Monte Carlo Simulation for the Evolution of Microstructure during Thermal Cycling†

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Abstract

The present paper deals with the development of modules for the simulation of microstructure changes during thermal cycling indicating a combination of precipitation and dissolution of precipitates. A Monte Carlo simulation technique based on the Potts model was utilized. Nucleation sites of precipitates were randomly generated both on grain boundaries and in grains. The ratio of the growth rates of the two different precipitates was revealed as an important factor that determines the process of microstructure evolution. Thermal cycling resulted in grain refinement by the division of phase-boundaries that were formed by the precipitation. The refined microstructure after thermal cycling was similar to that observed in a Cu-Be alloy which shows discontinuous precipitation.

KEY WORDS: (grain growth) (Potts model) (precipitation) (boundary migration) (thermal cycling) (Monte Carlo simulation)

1. Introduction

Microstructure in polycrystalline materials is described by shape and size of grains, grain orientation or texture, grain boundary character distribution and kind of phases. Welding changes both the fractions and the distributions of these microstructure parameters drastically since it gives both base metal and weld metal complicated heat treatments consisting of rapid heating and cooling. Thermal history due to welding brings about phase transformation during cooling and reversed transformation during re-heating in the case of multi-layered welding.

Mechanical properties of joints having complicated microstructures depend on the thermal history. Thus, in order to design and fabricate sound interfaces, the microstructure parameters should be optimized for given conditions of heat treatment. In addition to many experimental techniques of microstructure observation at elevated temperature, computer simulation is also a useful method to classify the evolution process of microstructure systematically.

The present work aims to develop basic modules for the simulation of microstructure evolution during thermal cycling to promote grain growth, precipitation, dissolution and so on.

2. Calculation method

2.1 Microstructure model and nucleation sites

Polycrystalline structure is well described by the "Potts model" which is shown in **Fig.1** for a two-dimensional structure[2]. This model was first developed for grain growth simulation of single-phase microstructures, but it is also adopted for multi-phase structures such as precipitated ones.

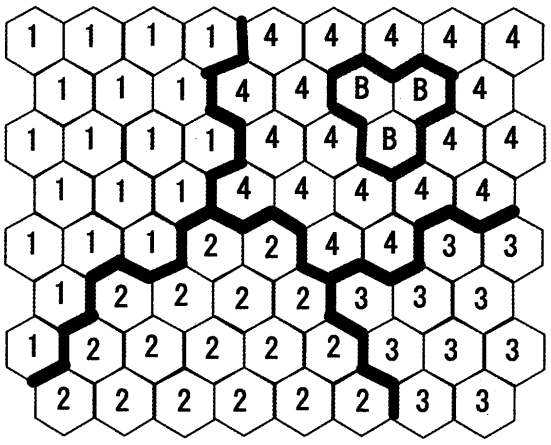

Fig.1 Potts model utilized in the present study.

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As shown in Fig.1, microstructure is composed of the "sites", which have their own number indicating grain orientation, kind of phase etc. In this figure, there are four different site numbers, from 1 to 4, and sites marked "B" indicating the second phase as highlighted by the yellow color. Grains are composed of sites with the same site number, and a grain boundary lies between sites with different numbers. In this figure the red and green lines are corresponding to grain boundaries and phase boundaries, respectively.

Figure 2 represents a two-dimensional single-phase microstructure generated by the module developed in the present study. No second phase or nuclei of precipitates is generated. The red and black boundaries are small angle and large angle boundaries, respectively. In the present simulation, all the grains were set to have <001> orientation, and a rotation angle around the <001> axis is randomly given to each grain, and is referred to site numbers.

Figure 3 represents an example of nuclei generated on boundaries in the initial microstructure shown in Fig.2. In this case one nuclei was set randomly on each boundary to simplify the role of grain boundary nucleation processes. The present module can generate any number of nuclei on a boundary.

The other type of nuclei within grains can be generated as shown in **Fig.4**. The number of nuclei is valuable and the position of each nuclei is set randomly in this module. The present study adopted one nucleus for each grain.

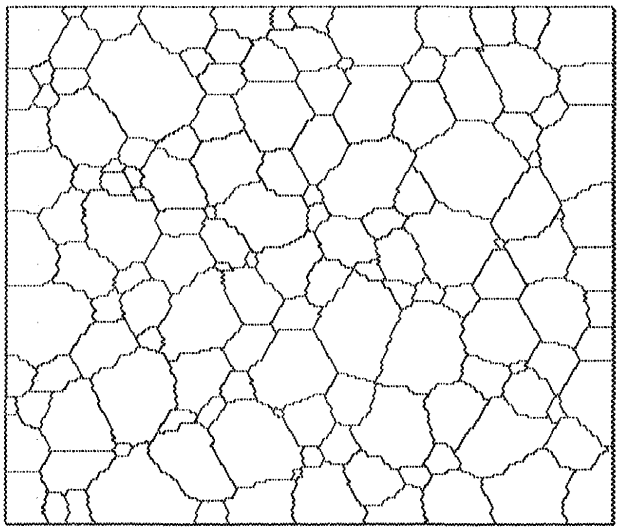

Fig. 2 An example of a two dimensional single phase structure generated.

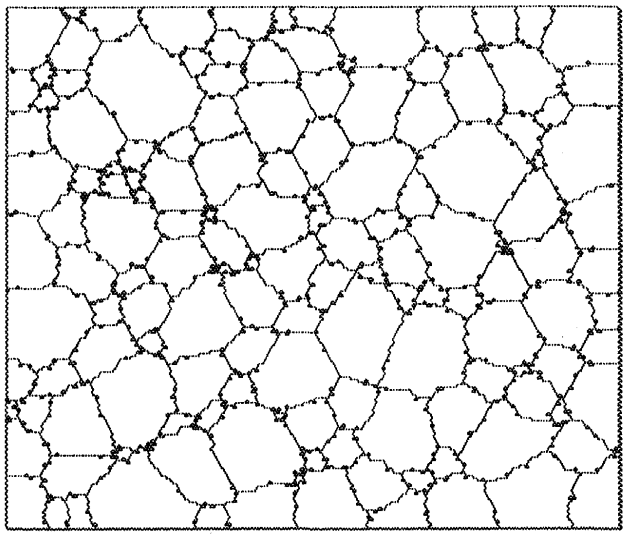

Fig. 3 An example of nuclei on grain boundaries randomly generated.

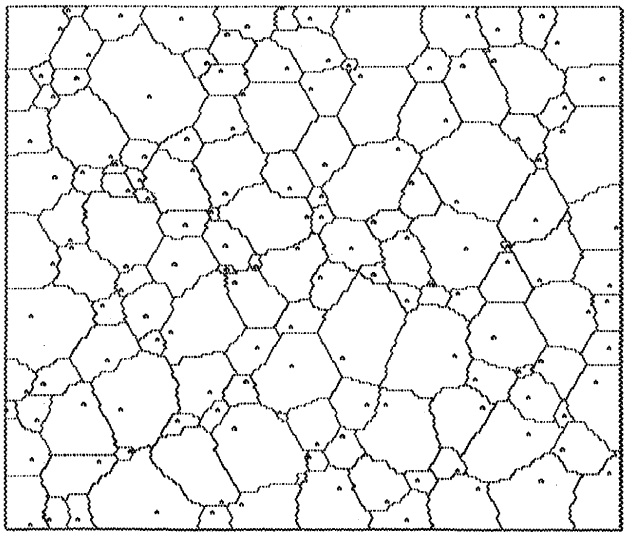

Fig. 4 An example of nuclei within grains randomly generated.

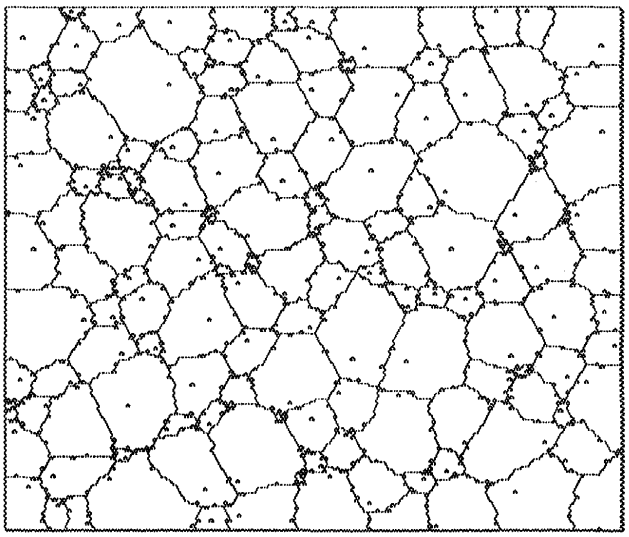

Fig. 5 An example of mixed nucleation.

Figure 5 shows an example of mixed nucleation for the initial microstructure, a combination of Figs. 3 and 4.

2.2 Simulation of boundary migration

The present calculation system was first designed to simulate the migration of both grain boundary and inter-phase boundary. Grain boundary migration and its related phenomena have been successfully described by many researchers utilizing the Monte Carlo simulation method based on the Potts model[2-4]. **Figure 6** represents the fundamental process of the grain boundary migration. The site having the site number "2", highlighted by green color, is now selected randomly, and one of the surrounding 6 sites become the target to be re-construction as shown in Fig.6(a). If the comparison of energy state of the site satisfy the preferential site-exchange condition, the number "2" turns to "4" as shown in Fig.6(b), involving boundary migration. The exchanging probability is a function of temperature, activation energy and some other parameters that are related to physical and chemical properties of given materials. Grain boundary character or grain boundary atomic structure are the most important to be considered in the migration function. For example the low angle boundary, (red colored boundaries in Fig.1), has been reported to be a less mobile boundary than high angle boundaries including coincidence boundaries. Present calculation modules can take these effects into account, but all the boundaries were set to have the same mobility in this study.

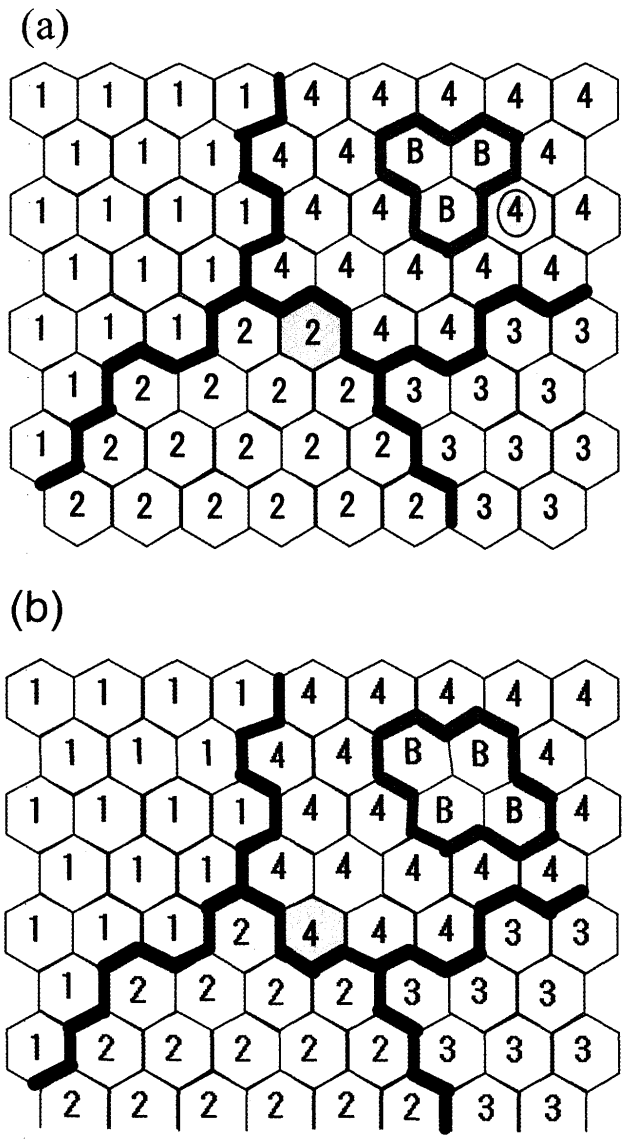

Fig. 6 Fundamental process of migration of grain boundary and phase boundary.

Migration of inter-phase boundary can also described by the exchange of site number, as shown in Figs.6(a) and (b). In this case, the site of the second phase, having the number "4" and highlighted by yellow color, is now selected for the calculation. The neighboring site "B" is selected and if the check routine of the probability allows the exchange, the interphase boundary moves by one site as shown in Fig.6(b). Migration rate of the boundary can also be defined as a function of some material properties. But in the present study the probability function was not constructed in detail since there are many unknown parameters which determine the mobility. A rational number ranging from zero to 1 was selected and the comparison with a random number decided for each iteration if the boundary migrates or not.

2.3 Thermal cycling

Thermal history involves successive alternations of the solution treatment process and the precipitation/phase transformation process. The present work designed a module that simulates the dissolution process of precipitates for a given precipitated microstructure. The dissolution temperature was set to be constant, and no grain growth occurs during dissolution. Back motion of inter-phase boundary can be calculated, but the precipitates were set to disappear at one time in the present work without the migration of phase boundaries. Thus, grain refinement occurs by the division of old grains before the precipitation by inter-phase boundaries of precipitates/second phase. The present paper reports the changes of microstructure during one cycle.

3. Results and Discussion

3.1 Precipitation process

Figure 7 shows an example of the precipitation process for the initial structure of a mixed nucleation type shown in Fig.5. Each grain boundary has two nucleation sites on both its sides, where the position was randomly set. A nucleation site of the grain interior type was also set randomly in each grain. The growth rates of grain boundary precipitates and grain-interior precipitates were set to be equal, and every precipitate grows equi-axially.

As the calculation proceeds, the grain boundary phases, indicated by blue color hatching, grow until they come into contact with each other. The precipitates nucleated in the grain interior, indicated by orange color hatching, are growing almost equi-axially until they come into contact with grain boundary precipitates. In this case 50 Monte Carlo steps (MCS) are needed to come to a full precipitated structure, which is shown in Fig.7(d).

As the migration rates is expected to have an important effect on the process of precipitation, the migration rate of the inter-phase boundary was then changed for the same initial structure. The result is shown in **Fig.8**. The ratio of migration rates of phase boundaries of the grain boundary phase to that of the grain interior phase was set to be 1/3. Therefore the grain boundary precipitates grow faster than the other type of precipitates

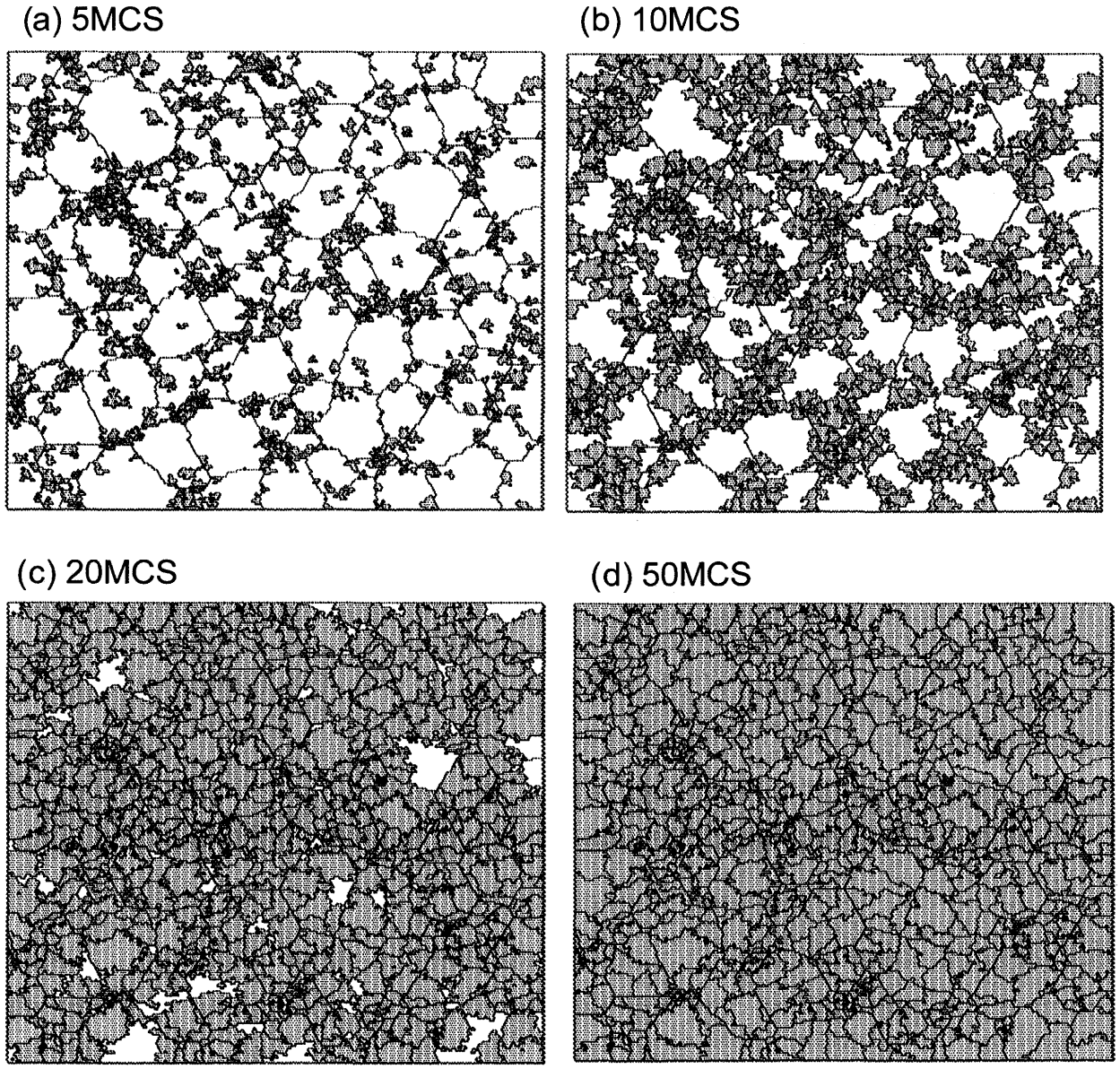

Fig.7 An example of precipitation process for the initial structure with mixed nucleation.

in this case. As shown in Fig.8, grain boundary precipitates grow dominantly from the beginning of the calculation, and finally almost all parts of the calculation field are occupied by the grain boundary originated precipitates.

A quantitative analysis was then performed for the microstructure changes shown in Figs.7 and 8 to discuss the role of growth rate of precipitates of the two types. **Figure 9** represents the changes of area fraction of precipitates for the case of the same precipitation rate. For both types of nucleation sites, the area fraction of precipitates increases rapidly up to 20MCS and little changes was obtained after 30MCS. The saturated values of the area fraction were 72.2% and 27.8% for the nucleation types of grain boundary and grain interior, respectively.

Figure 10 shows the changes of area fraction for the case that the ratio of growth rate is 1/3. In this case the fraction showed almost no change for the precipitates nucleated in grains. The area fraction at 50MCS was 3.2%. Meanwhile precipitates nucleated on grain boundaries showed the same tendency as that explained for Fig.9.

The competition of precipitation or phase transformation of different nucleation modes is a key to controlling microstructure during heat treatment. The

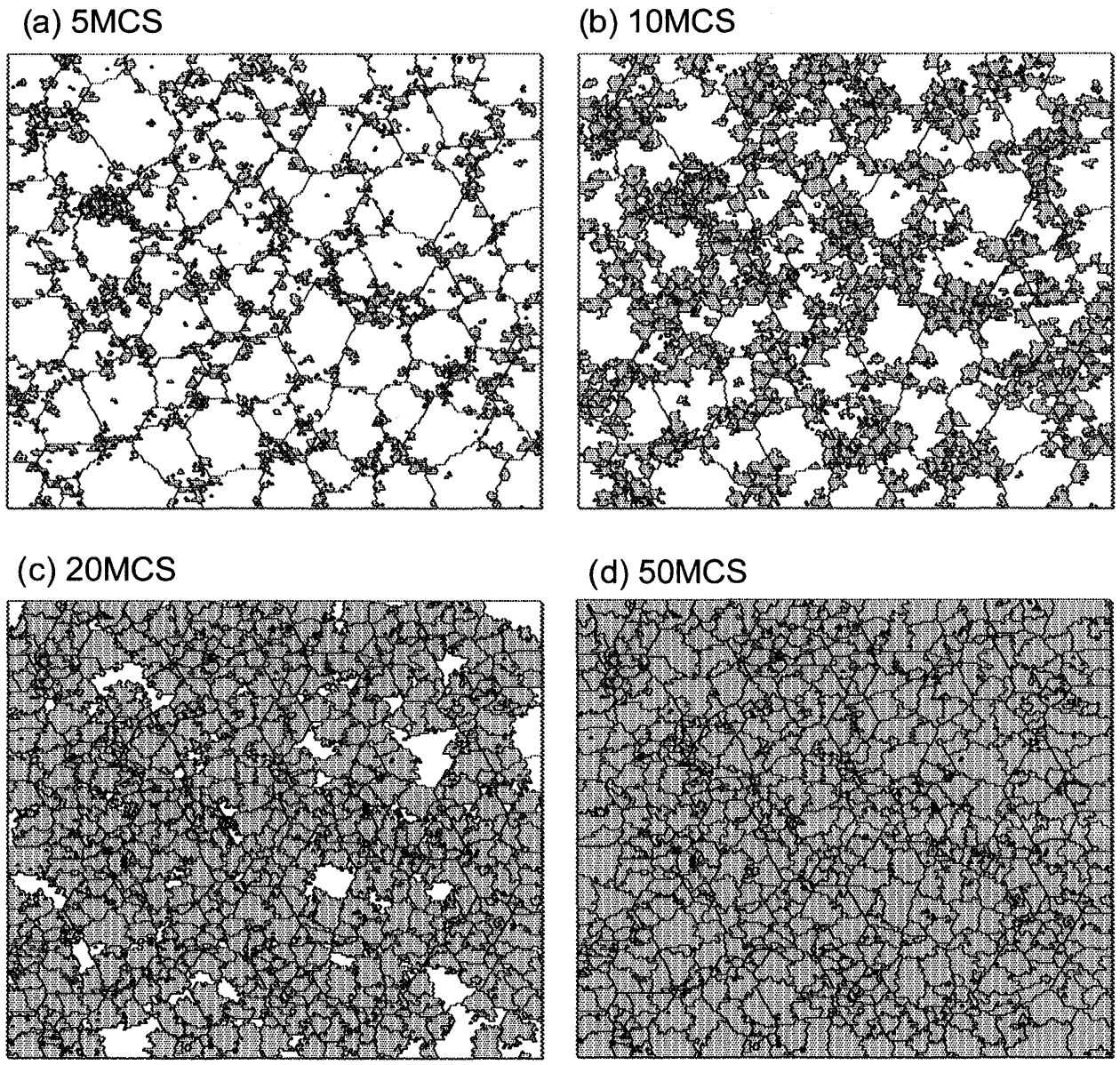

Fig.8 An example of precipitation process for the initial structure with mixed nucleation.

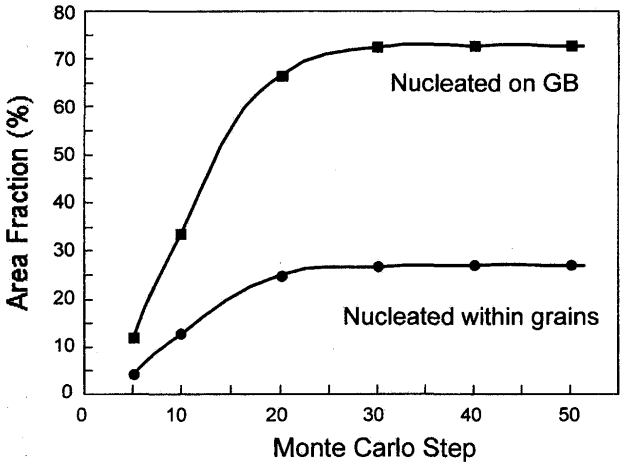

Fig. 9 Changes in the area fraction of precipitates of two types.

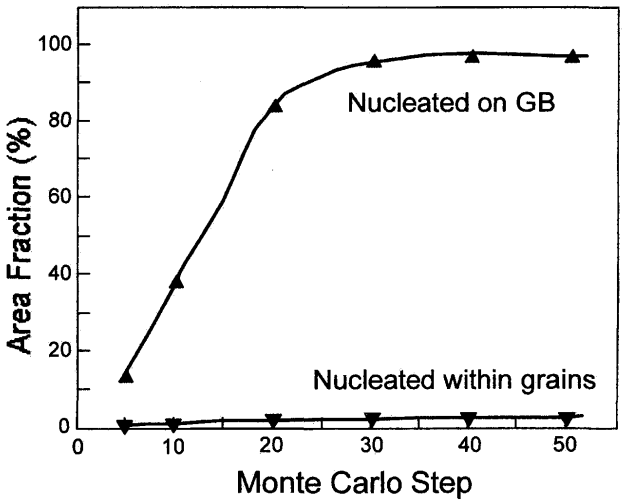

Fig. 10 Changes in the area fraction of precipitates of two types.

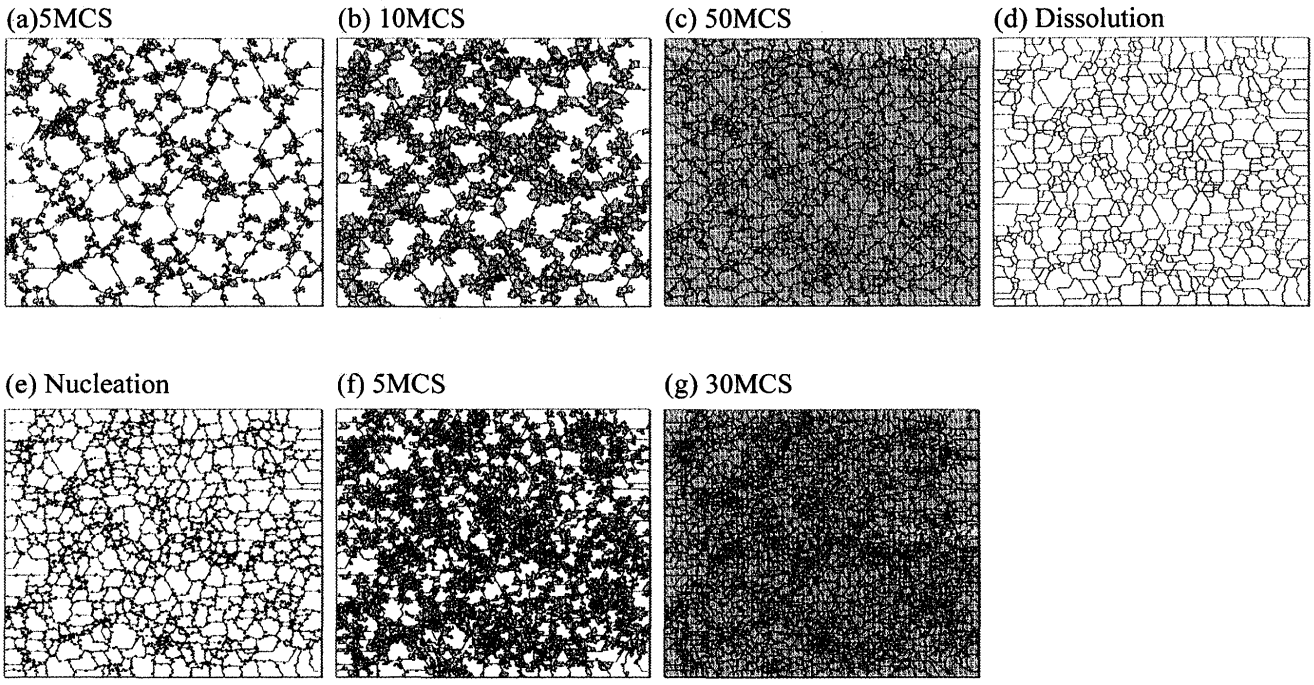

Fig. 11 Changes of microstructure during thermal cycling.

grain size at high temperature region is an important microstructural factor that determines the area fraction of precipitates starting from grain boundaries. Thus optimization of the precipitation process should be based on the grain size at elevated temperature. On the other hand, precipitates or transformed phases nucleated within grains act as obstacles to growth for the grain boundary phases. Thus the growth rate of the phases generated within grains should be controlled in order to obtain the most favorable microstructure if the grain boundary phases damage the mechanical properties.

The present simulation module can contribute to determining the heat treatment condition by optimizing the parameters that affect the behavior of precipitation or phase transformation. For this purpose, it is necessary to obtain the details of parameters describing the nucleation and growth process of precipitation and phase transformation such as nucleation probability, anisotropy of growth rate depending on crystallographic orientation. The system can also predict the alteration of orientation

distribution during thermal cycling if the orientation relationship of phases between low temperature and high temperature is given.

3.2 Microstructural change during thermal cycling

Figure 11 shows a change of microstructure during thermal cycling. Precipitation starts from grain boundaries and proceeds as shown in Fig.11(a) and (b). 50MCS of calculation resulted in a full precipitated structure as shown in Fig.11(c). Successively the re-solutionizing occurs and yields a grain refined structure as shown in Fig.11(d). In this calculation one nucleation site is given for each grain boundary. Thus each grain is divided by the number of its grain boundaries. A second nucleation process is performed for the grain refined structure as shown in Fig.11(e) and then the precipitation proceeds from grain boundaries as shown in Figs.11(f) and (g). The full precipitated structure is obtained after 30MCS which is faster than the first time of precipitation.

Grain refinement utilizing thermal cycling is realized in Cu-Be alloy that shows discontinuous precipitation[5]. In this alloy one cycle resulted in the grain refinement by a factor of one tenth. Similar microstructure is obtained in the present simulation. The present module is applicable for the analysis of this phenomenon and is able to propose an optimum condition for the heat treatment.

Further design of modules should take the diffusion field into account for the purpose of the precise calculation of phase transformations that change the solute content in front of the inter-phase boundaries.

4. Summary

The present study developed modules to simulate thermal cycling by the combination of precipitation process and dissolution of precipitates. The modules can generate any number of nuclei both on grain boundaries and within grains. The growth rates of precipitates nucleated on boundaries and within grains are important factors in the evolving process of microstructure. Thermal cycling was simulated for the case of one nucleation site on each grain boundary, and grain refinement by the division of phase boundaries within each grain was realized.

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