Transactions of the Materials Research Society of Japan 30[3] 865-868 (2005)

Computer Simulation of Grain Growth in Three Dimensions by Phase Field and Monte Carlo Methods

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Temporal evolution and morphology of grain structure in three dimensions were simulated by the phase field and the Monte Carlo simulations. The average area is found to be proportional to time in the phase field and the Monte Carlo simulations. The scaled grain size and the face number distributions become time-independent in both simulations. The scaled grain size and the face number distributions obtained by the phase field simulation are in good agreement with those by the Monte Carlo method. The nearest neighbor face correlation similar to the Aboav-Weaire relation is observed in simulated grain structures by both methods. The nearest neighbor face correlation for the phase field model is quite similar to that for the Monte Carlo method.

Key words: phase field method, Monte Carlo method, grain growth, topological properties

1. INTRODUCTION

Understanding of kinetics of grain growth is essentially of fundamental importance, not only for its intrinsic interest, but also for its technological significance. Due to the difficulty of incorporating topological features into analytical theories of grain growth directly[1]-[2] there has been increasing interest in the use of computer simulations to study grain growth. Among simulation models, the Monte Carlo and phase field[3]-[7] models are the arguably the most robust and versatile and certainly the most highly developed and widely applied.

Kinetics, grain size and edge distribution results obtained by the phase field model are reported to be in good agreement with those by the Monte Carlo method[6]. Krill and Chen compared kinetics and topological results in grain growth in 3-dimension given by the phase field simulations with results by various simulations[7]. However comparison of the phase field and the Monte Carlo results for similar condition is left unfinished problem.

In this paper, we execute simulation of grain growth in 3-dimensions by the phase field model and the Monte Carlo method with new algorithms in order to prevent large discontinuous changes in grain sizes. The phase field simulation results are compared with those by the Monte Carlo model. Kinetics of normal grain growth and topological results of grain structures such grain size distributions, grain face distributions simulated by both models under similar conditions are compared.

2. MODEL

In the phase field model for the grain growth of polycrystalline materials, microstructure of polycrystalline materials is described by set of orientation field variables, $\eta_1(r),\eta_2(r),....,\eta_Q(r)$, where $\eta_i(r)(i=1,2,....Q)$ are called orientation field variables that distinguish different orientations of grains and Q is the number of possible orientations. Within the grain labeled by η_1, the absolute value for η_1 is 1 while all other η_i for $i \neq 1$ is zero. Across the grain boundaries between the grain η_i, and its neighbor grains, the absolute value of η_i changes continuously from 1 to 0. According to Cahn's and Hilliard's treatment[8], the total free energy functional of an inhomogeneous system is given by

$$F=\int\left[f_0(\eta_1(\vec{r}),\eta_2(\vec{r}),\ldots,\eta_Q(\vec{r}))+\frac{\kappa}{2}\sum_{i=1}^{Q}(\nabla\eta_i(\vec{r}))^2\right]d\vec{r}, \tag{1}$$

where f_0 is the local free energy density which is a function of orientation field variables, η_i, and κ is the gradient energy coefficient. The spatial and temporal evolutions of orientation field variables are described by the time-dependent Ginzburg-Landau equations for nonconserved order parameter.

$$\frac{\partial\eta_i(\vec{r},t)}{\partial t}=-L_i\frac{\delta F}{\delta\eta_i(\vec{r},t)} \quad (i=1,2,\ldots,Q), \tag{2}$$

where L_i are the Onsager's phenomenological coefficients. We used the Ginzburg-Landau type free energy density functional for the present simulation

$$f_0(\eta_1(\vec{r}),\eta_2(\vec{r}),\ldots,\eta_Q(\vec{r}))= \sum_{i=1}^{Q}\left(-\frac{\alpha}{2}\eta_i^2+\frac{\beta}{4}\eta_i^4\right)+\gamma\sum_{i=1}^{Q}\sum_{(j=1,j\neq i)}^{Q}\eta_i^2\eta_j^2, \quad (3)$$

where α, β and γ are phenomenological parameters. The only requirement for f_0 is that it has $2Q$ minima with equal well depth at $(\eta_1,\eta_2,\ldots,\eta_Q)=$ $(1,0,\ldots,0),\ldots,(0,0,\ldots,1)$ $,(-1,0,\ldots,0),\ldots,(0,0,\ldots,-1)$. Therefore, γ has to be greater than $1/2$ when we assume $\alpha=1,\beta=1$. In order to simulate the ideal case of uniform mobility and energy, we set each order parameter equal to its absolute value, effectively restricting the available order parameter space to that containing only the Q degenerate minima of f_0 [5].

For the purpose of simulating the grain growth kinetics, the set of kinetic equation (2) have to be solved numerically by discretizing them in space and time. In this paper, the Laplacian is discretized by the following equation,

$$\nabla^2\eta_i=\frac{1}{(\Delta x)^2}\sum_j(\eta_i-\eta_j), \quad (4)$$

where Δx is the discretizing grid size, *j* represents the first nearest neighbors of site *i*. For discretization with respect to time, we used the simple explicit Euler equation,

$$\eta_i(t+\Delta t),=\eta_i(t)+\frac{d\eta_i(t)}{dt}\times\Delta t, \quad (5)$$

where Δt is the time step for integration.

In the Monte Carlo computer simulation model proposed by Exxon group[3], the microstructure is mapped onto discrete lattice. Kinetics of grain boundary motion can be studied by counting the number of change of the orientation assigned to each lattice (reorientation trial).

In order to prevent the impingement of grain of like orientation too frequently, we proposed a new algorithm[4] in which the grain number is allotted to each lattice point. The procedure of the simulation is as follows:

- A grain number from 1 to the system size, N, is assigned to each lattice point sequentially.
- A number corresponds to an orientation of a grain is randomly assigned to each grain.
- The evolution of microstructure is tracked by the change of orientation on each lattice.
- One lattice site is selected at random
- If the lattice site belongs to grain boundary, then a new orientation is generated.
- If one of the nearest neighbor lattices has the same orientation as the newly selected grain orientation, a re-orientation trial is attempted.
- The change in energy, δE, associated with the change of grain orientation is calculated.
- The re-orientation trial is accepted if δE is less than or equal to zero. If the value δE is greater than zero, the re-orientation is accepted with probability, $W=\exp(-\delta E/k_BT)$.

If the system is N, N re-orientation attempts are referred to 1 Monte Carlo step (MCS).

The interfacial energy is related to the interaction energy between nearest neighbor sites. The interfacial energy is a function of the grain misorientation:

$$E_0=-\sum_{<ij>}M_{s_is_j}, \quad (6)$$

where s_i is a grain orientation which takes a value from 1 to Q. The sum is taken over nearest neighbor sites. The matrix M_{ij} is given by

$$M_{ij}=J(1-\delta_{ij}), \quad (7)$$

where J is a positive constant which sets the scale of grain boundary and δ_{ij} is the Kronecker's delta.

3. RESULT AND DISCUSSION

Phase field simulation were performed on 3-dimentional lattice with size of $N=180^3$ and the number of orientations of Q=60. All simulations were performed on the lattice systems with periodic boundary condition. The lattice step size Δx was set to be 2.0 and a time step Δt of 0.05 was employed. We assumed the following numerical value for the parameters in the kinetic equations: $\alpha=1.0,\beta=1.0,\gamma=1.0$, and $\kappa=2.0$, and $L_i=1.0$ for *i*=1 to Q. All simulations were performed on the lattice systems with periodic boundary condition. In order to prevent large discontinuous change in grain size by coarsening of grains having the same orientation, the nucleation sites were situated so that grains with same orientation are located at distance of a pre-set minimum distance in each phase field.

To visualize the microstructure evolution using the orientation field variables, the following function was defined:

$$\varphi(\vec{r})=\sum_{i=1}^{Q}\eta_i^2(\vec{r}), \quad (8)$$

which takes on a value of unity within individual grains and smaller values in the core regeions of the boundaries [5],[7]. If we map the value of φ to a specturm of graylevels, then we obtain images like that of Fig.1, in which the grain boundaries appears as dark regions separating individual grains. The topological properties of the latter - such as number of side, cross-sectional area, or volume - can evaluated directly by choosing a threshold value in φ to establish the boundary positions. In this manner, it is possible to quantify the

evolution of local and averaged topological grain properties during coarsening. The average grain area versus time steps for the 180^3 system is shown in Fig.2. Excluding the early stage, the average area is found to be proportional to time. In order to get the grain size and grain face distributions 6 runs of simulation were performed.

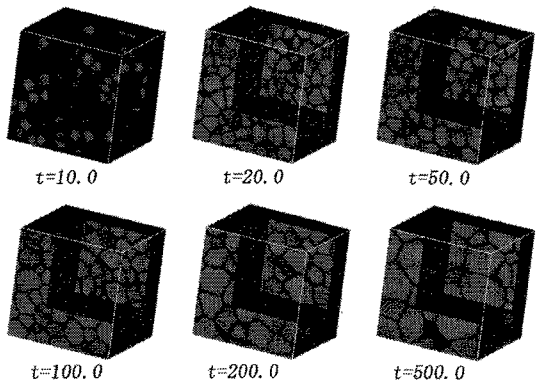

Fig.1. Microstructural evolution in 180x180x180 cells simulated by the phase field model

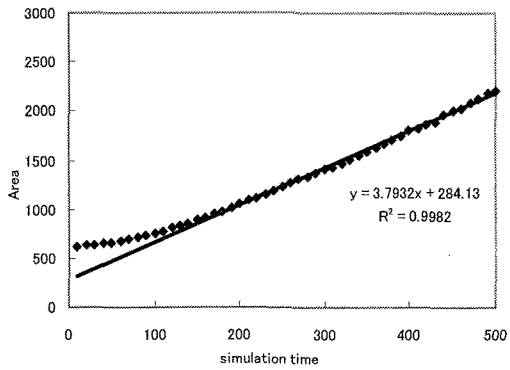

Fig.2. Average area versus time simulated by the phase field model

Monte Carlo simulations were performed on 3-dimentional fcc like lattice with size of $N = 128^3$. All simulations were performed on the lattice systems with periodic boundary condition. The number of orientation, Q is chosen to be $Q = 32$. The value J/k_BT is set to 2.0. As an initial microstructure, an orientation between 1 to Q was assigned to each grain at random. Figure 3 shows an example of temporal evolution of microstructure simulated by Monte Carlo method. The formation of grain structure is detected in the early stage of the simulation. The coarsening of large grains by absorbing small grain is observed. The uniform and isotropic grain structure is obtained. The average area A, against time t, is shown in Fig.4. The average area is found to be proportional to time.

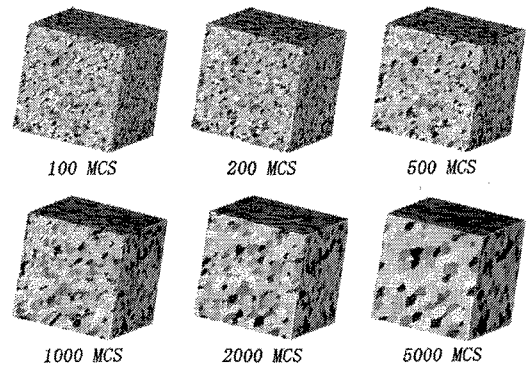

Fig.3 Microstructural evolution in 128x128x128 cells simulated by the Monte Carlo method

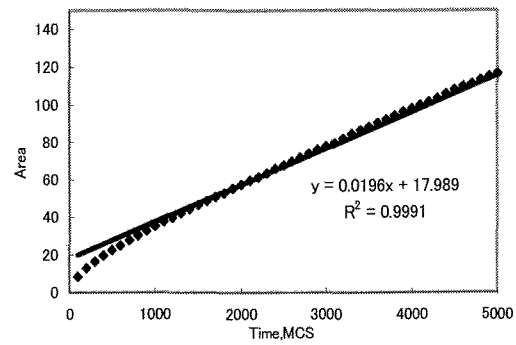

Fig.4. Average area versus time simulated by the Monte Carlo method

Figure 5 shows the scaled normalized grain size distribution obtained by phase field model is compared with that given by Monte Carlo simulation. For comparison the steady state distribution predicted by Hillert[2] is plotted. It is shown that the scale grain size distribution is quite good agreement with Monte Carlo grain size distribution. Krill and Chen pointed out that the distribution found by Monte Carlo method by one of the authors is significantly narrower than that found by the other method. The present results by phase field and Monte Carlo models are in good agreement with this distribution. Present distribution fall off to zero quite faster at large diameter. The reason of this behavior is due to prevention of coarsening of grain with same orientation.

The grain face distribution by phase field model is in good agreement with that by Monte Carlo method as shown in Fig, 6. Again, there is good agreement, well within the statistical error. The average numbers of faces for grain structures by the phase field model and by the Monte Carlo simulation are 13.7 and 13.9, respectively. Overall, there is excellent agreement between the phase field and the Monte Carlo

simulations.

The relationship between the average number of faces of grain adjacent to an N-faced grain, $m(N_f)$ and the face number in grains, N_f obtained by the phase field model and that by the Monte Carlo simulation is shown in Fig.7. It is shown that Aboav-Weaire type relations [9,10] obtained by both simulations are quite similar.

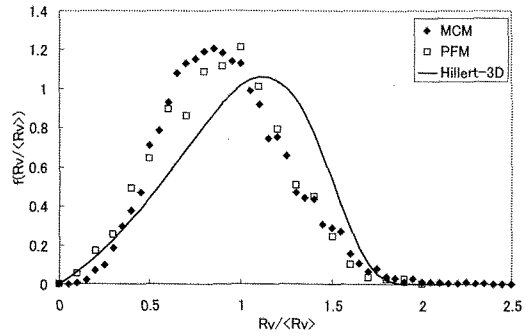

Fig.5 Comparison of the scaled grain size distribution function simulated by the phase field model with that by the Monte Carlo method

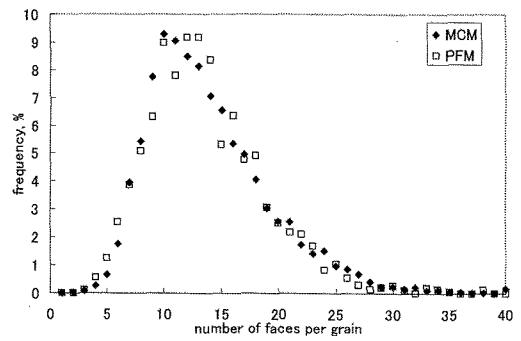

Fig.6 Comparison of the face number distribution function simulated by the phase field model with that by the Monte Carlo method

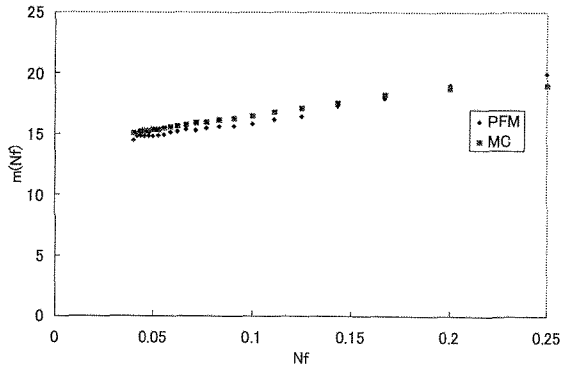

Fig.7 Comparison of the nearest neighbor face number correlation simulated by the phase field model with that by the Monte Carlo method

4. SUMMARY

(1) Excluding the initial stage the average area is found to be proportional to time in the phase field and the Monte Carlo simulations. The scaled grain size and the face number distributions become time-independent in both simulations.

(2) The scaled grain size and the face number distributions obtained by the phase field simulation are in good agreement with those by the Monte Carlo method. The nearest neighbor face correlation similar to the Aboav-Weaire relation is observed in simulated grain structures by both methods. The nearest neighbor face correlation for the phase field model is quite similar to that for the Monte Carlo method.

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(Received December 23, 2004; Accepted April 28, 2005)