have been made using proposed growth kinetics of rounded and faceted grains [3,4,10-12].

2. Kinetic Equations

The driving force for grain growth comes from the difference in size among grains and thus the capillary pressure of the grains, irrespective of their interface structure [12]. The capillary driving force of a grain is expressed as size difference between the grain of critical size r_c which is neither growing nor shrinking. For spherical grains with a rough interface, the rate of growth is linearly proportional to the driving force [1,2]. According to Ardell [3], the rate of continuous grain growth is in the form of

$$\frac{\mathrm{d}r}{\mathrm{d}t} = \frac{\mathrm{A}}{r}\left(\frac{1}{r_c} - \frac{1}{r}\right)(1 + \beta(\phi)\frac{r}{r_c}), \qquad (1)$$

where A is a constant depending on diffusion rate and $\beta(\phi)$ is a function of solid volume fraction (ϕ). For angular grains with faceted interfaces, however, grain growth proceeds with the step growth mechanisms (2DN, spiral growth, etc.) where the growth rate is a non-linear function of the driving force [12]. The growth rate of a faceted grain proceeding by the formation of two-dimensional nuclei is expressed as

$$\frac{\mathrm{d}r}{\mathrm{d}t} = \mathrm{B}\exp\left(-\frac{\mathrm{C}}{1/r_c - 1/r}\right), \qquad (2)$$

where B and C are constants dependent on temperature and materials. If intrinsic atomic steps by screw-dislocations or twins are present on the surface, the growth rate is promoted. On the other hand, continuous kinetics is applicable in the case of dissolution, since each corner acts as a dissolution source without energy barrier [4].

For calculation, appropriate and realistic values were assumed for physical constants except the driving force. The driving force was increased one hundred times higher to shorten the calculation time. The constants A, B, and C were taken to be 4.5×10^{19} , 5.0×10^{26} , and 0.1214 , respectively, as default values.

3. Results and Discussion

Normal Grain Growth. The normal grain growth is represented as a time-invariant form of size distribution with a uniform log-normal like shape. According to the simulation results, the maximum size of grain converges to about $1.5\bar{r}$, and the size distribution maintains a self-similar form as expected from the LSW theory. The average size increases with parabolic or cubic kinetics as the distribution maintains a homogeneous shape during NGG. The normal growth is characterized by a stability in size distribution irrespective of any disturbances; thus to investigate the variation in size distribution is crucial to determine NGG.

Abnormal Grain Growth. The AGG is characterized as a bimodal form of size distribution during grain growth [4,12]. In the microstructure the bimodal distribution means that there are two kinds of grains, abnormally large ones and small others. Fig. 1 shows a simulation result for the growth of grains with an initial Gaussian size distribution of $\bar{r} = 1.0$ m and $s = 0.2$ m. The average grain size increases as a form of stairs (step-wisely) in contrast to continuous growth of the largest grain. The normalized size of the largest grain fluctuates in the range of 2–3.5 with calculation time step (CTS), indicating a variation in the width of normalized size distribution. According to Fig. 1, there are three steps (stairs) for the growth of average sizes, which correspond to three fluctuations in normalized size distribution. The initial distribution becomes broad as crawling a tread of the step, and then converges narrow as the average size climbs up the step (step I). It is repeated after forming a narrow distribution at about 100 CTS (step II) and about 1500 CTS (step III). It implies that abnormal growth behavior appears during each step.

Grain growth proceeds by the mechanism that the group of large grains consume the other group of small grains until the small grains are entirely dissolved. The average grain size does not vary consideravely during AGG, while some of large grains outstretch the size gap from the average size. As the AGG finishes, the average increases abruptly to the mean of the surviving large grains. Moreover, this process can even repeatedly occurs during growth; it can be called as a primary, secondary, tertiary AGG, and so on.

4. Concluding Remarks

Model calculations for faceted grains were conducted using the proposed growth kinetics of NGG and AGG with respect to the grain morphologies. The grains under mixed controlled kinetics showed abnormal grain growth. In some cases, growth behavior varied from AGG to stagnation of growth (SGG) or NGG-like growth (pseudo-NGG) although the growth kinetics was still for AGG. Some typical variables in AGG kinetics such as liquid volume fraction, step free energy, and temperature were taken to examine their effects on grain growth. The increase in liquid volume fraction reduced the rafe of grain growth, showing NGG-like behavior. Increase in temperature or decrease in step free energy lowered the critical driving force for grain growth and induced NGG-like behavior. The variables thus affected critically the grain growth behavior in 2-phase systems.

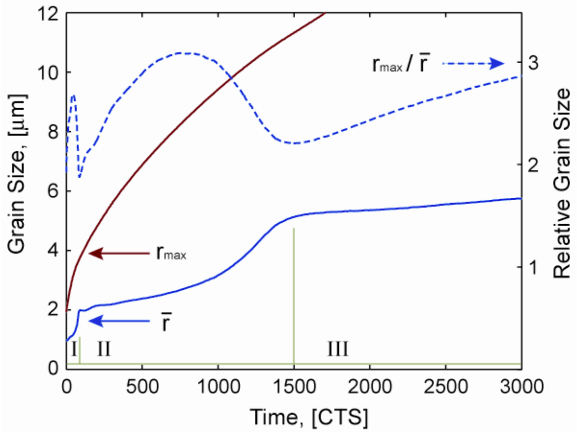

Fig. 1. Variations in the average grain size and the relative size of the largest grain to the average size. The variations consist three groups of growth step.

5. References

1. I.M. Lifshitz and V.V. Slyozov, J. Phys. Chem. Solids, 19, 35(1961).
2. C. Wagner, Z. Elektrochem., 65, 581(1961).
3. A.J. Ardell: Acta metall., 20, 61(1972).
4. P. Wynblatt and N.A. Gjostein, Acta metall., 24, 1165(1976).
5. H.-Y. Lee, J.-S. Kim, N.-M. Hwang and D.-Y. Kim, J. Eur. Ceram. Soc., 20 731(2000).
6. J.B. Koo and D.Y. Yoon, Metall. Mater. Trans. A, 32A, 1911(2001).
7. S.-J.L. Kang and S.-M. Han, MRS Bull., 20, 33(1995).
8. B.-K. Lee, S.-Y. Chung, and S.-J.L. Kang, Acta Mater., 48, 1575(2000).
9. B.-K. Yoon, B.-A. Lee, and S.-J.L. Kang, Acta Mater., 53, 4677(2005).
10. G.S. Rohrer, C.L. Rohrer and W.W. Mullins, J. Am. Ceram. Soc., 85, 675(2002).
11. M.-K. Kang, D.-Y. Kim and N.M. Hwang, J. Eur. Ceram. Soc., 22, 603(2002).
12. S.-J.L. Kang, Sintering: Densification, Grain Growth & Microstructure (Elsevier, Oxford, UK, 2005).