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The Phase Field Method to Simulate the Evolution of Two Phase

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Abstract. A phase field model which contains two phase grain growth in binary alloys was used to study the effect of the same or different initial grain fraction and the different diffusion coefficients on the two-phase grain structure evolution. The results show that the low volume fraction of grain, coarsening power is only controlled by the Ostwald coarsening and through distance interval of grain. The coarsening of the second phase particles in the dominant phase is affected by the number of grain boundaries, grain boundaries will be pinned by the grain, which is affected by the area fraction of the grain. When the diffusion coefficient is large, the diffusion rate is fast, and the grain boundary mobility rate is large.

Introduction

Most of the existing theoretical researches have been focused on the one-way grain growth stage [2, 3] or Ostwald single crystal coarsening [2, 4, 5], or small and cannot grow-up in the secondary phase particles. However, in the two-phase polycrystalline material coupling grain with austenite growth topological evolution attract less attention, part of the reason is the complexity of the topological evolution in the more than two phase in crystal system. In the two-phase polycrystalline solids (second-phase particle+ grain), There are three kinds of interfaces, second-phase particle/ second-phase particle interface, second-phase particle/ grain interface and grain /grain interface. Mullines - Von Neumann's law shows the grain size and its change rate of edge number. Study found that in general the law in the single-phase system is reasonable [6, 7], but whether it is still established in the two-phase system. Chen [1] established in a constant volume diffusion simulation of microstructure evolution in two-phase system model. According to the work of Cahn, Holm [8] et al simulated Monte Carlo in the same system for two phase solid volume fraction of conservation. This section use the phase field model of two-phase grew up, to studied the same initial grain size fractions, different initial grain size fraction, and different impact of the diffusion coefficient on the two phase structure.

Experimental Method

Phase Field Model of Two-phase Growth

Phase field model of two-phase growth, the free energy of the system includes two parts: interfacial energy and chemical free energy [9, 10]:

$$F = \int_V \left[f_{\mathrm{int}\,erf}(\eta_i) + f_{chem}(\eta_i, c) \right] dV \tag{1}$$

$$f_{\text{int}\,erf} = m\left[\sum_{i=1}^{p}\left[\frac{\eta_i^4}{4}-\frac{\eta_i^2}{2}\right]+\gamma\sum_{i=1}^{p}\sum_{j=i+1}^{p}\eta_i^2\eta_j^2+\frac{1}{4}\right]+\frac{\kappa}{2}\sum_{i=1}^{p}(\nabla\eta_i)^2 \tag{2}$$

Chemical energy according to the literature Folch [11]

$$f_{chem} = \frac{1}{2}\left(c-\sum_i A_i(T)\Phi_i\right)^2 \tag{3}$$

$$f_{chem} = \frac{1}{2}\left(c-\phi_\alpha c_{0,\alpha}-\phi_\beta c_{0,\beta}\right)^2 \tag{4}$$

Substitute the total free energy expressions of F:

$$\frac{\partial\eta_i}{\partial t} = -L\left[m\left[\eta_i^3-\eta_i+2\gamma\eta_i\sum_{j=1,\,j\neq i}^{p}\eta_j^2\right]-\kappa\nabla^2\eta_i-\left[c-\phi_\alpha c_{\alpha,0}-\phi_\beta c_{\beta,0}\right]\left[c_{\beta,0}-c_{\alpha,0}\right]\frac{2\eta_i\phi_\beta}{\sum_{j=1}^{p}\eta_j^2}\right] \tag{5}$$

$$\frac{\partial c}{\partial t} = -\nabla\cdot\left[-M(\eta_i)\nabla\frac{\partial f_{chem}}{\partial c}\right] = \nabla\cdot\left[M(\eta_i)\nabla\left[c-\phi_\alpha c_{\alpha,0}-\phi_\beta c_{\beta,0}\right]\right] \tag{6}$$

$$M(\eta_i) = \phi_\alpha D_\alpha + \phi_\beta D_\beta$$

Calculation Method of the Model

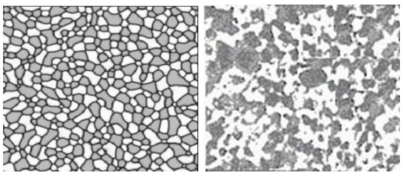
Finite difference is through a linear combination of the function values in a grid point, which is a method to solve the partial differential equation. For the two-dimensional case, set the boundary conditions, to calculate $c_{i,j}^{n+1}$

$$c_{i,j}^{n+1} = c_{i,j}^{n}+\frac{M\Delta t}{\Delta x^2}\left(c_{i+1,j}^{n}-2c_{i,j}^{n}+c_{i-1,j}^{n}\right)+\frac{M\Delta t}{\Delta y^2}\left(c_{i,j+1}^{n}-2c_{i,j}^{n}+c_{i,j-1}^{n}\right) \tag{7}$$

(5) and (6) are used the same method to calculate

Result and Analysis

Fig. 2.1 (a) is the picture of using the established model to simulate the evolution of the second phase particles pinning grain, By comparing with the system containing 50% and 70% second phase particles of grain growth, respectively, to study the effect of area fraction, Fig. 2.1 (b) is SEM photos of synthetic products of Ti-C-Ni, metal ceramic microstructure consists of TiC particles [12] (dark gray) and Ni binding phase (white). It can be seen that the qualitative simulation results are very similar to the experimental results, which shows the reliability of the established model and simulation results.



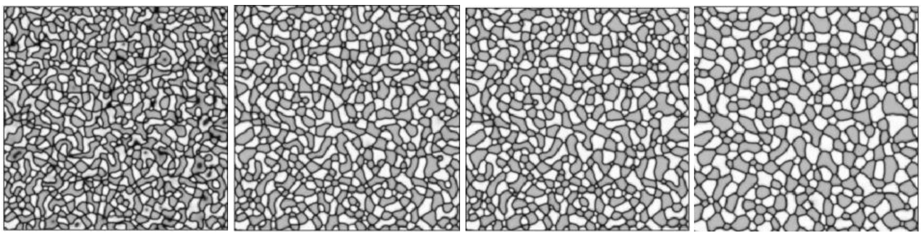
(a) (b)

Fig. 1.1 comparison of model and experimental results

By comparing with 50% and 70% of the second phase particle system of grain growth, respectively, to study the effect of area fraction. Fig.1.2 shows the microstructure evolution of the system containing 50% second phase particle containing 50% grain. the characteristics of microstructure are similar to the system contains 70% second phase particle containing 30% grain in Fig. 1.3 .

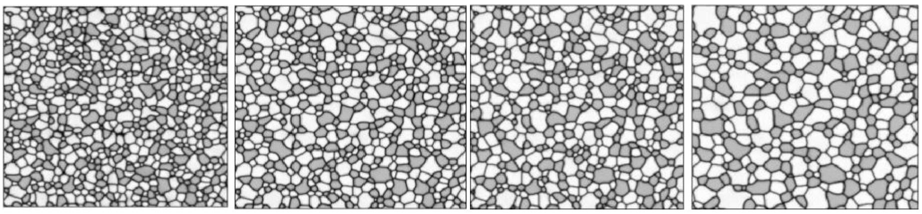
Fig. 1.5 is the radius of the phase under different conditions with the evolution of the time. Fig. 1.5 (a) shows that the growth rate of the radius of the second phase particles containing 50% is about 0.1777, while the growth rate of the radius of the second phase particle containing 70% is about 0.2847. As can be seen in Fig. 1.5 (b), the growth rate of the radius with 50% of the grain is about 0.0851, while the growth rate of the radius with the grain of 30% is about 0.0836. The obvious difference between the second phase particles is that the two phases have different diffusion distances in the coarsening process.

Fig. 1.4 is a system containing 70% second phase particle and 30% grain and both have different diffusion coefficients of the system (D second phase particle =1, D second phase particle =3). From Fig. 1.5, the growth rate of the second phase particle radius before and after is about 0.2847 and 0.2782, respectively and the growth rate of the grain radius before and after is about 0.0836 and 0.1183, respectively. This is due to the large diffusion coefficient, fast diffusion rate and large grain boundary mobility.



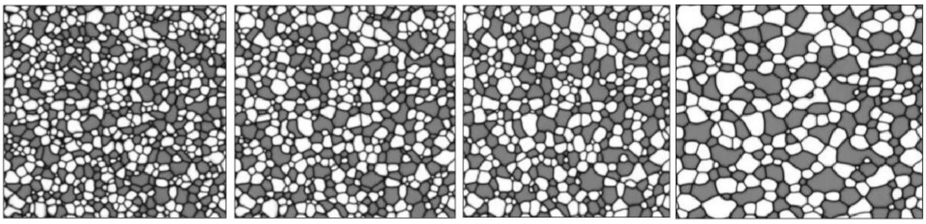
(a) (b) (c) (d)

Fig.1.2 Two phase growth with the same area fraction a) 2000 b) 5000 c) 8000 d) 20000



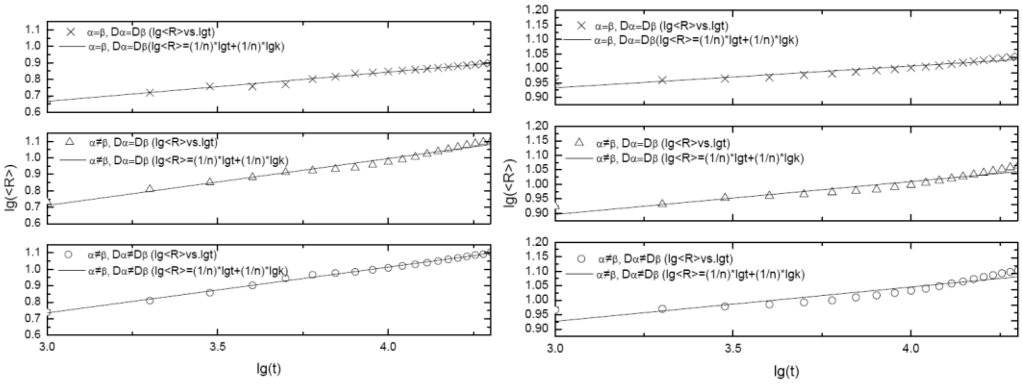
(a) (b) (c) (d)

Fig. 1.3 Two phase growth with different area fractions and same diffusion coefficient a) 2000 b) 5000 c) 8000 d) 20000



(a) (b) (c) (d)

Fig. 1.4 Two phase growth with different area fractions and different diffusion coefficient a) 2000 b) 5000 c) 8000 d) 20000.



(a) (b)

Fig.1.5 (a) Mean radius of second phase particle; (b) The evolution of the mean grain radius and fitting value with time.

Conclusions

The two-phase evolution model was established. In this model, the evolution of grain is described by non conservative phase field variables. Based on the established model, the effects of the same initial grain size, different initial grain size and different diffusion coefficient on the evolution of the two-phase structure were studied. The results show that:

(1)The low volume fraction of grain, coarsening power is only controlled by the Ostwald coarsening and through distance interval of grain.

(2)The coarsening of the second phase particles in the dominant phase is affected by the number of grain boundaries, grain boundaries will be pinned by the grain, which is affected by the area fraction of the grain. When the diffusion coefficient is large, the diffusion rate is fast, and the grain boundary mobility rate is large.

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References

[1] Chen L Q, Fan D. Computer simulation model for coupled grain growth to Al2O3-ZrO2 two-phase systems. J. Am. Ceram. Sot, 1996, 79: 1163~1168.

[2] Fan D, Chen L Q. Computer simulation of grain growth using a continuum field model. Acta mater. 1997 45: 611~622.

[3] Glazier J A, Weaire D J. The Kinetics of Cellular Patterns. Phys., Condens. Matter, 1992, 4: 1867~1894.

[4] Cahn J W, Kobayashi R. Exponentially rapid coarsening and buckling in coher- ently self-stressed thin plates. Acta Metall. Mater., 1995, 43:931~944.

[5] Holm E A, Srolovitz D J, Chan J W. Microstructural evolution in two-dimensional two-phase polycrystals. Acta Metall. Mater., 1993, 41: 1119~1136.

[6] Mullins W W. The statistical self - similarity hypothesis in grain growth and particle coarsening. J. Appl. Phys., 1986, 59: 1341~1349.

[7] Von Neumann J, Modeling of Coarsening and Grain Growth. Metal Interfaces. ASM. Cleveland, OH, 1952: 108.

[8] Holm E A, Srolovitz D J, Cahn J W. Microstructural Evolution in Two- Dimensional Two-Phase Polycrystals. Acta metall. mater., 1993, 41: 1119-1136.

[9] Moelans N, Blanpain B, Wollants P. Quantitative analysis of grain boundary properties in a generalized phase field model for grain growth in anisotropic systems. Physical Review B, 2008, 78: 024113.

[10] Fan D, Chen L Q. Computer Simulation of Grain Growth Using A Continuum Field Model. Acta Materialia, 1997.45: 611 - 622.

[11] Folch R, Plapp M. Quantitative phase-field modeling of two-phase growth. Physical Review E, 2005, 72: 011602.

[12] Huiping Wang, Zhiming Yin. TICN Study on the foundation of the ceramic blade. Cemented carbide, 2003, 3: 133~137(In Chinese).