Control of Grain Growth Process by a Local Heating Method†

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Abstract

The present work deals with a preferential grain growth process in a localized region utilizing a local heating method in order to fabricate some unique microstructures, different from those fabricated in the homogeneous way by microstructure evolution. A Monte Carlo simulation of grain growth under a heterogeneous temperature gradient, i.e. spot heating, was performed. A steep temperature gradient brought about preferential grain growth in the higher temperature region, showing that the local heating is effective for the control of grain structure of polycrystalline materials. Such a type of preferential grain growth became less significant under a mild temperature gradient. Local heating of pure copper foil of 0.2mm in thickness utilizing a laser beam was performed by changing the irradiation conditions. In the case of 200W of laser power and 18mm/s for sweep velocity, some grains were observed to have larger grain size than their neighbors, suggesting a possibility of preferential grain growth in localized regions.

KEY WORDS: (pure copper) (local heating) (laser beam) (grain growth simulation) (EBSP analysis)

1. Introduction

Microstructure controls aim to optimize distributions of microstructure parameters to ensure that given materials possess the best characteristics. The optimization of microstructure is realized by utilizing mechanical energy and thermal energy, and a combination of both energies in some cases. For example, improvement of mechanical properties is realized by grain refinement, and the reduction of grain size is performed by making use of well known metallurgical phenomena such as severe deformation, recrystallization, phase transformation and precipitation. Generally these important phenomena take place in the homogeneous fields of temperature and plastic strain in the materials during treatment.

Electron Back-Scattering Pattern (EBSP)analysis has revealed some important features of microstructure such as grain orientation and grain boundary characters that are correlated to their spatial positions in the materials(1).These spatial distributions of microstructure parameters are heterogeneous in many cases. Therefore some novel control methods of microstructure could be developed by taking into account the heterogeneity of the distributions.

Growth phenomenon of Goss oriented grains in Fe-Si alloy is a well-known example of microstructure control utilizing the heterogeneity of microstructure parameters (2). In this case, Goss oriented grains, existing in the primary recrystallized grain structure with quite low frequency, started to grow preferentially in the later stage of annealing and eventually occupy almost all the parts of the alloy.

Such abnormal growth of Goss-grains proceeds in a homogeneous temperature field but heterogeneous distribution of grain boundary characters, especially the sigma 9 coincidence boundary that migrates faster than the other types of boundary in the alloy. Meanwhile a heterogeneous temperature field would play a new role in the fabrication of peculiar textures since grain boundary migration is also a function of temperature. In other words, the introduction of thermal energy into target grains to be grown preferentially yielding the microstructure we desire.

The present study discuss the possibility of preferential growth of target grains by spot heating, by means of both computer calculation and spot annealing

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by a focused laser beam.

2. Experimental Procedure

2.1 Monte Carlo simulation of grain growth in the heterogeneous temperature field

The calculation of grain growth in the two dimensional microstructure is based on the algorithm of the Monte Carlo simulation method that has been adopted by many researchers so far. The present calculation adopted an initial grain structure generated in the calculation system. The polycrystalline structure is composed of many cells and each cell has its own number correlated to grain orientation. This polycrystalline model is called the "Potts model", and 200 x 200 cells were used for the description of microstructure. Grain boundaries are recognized between two adjacent cells having different orientations, and small angle boundaries are defined as the boundary with a misorientation less than 15 degrees, and larger misorientaion angles denote large angle boundaries. The misorientation angles of less than 2 degrees are taken as the same orientation, i.e. no grain boundary lies between the cells.

Figure 1 represents an initial structure adopted in the present calculation. The polycrystalline microstructure was generated in the present simulation system. Grain boundaries in red and in black color correspond to low angle and high angle boundaries, respectively. But the growth simulation in the present study did not take into account the effect of grain boundary characters.

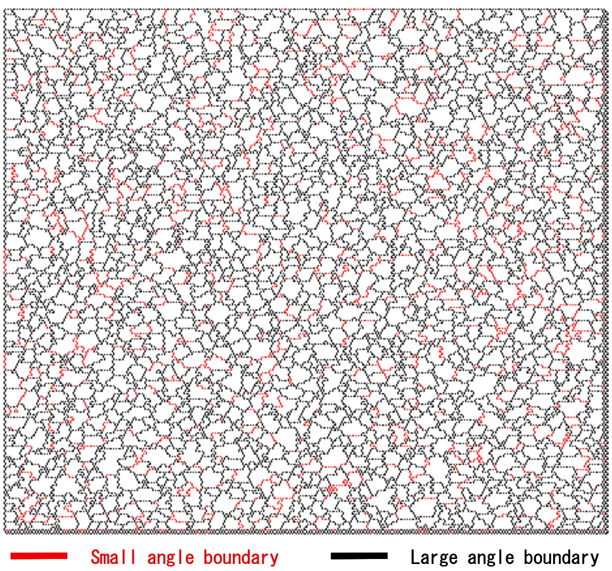

Fig.1 Initial grain structure adopted in the present grain growth simulation by Monte Carlo method.

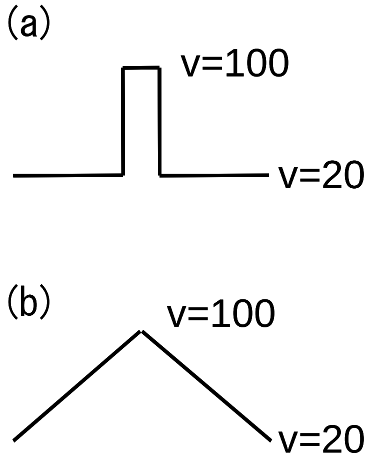

Fig.2 Temperature distributions utilized in the present grain growth simulation.
(a) a steep temperature gradient type,
(b) a gentle temperature gradient type

A special calculation field of 200 x 200 cells, the same size as that of the fundamental calculation field, was chosen to deal with only the degree of temperature, and the field was overlapped on the fundamental field. The double-layered calculation field can realize the simulation of grain growth under any kinds of temperature distribution.

The present calculation deals with microstructure evolutions under spot heating conditions, and adopted two kinds of heterogeneous temperature distributions such as (1) a steep temperature gradient field and (2) a gentle temperature gradient field. These two temperature distributions are shown schematically in **Fig.2**. In order to represent temperature dependence of grain boundary migration, the migration rate was represented as a ratio of migration.

2.2 Laser heating on pure copper sheets

Pure copper sheets of commercial grade of 0.2mm in thickness were used for the local heating by a Laser beam. The copper sheets are recrystallized. The laser heating system is shown schematically in **Fig.3**. The present system utilized a diode laser apparatus (Spectra Physics, GTS500 type) with the maximum power of 500W. The laser radiation was performed in an ambient atmosphere by changing incident power from 91 to 300W, and sweep rate from 12 to 18mm/s. so as to change the heat input to the sheet. The beam profile on the specimen surface was a rectangular shape of 400 μ m x 1800 μ m.

After the laser irradiation, samples for microstructure observation were machined and then

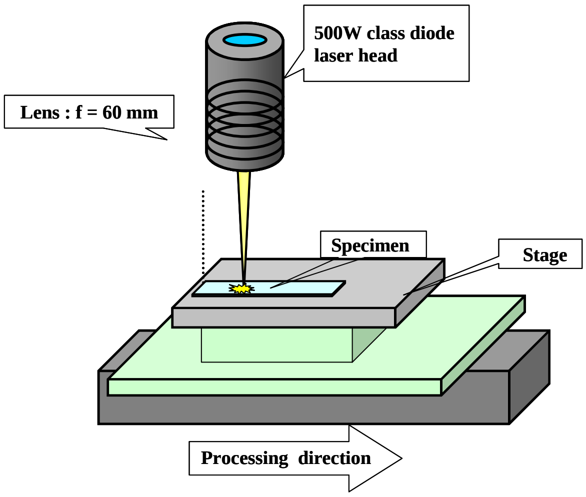

Fig.3 Schematic illustration of the Laser heating system utilized in the present study.

mechanically polished followed by an electrolytical polishing using a 30% nital solution. The amount of the polishing was about 100 μ m.

The EBSP measurement of the specimens was performed at an accelerating voltage of 30kV utilizing software (OIMDC ver. 3.5) provided by TSL Japan Inc. The distance between each measurement point was 1 μ m and the analysis focused on grain size distribution, grain orientation and grain boundary character distribution.

3. Results and Discussion

3.1 Calculation of grain growth during spot heating

Figure 4 shows an example of grain growth process under a spot heating condition simulated in the present system. The region highlighted by a red square is the boundary of two temperature regions which corresponds to Fig.2(a). In this high temperature region grain boundaries migrate five times faster than those in the outer region. So the red border represents a steep temperature gradient.

A slight coarsening was observed in the high temperature region after 10 MCS, as shown in (b), while few changes in microstructure occurred in the surrounding region. A significant grain growth occurred after 100MCS as shown in (c). Further calculation resulted in abnormally grown grains in the higher temperature region as shown in (d)of 500MCS, and the grain size difference was larger than ten times.

This microstructure change is similar to the case of anomalous grain coarsening where small amounts of grains grow preferentially by invading their surrounding grains. In this case the important feature of microstructure is the existence of fast moving boundaries that localize mainly around the growing grains. But the present case is brought about by the localization of the high temperature region although the microstructure change was driven by the fast moving grain boundaries.

Figure 5 shows an example of grain growth process under a gentle temperature distribution as indicated in Fig.2(b). No significant change occurred in the early stage as shown in (b), but many grains grew with different growth rates in a wider region than the case

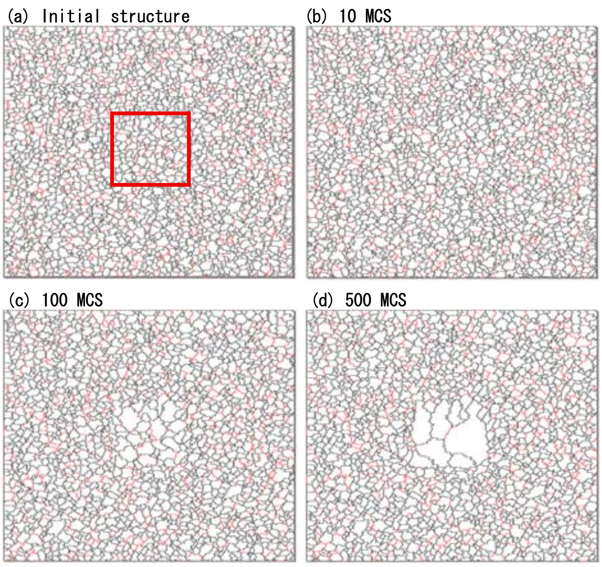

Fig.4 Grain growth process under the steep temperature gradient.

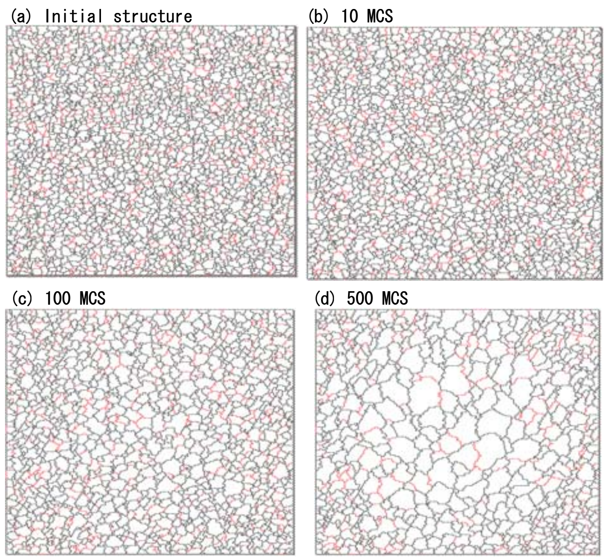

Fig.5 Grain growth process under the gentle temperature gradient.

of the steep temperature gradient. The largest grains existed in the center of the calculation field, i.e. in the highest temperature region. After 500MCS of the calculation many grains with different grain size came to be observed in a wider region than that observed in Fig.4(d). Larger grain size tended to be obtained in the region closer to the center position. Little change in grain structure occurred in the region close to the corner of the calculation field, where the lowest migration rate was set to be 0.2. These corner regions showed a similar tendency in microstructure change to those observed in the lower temperature region shown in Fig.4.

Comparing the two types of temperature distributions, it can be said that the temperature gradient should be a controlling factor for the sake of realizing the designed growth process of polycrystalline materials. Physical properties of materials such as specific heat, thermal conductivity etc. are important factors directly affecting the temperature distribution, although the same amount of heat input is given to the materials. Computer simulation techniques can show us the way to select appropriate conditions for local heating on given materials.

3.2 Laser local heating on pure copper sheets

As discussed in the previous section, the local heating could modify and control the grain growth process. Then an experimental trial was performed to investigate the possibility of such a method of microstructure control.

Figure 6 shows an appearance of the copper sheet that was heated by a scanning laser beam under the incident power of 200W and the sweep rate of 18mm/s. Fig.6(a) and (b) represent the top and the bottom surfaces of the sheet, respectively. A change of color was observed on both sides, indicating that the laser energy was transformed into the heat energy at the specimen surface since the color change is attributed to the oxidation caused by raising the temperature. Larger heat input resulted in the melting of the sheet. Lower heat input resulted in little change of color on the surfaces, suggesting less effective heat input were given to the material. But it should be noted that heat input was possibly introduced into the material even though there was no change of color.

Figure 7 shows a result of EBSP analysis performed for the same specimen. Fig.7(a) represents a spatial distribution of grain orientations on the ND plane,

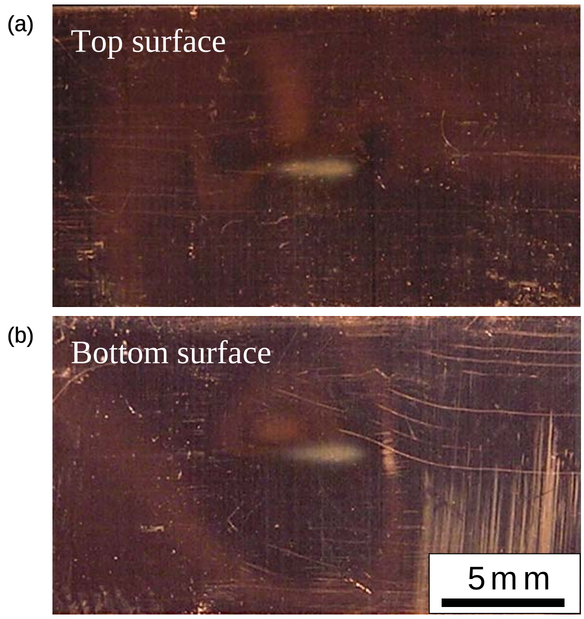

Fig.6 Appearance of both top and bottom surfaces of pure Cu plate heated by a Laser beam with 200W and 18mm/s of the sweep velocity.

which is commonly called “Orientation Imaging Map (OIM)”. In this figure, the horizontal and the vertical direction correspond to the rolling direction and the laser sweep direction, respectively. The color of each grain represents crystallographic orientation indicated in the unit triangle of the cubic system. The red, blue and green colors correspond to (001), (011) and (111) orientations, respectively. Mixing of these three colors depending on the disorientation from these three orientations represents any orientation.

As shown in Fig.7(a), no significant change seems to occur during the irradiation due to the short time in heating of this area. But as highlighted by a white circle, a blue color grain has larger grain size than its surrounding grains. This grain seems to have just started to grow by consuming the other grains, and such grains exist in the other area of this figure.

Fig.7(b) is a {111} pole figure on the ND plane, showing a higher density of the {111} orientation along the rolling direction and particularly similar types of <111>//RD fiber texture. The statistical distribution of orientation is not always representing local distributions, for example a different orientation distribution exists in the region inside the white circle in Fig.7(a). The blue color grain in this region is not the main component of the fiber texture, so the growth of this grain means that the texture component would be changed by the selected heating of the grains that we want to grow.

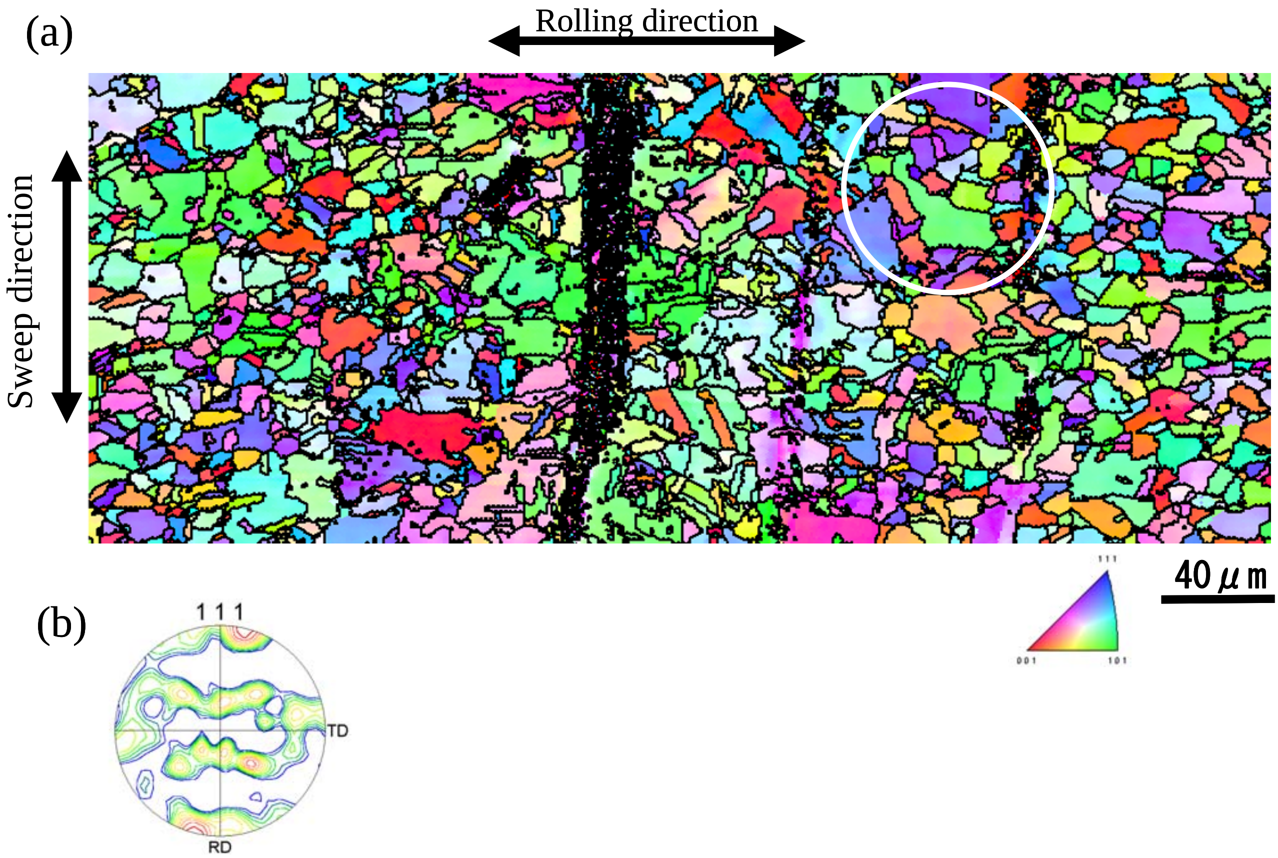

Fig.7 Orientation distribution in the Laser heated area of pure Cu plate.
(a) a spatial distribution of grain orientation, (b) {111}pole figure

The area of EBSP measurement is about 400 μ m in the horizontal direction and this value is the same as the beam size of the laser in the same direction. Taking into account the thermal conductivity of pure copper, the observed area was mainly heated in the present study. But the area is still large compared with the size of spot heating in the present simulation. In this respect, the present laser heating system could not achieve the pin-point heating on the target grains.

Since actual heat input to the copper sheet could not be enough, grain boundary migration must have taken place for only a few grain boundaries that satisfied a preferential migration condition. Thus the laser heating did not yield a homogeneous grain growth. Hereafter the heterogeneous grain boundary migration will be discussed concerning local grain boundary character distribution.

3.3 Role of local grain boundary character distribution in migration behavior of grain boundary

Grain boundary migration is a fundamental process of grain growth phenomenon, and the migration velocity is a function of the driving force and the mobility of the boundary [(5)]. The driving force of grain boundary migration is given by the difference of dislocation density, imbalance of grain boundary energy at triple junctions, difference of surface energy, difference of grain size etc. The mobility is strongly related to grain boundary structure.

Assuming that the energy balance at the triple junction mainly gives the driving force, each boundary may possess different driving forces since each triple junction has different sets of grain boundary structures or grain boundary energies. Thus local grain boundary character distribution or local distribution of grain orientation are playing a dominant role in the grain boundary migration and grain growth process.

Therefore grain boundary migration and grain growth do not always take place homogeneously. The most active triple junction can migrate at first and grains having such triple junctions can grow preferentially. The present laser heating did not give sufficient energy to the material, so the most active junctions could contribute the growth of a few grains pointed out in Fig.7.

Local heating or spot heating utilizing a laser beam will be a promising method for fabricating peculiar grain size distributions in given materials, also creating some new types of texture.

4. Summary

The present work performed a Monte Carlo simulation of grain growth in the heterogeneous temperature distribution for an initial single-phase polycrystalline microstructure that was generated by the calculation system. A laser heating experiment was then performed on pure copper sheets to investigate changes of microstructure, especially during early stages of grain growth in localized areas. The following results were obtained.

(1) A steep temperature gradient field yielded a preferential grain growth inside the higher temperature region, resulting in the enhancement of heterogeneity in grain size distribution. After 50MCS of calculation, the higher temperature region consisted of some large grains with grain size more than ten times greater than those in the surrounding lower temperature area.

(2) A gentle temperature gradient field yielded a wider grain size distribution since grain growth took place with different growth rates depending on temperature in larger areas than the case of a steep temperature gradient field.

(3) Laser heating on pure copper sheets of 0.2mm thickness was carried out under the condition of 200W of incident power and 18mm/s of sweep rate. In this case some grains seemed to have just grown preferentially, indicating the possibility of artificial microstructure control by the laser spot heating technique.

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