

Computer Simulation of Grain Growth in Three Dimensions by the Phase Field Model and the Monte Carlo Method

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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. In order to prevent impingement of grain of like orientation, a new algorithm was adopted for both simulations. 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. 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. The Allen–Cahn type equation for the phase field simulation can be derived from the master equation of the Monte Carlo Model.

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1. Introduction

Control of microstructure of a polycrystalline material is one of most important factors that determines properties of the materials such as strength, toughness, electrical conductivity and magnetic susceptibility. Computer simulation models based classical thermodynamics and phase transformation theory have been successfully applied to prediction of microstructural evolutions in materials. However, inhomogeneity in microstructure in materials affects mechanical properties such as impact and corrosive properties. The incorporation of factors which characterize spatial and temporal distributions of microstructure is essentially important.

Understanding of kinetics of grain growth is essentially of fundamental importance, not only for its intrinsic interest, but also for its technological significance.^{1,2)} Due to the difficulty of incorporating topological features into analytical theories of grain growth directly^{3–5)} there has been increasing interest in the use of computer simulations to study grain growth. A variety of models have been proposed during the past decades.^{6–14)} Among these models, the Potts and phase field^{11–14)} are the arguably the most robust and versatile and certainly the most highly developed and widely applied.

The Potts model was first proposed by Potts as a generalization of the Ising model for simulating the critical transitions in magnetic materials with more than two degenerate states.^{6–12)} The Potts model treats the evolution of a nonequilibrium, discrete ensemble which populates a regular lattice. The ensemble can represent the composition and structure of materials. In the early 1980s, when computational facilities became sufficiently inexpensive to make it readily accessible, the Potts model was applied to coarsening phenomena, namely grain growth^{11,12)} and soap froth coarsening.¹⁵⁾ Since then, it has been modified to study many microstructural evolution problems including normal¹⁶⁾ and abnormal grain growth,¹⁷⁾ recrystallization,¹⁸⁾ coarsening in two phase system, Ostwald ripening,¹⁹⁾ and

microstructural evolution in thermal gradient.²⁰⁾

Phase field model is based on the Onsager's linear irreversible thermodynamics.²¹⁾ It has been extensively applied to simulation of temporal and spatial evolution of microstructure. This model represents temporal evolutions in the chemical, crystallographic and structural fields. In this model phase boundaries are assumed to be diffuse with finite thickness. The free energy density functional is defined to have continuous local order parameters. Time history of the whole microstructure is calculated by the temporal evolutions of local order parameters. In this paper, we will deal with single-phase polycrystalline materials. The polycrystalline microstructure is described by a set of orientation field variables; $\eta_1(r), \eta_2(r), \dots, \eta_Q(r)$. The interfacial energy of a material is related to parameters in fundamental equations of the phase field models, *i.e.* the gradient energy coefficient, κ , and a parameter in a local free energy function, γ .

One of the serious problem in grain growth simulation is that large discontinuous changes in the area of individual grain can occur when one grain meets and coalesces with another grain having the same orientation. In order to prevent the impingement of grain of like orientation too frequently, the large number of Q , the total number of grain orientations, is chosen. The growth rate is inversely proportional to Q . To overcome the above problems, we proposed new algorithm²²⁾ in which the grain number is allotted to each lattice point in the Monte Carlo simulation. In the phase field simulation initial structure is prepared in the way that grains have the same orientation are situated at a certain distance.

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.¹⁹⁾ 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.²³⁾ 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. With these results, we will discuss the interrelations of the master equation of the Monte Carlo simulation and continuum thermodynamic equations of interface motion.

2. Model Description

2.1 Phase field 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, $\eta_1(r), \eta_2(r), \dots, \eta_Q(r)$, where $\eta_i(r)$ ($i = 1, 2, \dots, Q$) are called orientation field variables that distinguish different orientations of grains and Q is the number of possible orientations. A schematic microstructure represented by orientation fields in 2-D is shown in Fig. 1. 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_1 , and its neighbor grains, the absolute value of η_1 changes continuously from 1 to 0. The schematic profiles of η_1 and η_2 across the grain boundary between the grain η_1 and η_2 are shown in Fig. 2. All other field variables this grain boundary having zero values. According to Cahn's and Hilliard's treatment,²⁴⁾ the total free energy functional of an inhomogeneous system is given by

$$F = \int \left[f_0(\eta_1(r), \eta_2(r), \dots, \eta_Q(r)) + \sum_{i=1}^Q \frac{\kappa_i}{2} (\nabla \eta_i(r))^2 \right] d^3r, \quad (1)$$

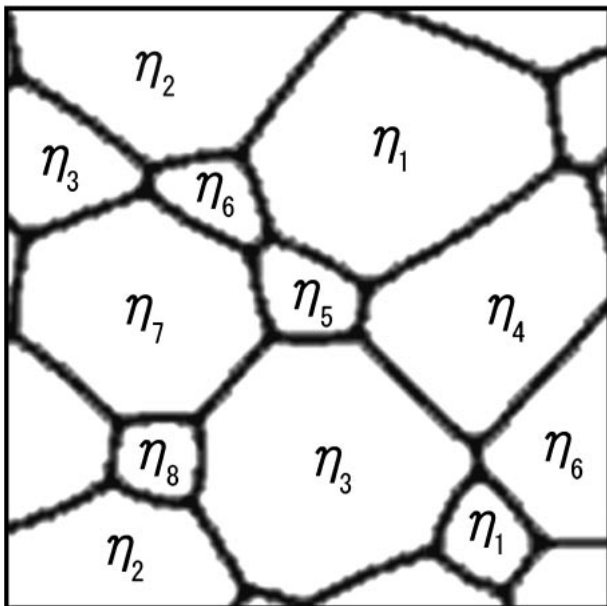


Fig. 1 Schematic illustration of microstructure described using orientation variables.

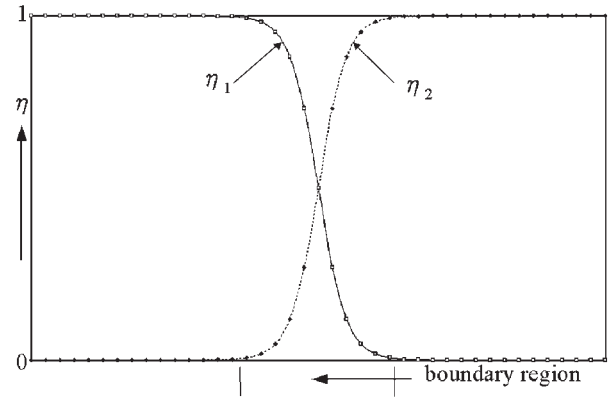


Fig. 2 Schematic illustration of microstructure described using orientation variables.

where f_0 is the local free energy density which is a function of orientation field variables, $\eta_i(r)$, and κ_i 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.²⁵⁾

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

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

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

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 $(\eta_1, \eta_2, \dots, \eta_Q) = (1, 0, \dots, 0), (0, 1, \dots, 0), \dots, (0, 0, \dots, 1), (-1, 0, \dots, 0), (0, -1, \dots, 0), \dots, (0, 0, \dots, -1)$. Therefore, γ has to be greater than $\beta/2$ 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 .¹³⁾

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

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

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,

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

where Δt is the time step for integration.

2.2 Monte Carlo simulation algorithm

In the Monte Carlo computer simulation model proposed by Exxon group,^{11,12)} the microstructure is mapped onto discrete lattice. To each lattice is assigned a number that corresponds to an orientation of the grain. The 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 algorithm²²⁾ 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, $W = \exp(-\delta E/k_B T)$.

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

The change of interfacial energy accompanying re-orientation is a driving force of interface migration. The interfacial energy is related to the interaction energy between nearest neighbor sites. The interfacial energy is a function of the grain misorientation:

$$E_0 = - \sum_{\langle ij \rangle} M_{s_i s_j}, \quad (6)$$

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. Numerical Simulation Result and Discussion

3.1 Phase field simulation

Simulation were performed on 3-dimensional lattice with size of $N = 180^3$ and the number of orientations of $Q = 60$. The lattice step size Δx was set to be 2.0 and a time step Δt of 0.05 was employed. 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.

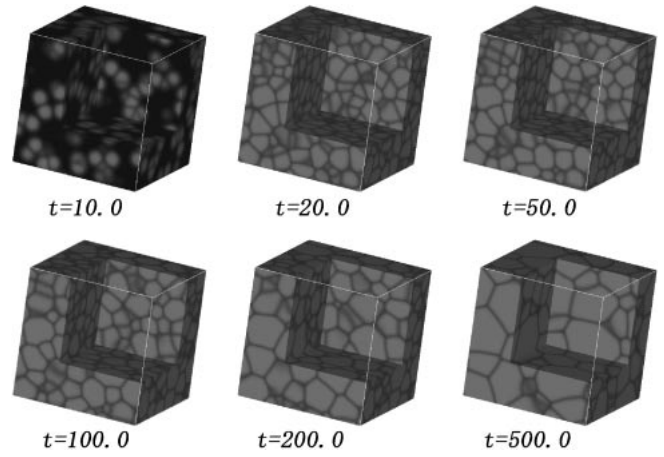


Fig. 3 Microstructural evolution in $180 \times 180 \times 180$ cells simulated by the phase field model.

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

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

which takes on a value of unity within individual grains and smaller values in the core regions of the boundaries.^{13,14)} If we map the value of φ to a spectrum of graylevels, then we obtain images like that of Fig. 3, 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 be 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. 4. 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. The scaled grain size distribution is shown in Fig. 5. After a short transient time, the grain size distribution becomes time-independent. The distributions of the number of face, N_f , for individual grains of the simulated microstructures is shown in Fig. 6. The distribution becomes time-invariant at the longer time. The frequency increase

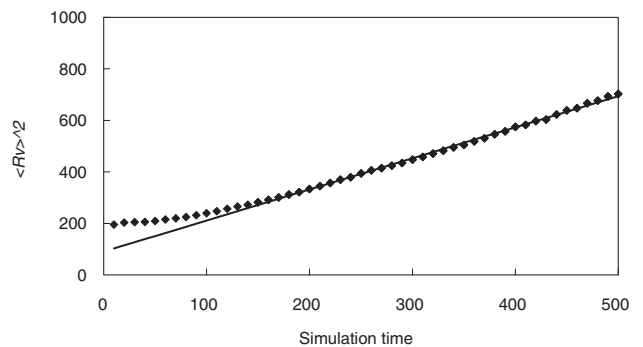


Fig. 4 Average area versus time simulated by the phase field model.

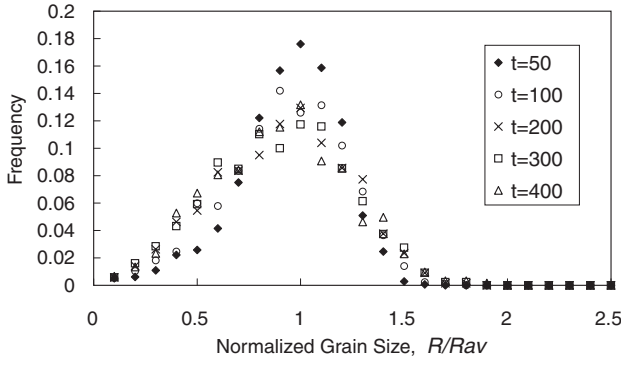


Fig. 5 Variation in the scaled grain size distribution function with time simulated by the phase field model.

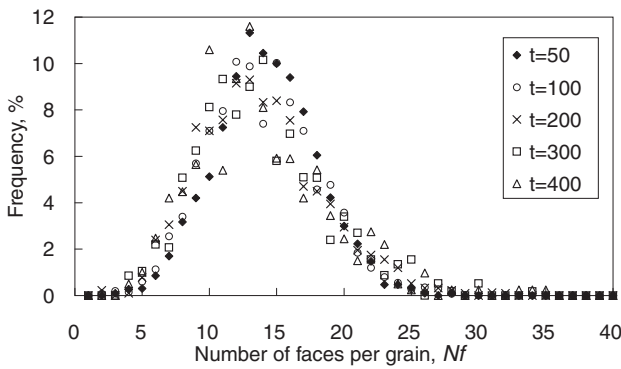


Fig. 6 Variation in the face number distribution function with time simulated by the phase field model.

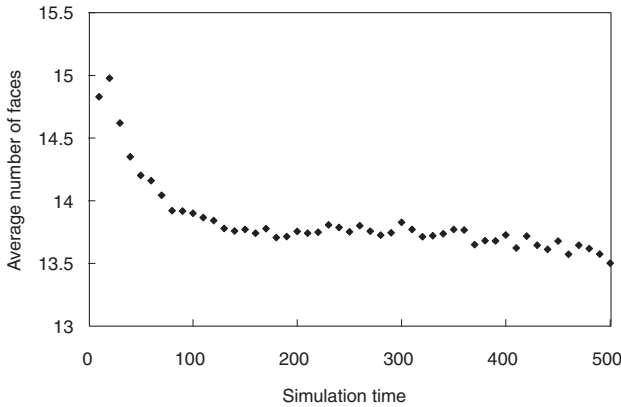


Fig. 7 Variation in the average face number with time simulated by the phase field model.

rapidly for a small number of faces and peaks at a value of 12 to 14 and decays quickly. Figure 7 shows variation in the average face number with time. The initial value of 15.0 decreases with time and approaches a constant value of about 13.7.

The relationship between the average number of faces of grain adjacent to an N_f -faced grain, $m(N_f)$, and the face number in grains, N_f , is shown in Fig. 8. The linear relation equal similar to Aboav–Weaire relations^{26,27} is obtained between $m(N_f)$ and N_f as;

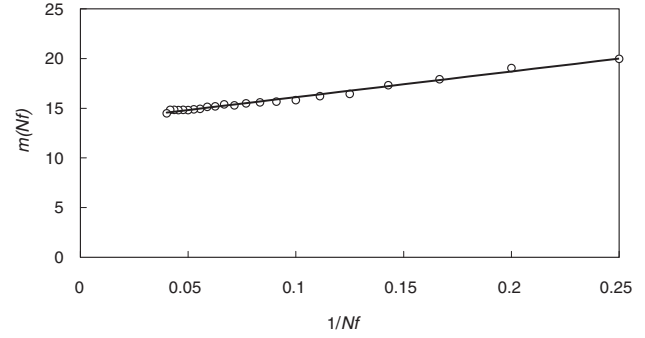


Fig. 8 Relation between the average number of faces of neighbor of N_f -face grain, $m(N_f)$ and the face number, N_f simulated by the phase field model.

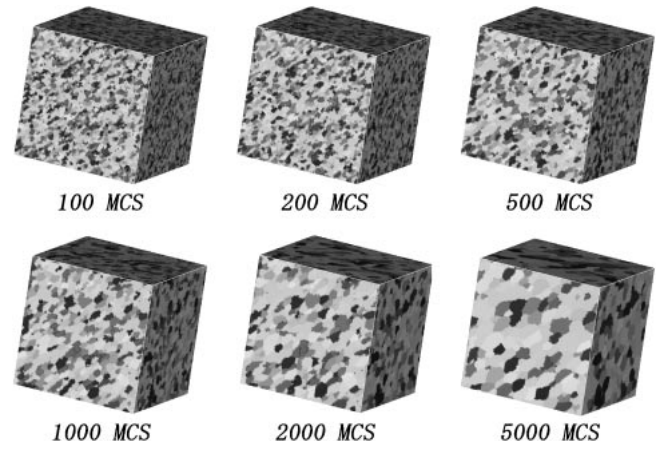


Fig. 9 Microstructural evolution in $64 \times 64 \times 64$ cells simulated by the Monte Carlo method.

$$m(N_f) = -13.5 + 25.9/N_f. \quad (9)$$

3.2 Monte Carlo simulation

Simulation were performed on 3-dimensional 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 $Q = 32$. In the following simulation, the value $J/k_B T$ is set to 2.0. As an initial microstructure, an orientation between 1 to Q was assigned to each grain at random. Figure 9 shows an example of temporal evolution of microstructure. 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. 10. The average area is found to be proportional to time. The average grain size, R_{av} , is described as a power-law kinetics:

$$R_{av} \propto Bt^{0.5}, \quad (10)$$

where B is a constant which is temperature dependent. The exponent is the same as that by analytical model by Hillert.³⁾

Figure 11 shows the variation of the scaled grain size distribution function for the simulated microstructures. The distribution function becomes time-invariant at the longer time. The distributions of the number of face, N_f , for

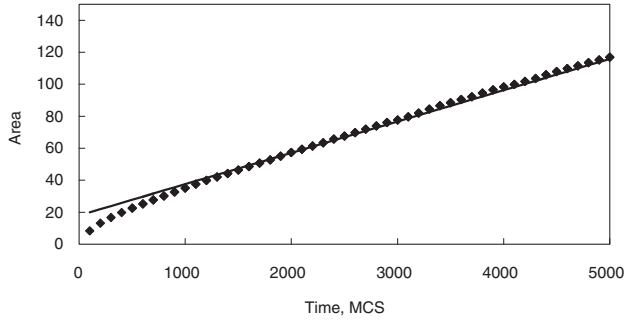


Fig. 10 Average area versus time simulated by the Monte Carlo method.

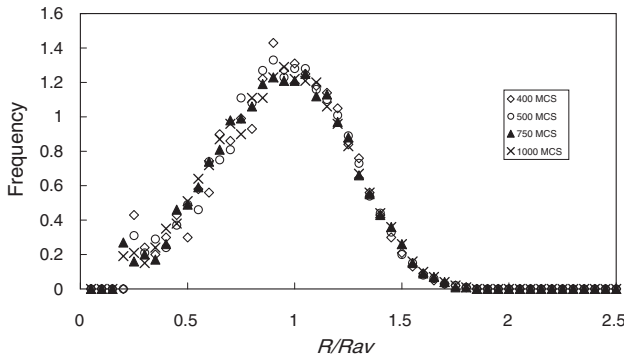


Fig. 11 Variation in the scaled grain size distribution function with time by the Monte Carlo method.

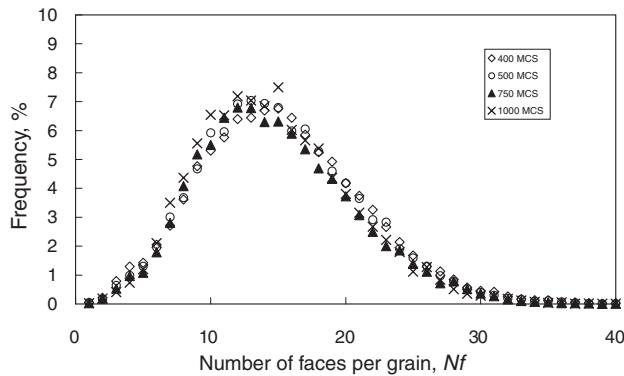


Fig. 12 Variation in the face number distribution function with time by the Monte Carlo method.

individual grains of the simulated microstructures is shown in Fig. 12. The distribution becomes time-invariant at the longer time. The frequency increase rapidly for a small number of faces and peaks at a value of 12 to 14 and decays quickly.

The relationship between the average number of faces of grain adjacent to an N_f -faced grain, $m(N_f)$, and the face number in grains, N_f , is shown in Fig. 13. The linear relation equal is obtained between $m(N_f)$ and N_f as;

$$m(N_f) = -14.0 + 23.6/N_f. \quad (11)$$

3.3 Comparison of phase field and Monte Carlo results

Figure 14 shows the scaled normalized grain size distribution obtained by phase field model is compared with that

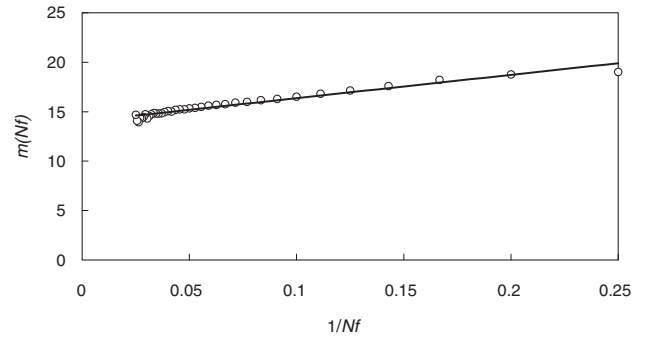


Fig. 13 Relation between the average number of faces of neighbor of N_f -face grain, $m(N_f)$ and the face number, N_f by the Monte Carlo method.

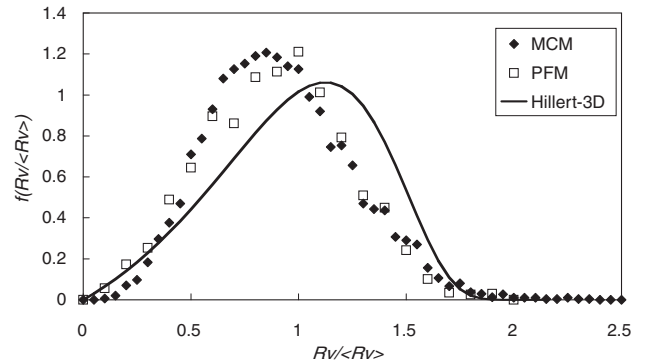


Fig. 14 Comparison of the scaled grain size distribution function simulated by the phase field model with that by the Monte Carlo method.

given by Monte Carlo simulation. For comparison the steady state distribution predicted by Hillert³⁾ 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. 15. 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.

Figure 16 shows comparison of $m(N_f)$ versus N_f relation obtained by the phase field model and that by the Monte Carlo simulation. It is shown that relations by both simulations are quite similar.

We find that topological results obtained by the phase field model are in good agreement with those by the Monte Carlo method. However it should be noted that the grain size and grain face distributions are affected by the J/kT value. Effect of the J/kT value on topology of grain structure is left as a future work.

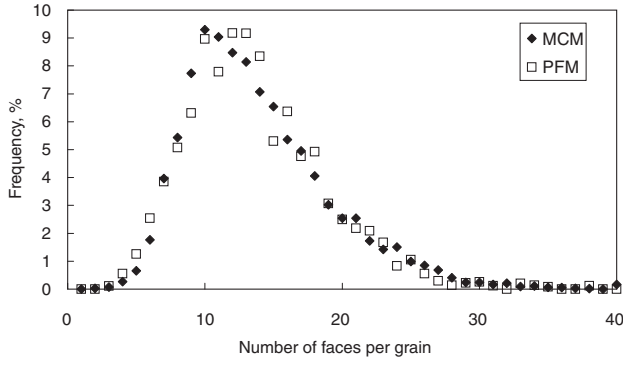


Fig. 15 Comparison of the face number distribution function simulated by the phase field model with that by the Monte Carlo method.

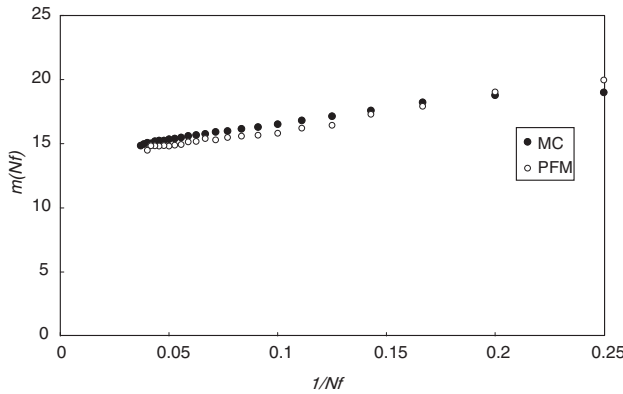


Fig. 16 Comparison of the nearest neighbor face number correlation simulated by the phase field model with that by the Monte Carlo method.

3.4 Interrelation of the phase field and the Monte Carlo models

In previous section we found that grain size and grain face distributions given by phase field model were in good agreement with those by Monte Carlo method. So we try to interrelate a master equation of Monte Carlo method to a continuum model.

In the Monte Carlo algorithm a sequence of successive configurations are generated with help of (pseudo) random numbers and a suitably chosen transition probability. An efficient sampling technique to sample configurations from phase space was given by Metropolis.²⁸⁾ In the Metropolis algorithm the successive configurations are not chosen independently but rather via a Markov chain. A possibility is to use a Markov process which generates a configuration $\{s'\}$ from the knowledge of a configuration $\{s\}$. Let $W(\{s\}, \{s'\})$ be the conditional probability to select $\{s'\}$ stating from $\{s\}$, thus defining the Markov process. The successive states are generated with a particular transition probability $W(\{s\}, \{s'\})$, which is chosen so that in the limit of a large number of configurations the probability $P(\{s\})$ tends toward the equilibrium distribution:

$$P_{\text{eq}} = \exp[-E(\{s\})/k_B T]/Z, \quad (12)$$

where E is an internal energy function, k_B is the Boltzmann constant, T is the temperature and Z is a canonical partition function. A sufficient condition to ensure this is the principle of detailed balance:

$$P_{\text{eq}}(\{s\})W_j(\{s\}, \{s'\}) = P_{\text{eq}}(\{s'\})W_j(\{s'\}, \{s\}). \quad (13)$$

The Monte Carlo algorithm may be interpreted via a master equation as describing a dynamical model with stochastic process.²⁹⁾ It satisfies the Markovian master equation as:

$$\frac{\partial P(\{s\}, t)}{\partial t} = \sum_{\{s'\}} P(\{s'\}, t) W(\{s'\}, \{s\}) - \sum_{\{s'\}} P(\{s\}, t) W(\{s\}, \{s'\}). \quad (14)$$

The master equation is reduced to a differential equation of the Fokker-Planck type.³⁰⁾ It will be helpful conceptually to divide the alloy into microregions, each containing ν sites. We define the average value s_α . We can choose the transition mechanism so that a particular s_α changes by $+\epsilon$ (the order parameter s is non-conserved). This transition mechanism can be expressed mathematically by writing W in the form:

$$W(\{s\}, \{s'\}) = \sum_{\alpha} \prod_{\beta \neq \alpha} \delta(s'_\beta - s_\beta) \times \int_{-\infty}^{\infty} R(\{s'\}, \{s\}) \delta(s'_\alpha - s_\alpha - \epsilon) d\epsilon. \quad (15)$$

The sum over α assures that the thermal mechanism acts uniformly on all the sites in the system. The transition rate $R(\{s\}, \{s'\})$ can be written as

$$R(\{s'\}, \{s\}) = \exp\left(-\frac{F\{s'\} - F\{s\}}{2k_B T}\right) \Omega(\{s'\}, \{s\}), \quad (16)$$

where $\Omega(\{s\}, \{s'\})$ is a symmetric function in the initial and the final state, $\{s\}$ and $\{s'\}$, and $F\{s\}$ is a coarse-grained free energy given by

$$F\{s\} = E\{s\} - k_B T \ln W\{s\}, \quad (17)$$

where $W\{s\}$ is the number of configuration consistent with a specific choice of average variable s_α . Note that the introduction of the factor $W\{s\}$ for computation of the transition rate required by the use of average variables s_α , has justified replacing the energies by free energies in eq. (17). Because of the restricted class of transitions ($\{s\}$ to $\{s'\}$) which is permitted by the form eq. (16), Ω is a function only of ϵ , change in s . Since the coarse-grain cell contains a large number of sites, the change in s corresponding to a single transition is small. Thus $\Omega(\epsilon)$ must be sharply peaked around $\epsilon = 0$. For convenience, we introduce the jump rate, Γ , though

$$\int_{-\infty}^{\infty} \epsilon^2 \Omega(\epsilon) d\epsilon \equiv \nu^{-1} \Gamma, \quad (18)$$

where ν is the number of sites in the cell. Thus Γ is the only adjustable phenomenological parameter. By defining the probability current vector by

$$J_\alpha = \frac{\Gamma}{2\nu} \left[\frac{1}{k_B T} \frac{\partial F}{\partial s_\alpha} P + \frac{\partial P}{\partial s_\alpha} \right], \quad (19)$$

we can rewrite the master equation in the form of the Fokker-Planck equation as

$$\frac{\partial P\{s\}}{\partial t} = - \sum_{\alpha} \frac{\partial J_\alpha}{\partial s_\alpha}. \quad (20)$$

In a continuum representation where $\vec{r}$ is the position corresponding to site α the summation on the cells become integral over the space according to

$$\sum_{\alpha} \dots = \frac{1}{v a^d} \int d\vec{r} \dots \quad (21)$$

It will be also convenient to introduce the functional derivative notation

$$\frac{\partial}{\partial s_{\alpha}} = v a^d \frac{\delta}{\delta s(\vec{r})}, \quad (22)$$

where d is the dimensionality of the model and a is the lattice constant. A Langevin type equation is simply the first moment of eq. (20). To see this we multiply eq. (20) by s_{α} and integrate over all the s 's. The result is

$$\begin{aligned} \frac{\partial \bar{s}_{\alpha}}{\partial t} &= \int \delta s \left(\frac{\partial P}{\partial t} \right) s_{\alpha} = \int J_{\alpha} \{s\} \delta s \\ &= - \left(\frac{\Gamma}{2 v k_B T} \right) \int \delta s \left(\frac{\partial F}{\partial s_{\alpha}} \right) P. \end{aligned} \quad (23)$$

In the continuum representation, eq. (23) becomes

$$\frac{\partial \bar{s}_{\alpha}}{\partial t} = - \left(\frac{\Gamma a^d}{2 k_B T} \right) \left\langle \frac{\partial F}{\partial s_{\alpha}} \right\rangle, \quad (24)$$

where angular brackets denote the statistical average. Let us suppose that P is a sharply peaked function of the s in the neighborhood of $\{s\} = \{\bar{s}\}$, so that average with respect to P of any function of $\{s\}$ is well approximated by the same function of $\{\bar{s}\}$. Then eq. (24) becomes

$$\frac{\partial \bar{s}_{\alpha}}{\partial t} = - \left(\frac{\Gamma a^d}{2 k_B T} \right) \frac{\delta \bar{F}}{\delta \bar{s}_{\alpha}}. \quad (25)$$

Thus we obtain the time-dependent Ginzburg–Landau equation for nonconserved order parameter from the master equation of the Monte Carlo method.

4. Summary

Temporal evolution and morphology of grain structure in three dimensions were simulated by the phase field and the Monte Carlo simulations. In order to prevent impingement of grain of like orientation, a new algorithm was adopted for both simulations.

The following results are obtained.

- (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.
- (3) Interrelation between the phase field model and the Monte Carlo method is discussed.

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