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Grain growth simulation of two phase structures under temperature gradient†

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Abstract

The role of second phase and temperature gradient in the grain growth process has been investigated utilizing a Monte Carlo simulation method. A grain structure containing periodic arrays of second phase grains was constructed as the initial structure for the calculation. Two kinds of grain boundary migration rate were set depending on the character of grain boundaries, i.e, low angle boundaries and high angle boundaries. The migration rate was also set to be a function of temperature, and the temperature gradient field was applied to the calculation field.

Grain growth was retarded around the second phase and also a lower growth rate was observed in the lower temperature region. Grain boundary character distribution was found to be affecting the growth process, and triple junctions containing many low mobility boundaries tended to act as passive junctions as if its vicinity region were lower temperature field..

KEY WORDS: (Monte Carlo simulation)(Potts model) (grain boundary migration) (migration rate) (local microstructure parameter)

1. Introduction

Grain growth is well known as a fundamental microstructure evolution that takes place in many fields of fabrication such as casting, heat treatment, welding, brazing and so on.

In particular welding brings about a temperature gradient field in the heat affected zone(HAZ) and also in the weld metal. Although grain size control in the HAZ and other temperature gradient regions has been a target of intensive research work, grain boundary character distribution(GBCD) ¹⁾ or the role of local GBCD in grain growth are still important problems that have been unsolved so far.

The present paper tries to make clear the role of local microstructure parameters such as GBCD and second phases in the grain growth process under the temperature gradient field utilizing the Monte Carlo simulation with a Potts model.

2. Simulation procedure

200 x 200 cells in hexagonal arrays were generated as the calculation field, and each cell was given a different number with. The number corresponds to a rotation angle around the <001> axis in the present calculation. This kind of grain structure is called "2 dimensional Potts model" ²⁾. The grain boundary was characterized by the difference in the number of the neighboring grains, i.e. the disorientation angle. Low and high angle boundaries were defined as the angles smaller and larger than 15 degrees, respectively. The velocity of grain boundary migration is well known to be affected by the boundary structure, temperature, obstacles such as precipitates and second phase grains and so on. In the present calculation the velocity of high angle boundaries was set to be 10 times faster than that of low angle boundaries. In addition to this, the dissimilar interface was set to be immobile. The temperature gradient is, in the present study, represented as the alteration of the velocity that decreases linearly from 100% of the highest velocity to zero.

After the growth simulation of 10 Monte Carlo steps (MCS) for the single-phase structure under the conditions of the same mobility and uniform temperature field, the second phase grains were periodically arranged in the initial microstructure as shown in **Fig.1**. In this figure, two kinds of initial grain structures are shown with

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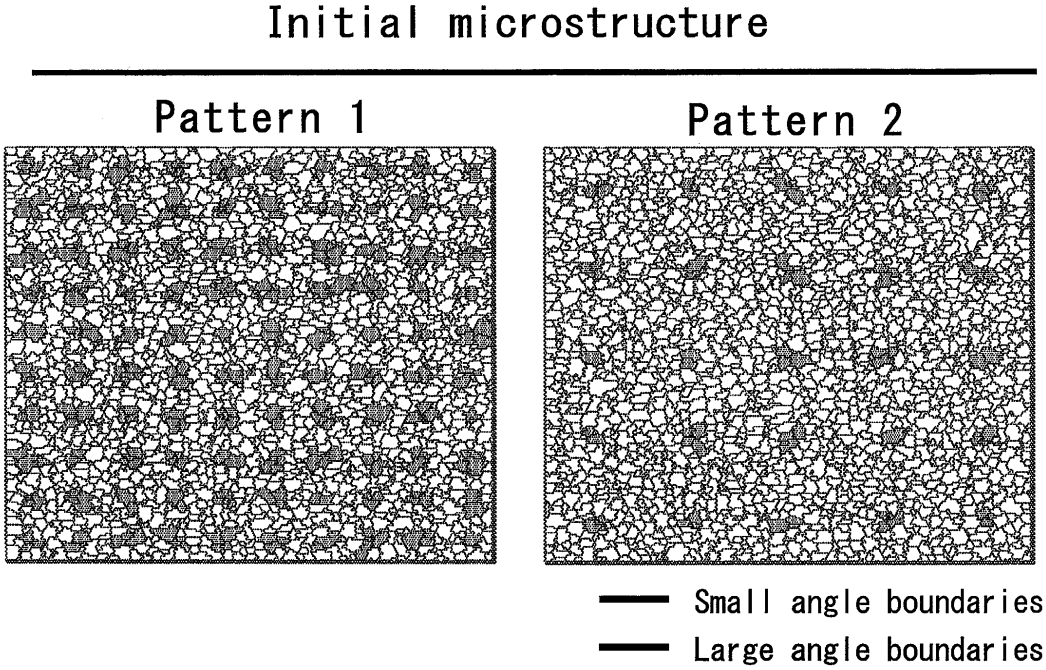

Figure 1 Two initial structures adopted in the present calculation. The blue hatched grains are second phase grains, and red colored boundaries correspond to low angle boundaries.

hatched blue grains as second phase and red colored grain boundaries as low angle boundaries. Fig.1(a) and (b) represent a dense and a coarse arrays of second phase grains, respectively.

The Monte Carlo method was utilized for the simulation of grain growth starting from the two initial microstructures. The second phase grains do not change their size, shape and volume fraction throughout the present calculation. The temperature was set to be highest at the left end side, and linearly decreasing towards the right side. There was no temperature gradient along the top and bottom direction. After calculating the settled steps such as 100, 200, 500 and 1000 MCS, each set of data was analyzed concerning (1)grain structure, (2) local grain boundary character distribution.

3. Results and Discussion

Figure 2 represents an example of the grain growth process simulated for the case of a dense array of second phase grains. In the higher temperature region grain boundary migration tended to occur frequently and consequently growth rate was higher than the other region of lower temperature field. After 1000MCS of the calculation, most of grain boundaries are impinged by second phase grains in the higher temperature region, suggesting that the second phase grains act as a trap site of grain boundaries as well known from the observation of actual materials. The impingement effect of the second phase is, in other words, regarded as if cold regions were embedded locally. Therefore the grain growth process of two phase structures under a temperature gradient contains two distinct characteristics of microstructure such as (1) alteration of grain boundary mobility ratio and (2)impingement of grain boundaries.

Figure 3 shows a microstructure change during grain growth for the case of a coarse array of second phase grains. The effect of temperature field is seen to be similar to that observed in the case of the dense array as shown in Fig.1. In the vicinity region of second phase grains, grain boundary migration is still effectively suppressed. But the trap effect by the second phase tended to be less effective for the region where the distance from the second phase grains becomes longer. In such regions, grain growth proceeds likewise in the single-phase microstructure, and grain boundary migration is thought to be affected by the other microstructure parameters such as local GBCD or the character of triple junctions.

A triple junction is one of the most important defects in materials, and is characterized commonly by the character of three grain boundaries connecting at the junction. If the junction is composed of boundaries with similar energy, the equilibrium angle between two neighboring boundaries is 120 degrees [3]. But in the case of junctions with boundaries of different energy, the equilibrium angles deviate from 120 degrees. The boundaries at the non-equilibrium junction migrate in

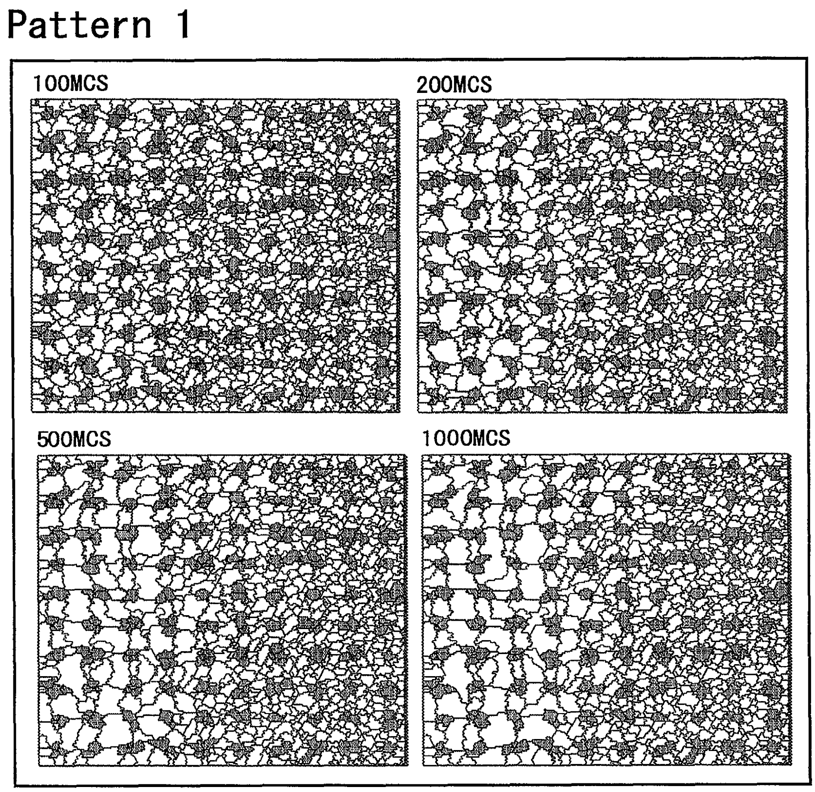

Figure 2 Grain growth process calculated for the dense array of second phase grains.

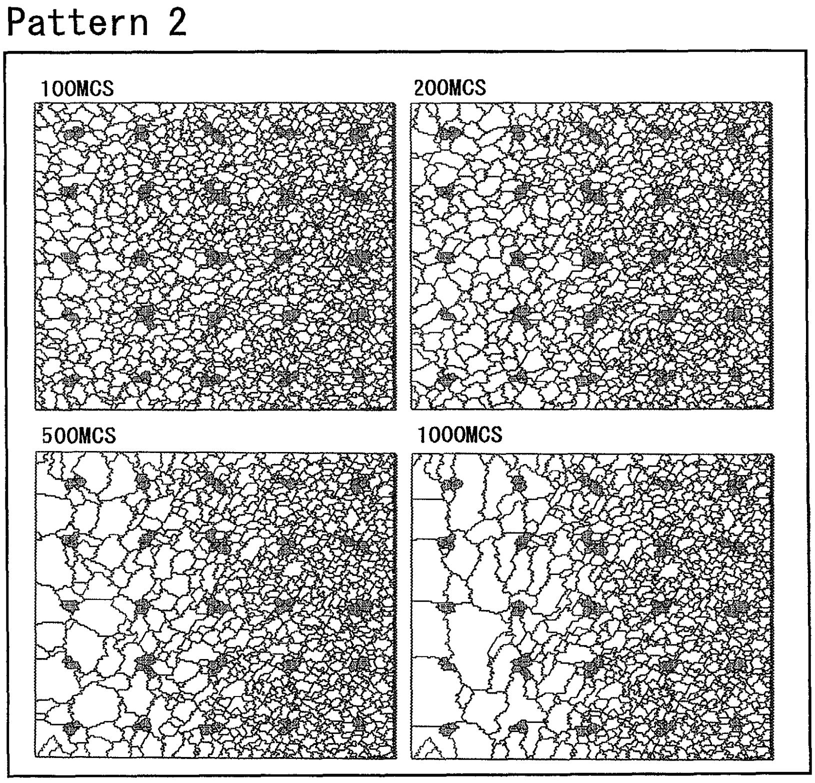

Figure 3 Grain growth process calculated for the coarse array of second phase grains.

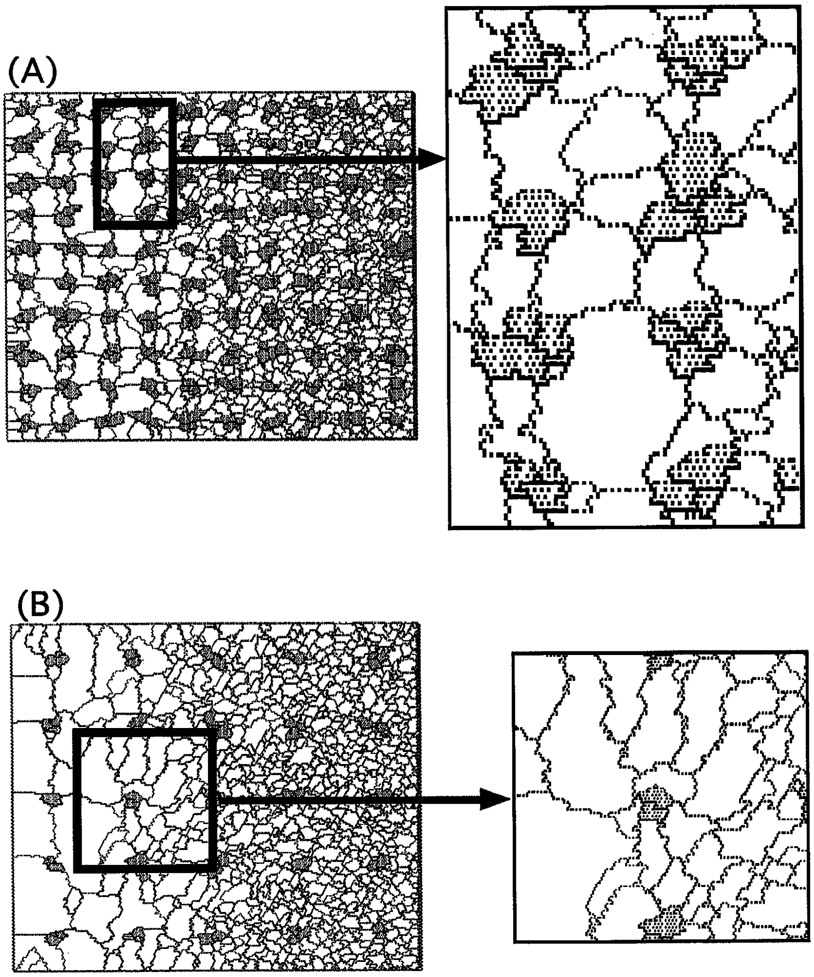

Fig. 4 Typical local GBCDs observed after 1000MCS, showing the segregation of low mobility boundaries.
(a) connections of low mobility boundaries to form passive triple junctions.
(b) low mobility boundaries around second phase grains.

order to form the equilibrium junction. This is one of the driving forces of grain boundary migration. Beside the driving force of migration, the mobility of the grain boundary is another important parameter. Grain boundary structure or character is well known to have a strong effect on mobility and coincidence boundaries have been revealed experimentally as fast moving boundaries rather than random boundaries [4]. Thus the active triple junctions are concluded to consist of boundaries with higher mobility. Passive junctions are composed of boundaries, either in an equilibrium and balanced state of energies or with low mobility. Grain growth proceeds preferentially in the region where active triple junctions exist. Evolution of microstructure observed in Fig.3 proceeds under the control of both the impingement effect of second phase grains and the behavior of active triple junctions in the region where the second phase grains are less effective for the migration.

As seen in Figs. 2 and 3, GBCD was not homogeneous and concentration of low angle boundaries was observed in some regions. This characteristic of local GBCD is frequently observed in actual materials.

Figure 4 shows two typical spatial distributions of low mobility boundaries observed after 1000MCS. As shown in Fig.4(a), once red colored low mobility boundaries connect with each other to form a stable or a passive triple junction, the vicinity region around such a junction changes into a region of low growth rate as if the temperature is lowered. The combined effects of second phase grains and passive junctions are observed in Fig.4(b), where low mobility boundaries are segregated around second phase grains. These particular regions make the growth process and microstructure more complicated and have wide variety. Thus the fraction of these passive triple junctions should be a target of investigation.

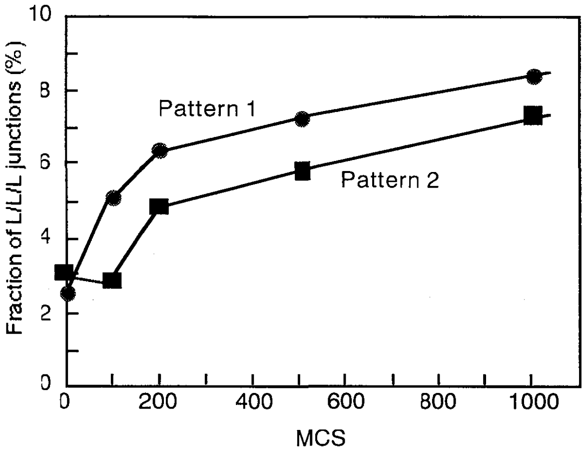

Fig. 5 Changes in the fractions of passive triple junctions as a function of MCS.

Figure 5 shows the fraction changes of passive triple junctions as a function of MCS for two initial patterns of microstructures explained in Fig.1. The fractions at the initial state were 2.6 and 2.9% for pattern 1 and 2, respectively. As grain growth proceeded, the values increased in the similar manner, and reached 8.4 and 7.3% at 1000MCS for pattern 1 and 2, respectively. At the initial stage of the growth process until 200MCS, passive triple junctions increased their fraction drastically, and the values turned into a gentle change. Pattern 1 brought about larger values than pattern 2, except for the initial value. This result suggests that the dynamic change of local GBCD and its related distribution of triple junction character are affected by the constraint of the second phase grains, and their denser distribution makes the local GBCD reach a saturated state earlier.

Temperature gradient also has a controlling affect on the evolution of microstructure during grain growth. Since grain boundary energy and other properties of boundaries are a function of temperature 5), active and passive triple junctions can be altered into the other state depending on the temperature. Thus, localized heating such as spot welding would yield some peculiarity in microstructure parameters such as GBCD and texture.

4. Conclusion

Growth process of two phase microstructure under temperature gradients has been calculated utilizing a Monte Carlo simulation method. The following results were obtained.

(1) Growth rate in the higher temperature region was larger than the other regions of lower temperature field. No abnormal grain growth was observed.

(2) Second phase grains effectively suppressed grain boundary migration in their vicinity region. This effect is equivalent to the reduction of temperature in the localized area.

(3) Triple junctions composed of low mobility boundaries such as small angle boundaries also stabilized the microstructure locally. The junctions with three low mobility boundaries increased as grains grew. The fraction of such passive junctions in the microstructure with a dense array of second phases was higher than that in the microstructure with coarsely distributed second phase grains.

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