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# Simulation of the effect of anisotropic grain boundary mobility and energy on abnormal grain growth

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Abnormal grain growth (AGG) can take place when the grain boundaries of a given grain have the growth advantage exclusively over those of the other grains. The growth advantage can be provided either by high mobility or by low energy of the grain boundaries. Monte Carlo simulation is done to determine which of the two factors is more important in inducing AGG. The results of the simulation indicate that the growth advantage by the low energy induces AGG under a more realistic condition if the grain boundary energy is low enough to allow the AGG grain to grow by solid-state wetting. Grain growth by wetting will take place at the triple junction when the sum of the two grain boundary energies is smaller than the other grain boundary energy. Island grains inside the AGG grain are formed both by anisotropic mobility and energy of grain boundaries. High frequency of island grains, however, comparable to that observed in the initial stage of AGG in an Fe-3%Si alloy, is induced under a condition where growth by wetting is favored while the grain boundary migration is suppressed. 

## 1. Introduction

Abnormal grain growth (AGG), which is also called discontinuous grain growth or secondary recrystallization, often takes place after recrystallization of the deformed polycrystalline materials. Although AGG is an important phenomenon both scientifically and technologically, its mechanism has not yet been fully understood. Phenomenological understanding is that AGG takes place in a condition where most of the grains are suppressed and only a few are allowed to grow [1–3]. AGG tends to be pronounced when growth of most grains is inhibited [1–3]. The inhibition is normally achieved by the second phase particles.

Monte Carlo (MC) simulations introduced by the Exxon group [4–6] have turned out to reproduce the important feature of the microstructure evolved during grain growth. By MC simulation based on the modified Potts model, Rollett *et al.* [7] examined the effect of anisotropic grain boundary mobility and energy on AGG. Even though they used the simple system with two different values of mobility or energy, they showed that AGG can take place by anisotropic mobility or energy. In the case of anisotropic energy, they determined growth by wetting, where high energy grain boundary can be replaced by two low energy grain boundaries. They found out further that this solid-state wetting is critical to AGG. They also found out that island-like grains inside the AGG grain are not formed by anisotropic mobility but formed by anisotropic energy. Previously, the formation of island-like grains was attributed to anisotropic mobility like breakaway of the second phase particle from the migrating grain boundary [8]. Since island-like grains are so frequently observed in the systems of AGG [2, 8–12], the formation of these grains seems to be closely related to AGG.

On the other hand, the assumption of Rollett *et al.* was unrealistic in that 100% of the grain boundaries shared by the AGG grain have high mobility or low energy. With grain growth, the AGG grain continues to have new neighboring grains and thus continuously changes its grain boundaries. Therefore, only a perfect texture can satisfy the assumption. It is worth examining the effect of anisotropic grain boundary mobility and energy under a more realistic condition that only a fraction of the grain boundaries shared by the AGG grain has high mobility or low energy. In this paper, the aspect of AGG was examined under such a condition of anisotropic mobility and energy in MC simulation. We will focus on which of the two factors, anisotropic mobility or anisotropic energy, is mainly responsible for AGG. Analysis of the island grain formation will be made in relation to the mechanism of AGG. Based on the analysis, a new mechanism of AGG will be suggested.

## 2. Monte carlo simulation

The simulation scheme is the same as in the previous papers [13, 14], which were based on the Potts model [4–6]. Simulations were done on the two-dimensional triangular lattice of 150 by 150 sites. Orientation of each grain was represented by integers from 1 to $Q$.

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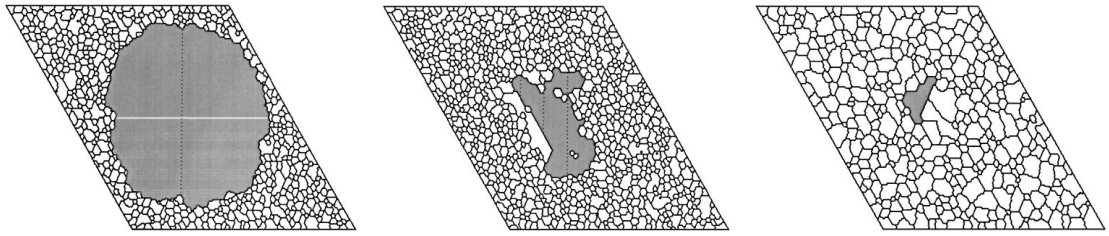

(a) (b) (c)

*Figure 1* Microstructure evolution after (a) 500 MCS, (b) 500 MCS and (c) 3000 MCS with the percentages of type II grains, (a) 100%, (b) 90% and (c) 80%. The grain boundary between AGG and type II grains has mobility 100 times higher than that between AGG and type I grains or between type I and type II grains.

$Q$ was chosen to be 50 in the simulation. The grain boundary energy function is given by

$$E = -J \sum_{nn} \left(\delta_{s_i s_j} - 1\right) \tag{1}$$

where $S_i$ is one of the $Q$ orientations on site $i$, and $\delta_{ab}$ is the Kronecker delta function. $J$ is a positive constant which represents the grain boundary energy. The sum is taken over all nearest neighbor sites. A lattice site is selected at random and the energy given by Eq. (1) is calculated with the nearest neighbors. This energy is compared with the energy when orientation of the site is replaced by that of one of the nearest neighbors. If the energy change is zero or negative, the new orientation is accepted. This corresponds to the temperature far below the melting point. Reorientation attempts of 150 by 150 are referred to as 1 Monte Carlo step (MCS). The initial structure of the simulation has 2500 grains, which are of uniform size and whose orientations are randomly chosen.

One specific grain with a unique orientation number is chosen at the center of the lattice. This grain will be called an AGG grain. Even if this grain is given high mobility, the grain sometimes shrinks rather than grows. In order to prevent this grain from shrinking, it is made initially four times bigger than the other grains. The AGG grain will be shaded in the figures. In order to implement the effect of anisotropic grain boundary mobility or energy on AGG, the matrix grains will be classified into type I and type II grains. A parameter C was introduced to distinguish between type I and type II grains. If $\mathcal{S}_i \leq \mathcal{C}$, the grain is type I, whereas if $S_i > C$, the grain is type II.

For simplicity, we use only two kinds of grain boundary mobility: low and high. The grain boundary between type I and AGG grains will have low mobility. The grain boundary between type II and AGG grains will have high mobility. All the other grain boundaries between type I and type II grains have low mobility. The low mobility grain boundary is 100 times slower than the high mobility one. This means that the mobility of grain boundaries between type I and AGG grains is 100 times lower than that between type II and AGG grains. Also the grain boundaries between type I and type II grains have the mobility 100 times lower. It should be noted that in the simulation we cannot increase the mobility higher than the normal one. Since mobility anisotropy can be made by reducing the mobility of the specific grain boundary, the overall growth rate decreases compared with that of the normal isotropic mobility. Isotropic grain boundary energy is assumed in the simulation for the effect of anisotropic grain boundary mobility.

Figs 1(a), 1(b) and 1(c) show the effect of the percentage of type II grains on AGG. Fig. 1(a) shows the microstructure evolution of AGG after 500 MCS when the percentage is 100%. All the grain boundaries have low mobility except those shared with the AGG grain. The AGG grain has growth advantage exclusively over the other grains. It is quite natural that AGG should take place in such a case. This result is practically the same as that shown by Rollett *et al.* [7].

Fig. 1(b) shows the microstructure evolution after 500 MCS when the percentage is 90%. It should be noted that island grains, which are not observed in Fig. 1(a), are observed in Fig. 1(b), though their frequency is low. As expected, all island grains in Fig. 1(b) turn out to be type I grains. The grain boundary of the AGG grain migrates away from them because of the mobility difference. In this case, the phenomenon is the same as the second phase particles break away from the grain boundary after overcoming the Zener's drag [15]. In the simulation by Rollett *et al.* [7], the island grain did not appear when AGG took place by mobility anisotropy. This might be due to the assumption that all the grain boundaries shared by the AGG grain have high mobility as in the case of Fig. 1(a). The size of the AGG grain in Fig. 1(b) is much smaller than that of Fig. 1(a), which implies that growth of the AGG grain must have been markedly inhibited by type I grains of 10%.

Fig. 1(c) shows the microstructure, where the percentage of type II grains is 80%. The shaded AGG grain grows in an abnormal manner initially; the size becomes about 10 times larger than the average size after 500 MCS. Then the relative size gradually decreases with further MCS. The microstructure in Fig. 1(c) is after 3000 MCS. When MCS increases further, the AGG grain tends to shrink. Comparison of the size of the AGG grain in Fig. 1(c) and that in Figs 1(a) and 1(b) indicates that growth of the AGG grain in Fig. 1(c) was inhibited markedly, implying that the high mobility grain boundary of 80% was inhibited due to the low mobility of grain boundary of 20%.

In this sense, low mobility grain boundaries have a pinning effect on high mobility grain boundaries. If a grain boundary of the AGG grain overcomes the

pinning effect, it will migrate away, leaving type I grains behind. That is, type I grains become island grains. If not, however, growth of the AGG grain is pinned by type I grains. This pinning effect comes from the coupled motion between grain boundaries through the triple junction. Fig. 1(c) indicates that even when 80% of the grain boundaries of the AGG grain have mobility 100 times higher than that of 20% of them, AGG cannot take place.

For the effect of anisotropic grain boundary energy, we also use two kinds of grain boundary energy: low and high. High grain boundary energy is assumed to be three times larger than low grain boundary energy. Under this condition, the high energy grain boundary can be replaced energetically by the two low energy grain boundaries, which corresponds to solid-state complete wetting and will be called simply wetting hereafter. Grain boundaries between type I and AGG grains have high energy. And the grain boundaries between type II and AGG grains have low energy. All the grains boundaries between type I and type II grains will have high energy.

Figs 2(a), 2(b) and 2(c) show the effect of the percentage of type II grains on the microstructure evolution. Fig. 2(a) shows the microstructure after 500 MCS with 100% type II grains. The AGG grain can continue to grow by wetting through the grain boundaries between matrix grains. Island grains, which are shown in the figure, are formed by solid state wetting. This mechanism of the island grain formation is quite different from that shown in Fig. 1(b). This aspect will be dealt with in more detail in the discussion.

Fig. 2(b) shows the microstructure after 500 MCS with 70% type II grains. Compared with Fig. 2(a), the growth rate is retarded but the growth mode is definitely AGG. Fig. 2(c) shows the microstructure after 2000 MCS with 40% type II grains. In this case, the growth mode of AGG was not marked in the initial stage but became marked in the later stage. We observed that even at 30% type II grains, AGG took place eventually in some cases and it did not in other cases; it depended on the initial condition, which is randomly determined. As shown in Figs 2(b) and 2(c), with decreasing percentage of type II grains, frequency of island grains decreases markedly.

The frequency of island grains shown in Fig. 1(b) and Fig. 2(a) is much lower than we experimentally observed in the systems during AGG, especially in the initial stage. For example, the number of island grains in the initial stage of AGG in the Fe-3%Si alloy [16] is more than one hundred in one AGG grain. According to our observation, frequency of island grains tends to be high in the system with second phase particles, which inhibit the grain boundary migration. Such high frequency might come from the difference in the effect of second phase particles on growth by wetting and by grain boundary migration. Second phase particles would not have a pinning effect on wetting as they have on grain boundary migration since wetting is determined purely energetically by the anisotropy of the grain boundary energies at the triple junction. Therefore, in the presence of inhibitors, the growth by wetting will be more dominant over that by the boundary migration. In such a case, formation of island grains can be favored.

These possibilities are tested by the simulation in Fig. 3. In Fig. 3, frequency of atomic jumps is reduced by the factor of 10 except at the triple junction. In other words, the mobility of the grain boundary is reduced but the wetting kinetics is not reduced. Therefore, solid-state wetting is not affected by the reduced boundary mobility. The anisotropy in grain boundary energies

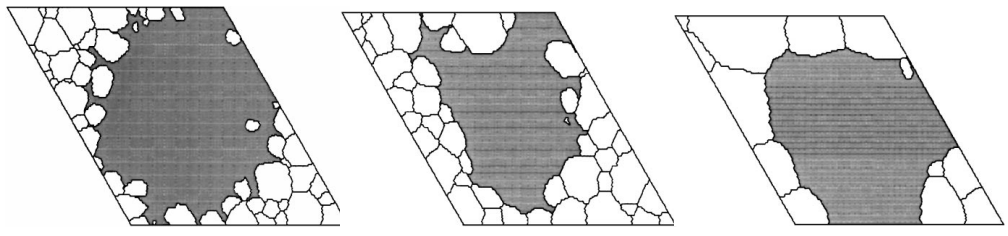


*Figure 2* Microstructure evolution after (a) 500 MCS, (b) 500 MCS and (c) 2000 MCS with the percentages of type II grains, (a) 100%, (b) 70% and (c) 40%. The grain boundary between AGG and type I grains has energy 3 times that between AGG and type II grains or between type I and type II grains.

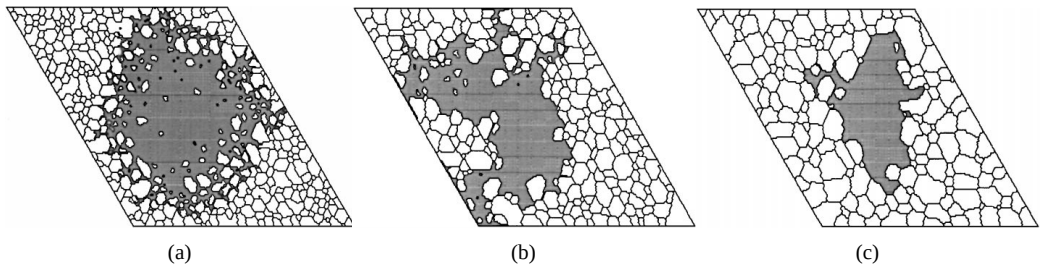


*Figure 3* Microstructure evolution after (a) 500 MCS, (b) 500 MCS and (c) 1000 MCS with percentages of type II grains, (a) 100%, (b) 80% and (c) 60%. The overall mobility except at the triple junction is reduced by 10 times. Conditions for anisotropy in grain boundary energy are the same as Fig. 2.

between AGG, type I and type II grains is the same as that of Fig. 2.

Figs 3(a), 3(b) and 3(c) show the microstructures with percentages of type II grains 100%, 80% and 60%, respectively. Figs 3(a) and 3(b) are after 500 MCS and Fig. 3(c) is after 1000 MCS. Frequency of island grains in Fig. 3(a) is much higher than that in Fig. 2(a). The high frequency of island grains in Fig. 3 is comparable to that observed experimentally in the initial stage of AGG in the specimen of the Fe-3%Si alloy [16]. It should be noted that the Fe-3%Si steel contains the second phase particles such as MnS and AlN, which have a strong pinning effect on grain boundary migration. Fig. 3 indicates that frequency of island grains increases with reducing the grain boundary mobility and decreases with decreasing fraction of type II grains.

The AGG grain in Fig. 3(a) is slightly smaller than that in Fig. 2(a). If the size is normalized by the average size of matrix grains, however, the AGG grain in Fig. 3(a) is much larger than that in Fig. 2(a). Therefore, AGG induced by wetting tends to be more pronounced when the migration of the grain boundary is suppressed.

## 3. Discussion

The result of Fig. 1 indicates that AGG cannot take place by anisotropic mobility unless the percentage of high mobility boundaries is unrealistically high; even 80% is not enough. This result is against some of previous treatments of AGG, which were based on advantage in grain boundary mobility over the other grains [3, 8]. The reason why such high fraction of high mobility boundaries cannot lead to AGG seems to be the triple junction constraint. The triple junction imposes a constraint on the grain boundary migration, which is coupled with the migration of the two other grain boundaries at the junction. If the triple junction is immobile, it imposes a strong pinning effect on the grain boundary, which is similar to that imposed by the second phase particle. Therefore, even if a specific grain boundary has extremely high mobility, it cannot migrate with that mobility unless the triple junctions connected to the grain boundary migrate sufficiently fast. For this reason, only almost a perfect texture as the cases of Figs 1(a) and 1(b) can induce AGG by anisotropic grain boundary mobility.

The fraction of the high mobility grain boundary in a real system, where AGG takes place actively, needs to be mentioned for comparison with fractions in Fig. 1. Grain boundary mobility depends on crystallographic orientation and impurity [17–19]. In a polycrystal, the coincidence site lattice (CSL) boundary is known to have high mobility [17]. Harase and Shimizu [3] reported that frequency of the CSL grain boundary between the hypothetical abnormal nuclei and the other grains is relatively high, based on the experimental determination of orientations for thousands of grain after primary recrystallization of the Fe-3%Si steel. They attributed this relatively high frequency to the high growth rate of AGG. But the frequency is at most 20%. Fig. 1 indicates that even if uncertainties are considered, this frequency cannot explain AGG by anisotropic grain boundary mobility.

On the other hand, considering that the relative size of the AGG grains in Fig. 1(c) decreases after the initial growth to the size about 10 times larger than average matrix grains until 500 MCS, it can be said that neither mobility advantage nor driving force advantage can induce AGG. Most conventional approaches to AGG [20–23] belong to this category: mobility advantage or driving force advantage. Even if a specific grain has both size and mobility advantages, the grain does not undergo AGG because of the triple junction constraint.

The result of Fig. 2 indicates that AGG can eventually take place with type II grains as low as 40%. The limit of AGG can decrease to 30%. Although 30% or 40% is still higher than a real condition, AGG takes place under a much more realistic condition by anisotropic energy than by anisotropic mobility. The important point to be noted is that growth by solid-state wetting is free from the triple junction constraint. This fact seems to be related to the present simulation results that AGG is favored more by anisotropic energy than by anisotropic mobility of grain boundaries.

Fig. 2 also indicates that island grains, which are observed inside AGG grains in many systems [2, 8–12], can easily be developed by wetting. In the Fe-3%Si alloy, the frequency of island grains is extremely high, especially near the growing front of AGG [16]. Large aggregates of the grains, which are isolated inside the AGG grain, are also commonly observed. These island aggregates are much larger than the dimension of the grain boundary. Therefore, it is difficult to explain island aggregates by anisotropic grain boundary mobility. The high frequency of island grains cannot be explained by the mobility effect, either. These aspects can be best explained by grain boundary wetting with suppression of grain boundary migration as shown in Fig. 3.

The Fe-3%Si alloy contains grain growth inhibitors such as MnS or AlN, which play a critical role in inducing AGG. From the viewpoint of AGG by wetting, the role of these second phase particles is twofold; one is to favor growth by wetting over growth by grain boundary migration and the other is to inhibit the grain growth of the matrix grains. Since the first role is revealed in Fig. 3, the second role will be mentioned. In order to favor AGG by wetting, the grain boundary energy among the matrix grains should remain high. We previously showed that the grain growth makes high energy boundaries replaced by low energy ones [13]. This means that if the grain growth is not suppressed by the second phase particles, the fraction of the high energy grain boundary will decrease and then AGG by wetting will be disfavored. This new possibility in the role of the second phase particles in inducing AGG would not be valid if AGG does take place by wetting.

On the other hand, the present simulations are done on a two-dimensional lattice but the real system is three-dimensional. In the two dimensional case, grain boundary wetting is the only possibility. In the three dimensional case, however, wetting along the triple junction is also possible. For a given anisotropic grain boundary energy, triple junction wetting can be more easily

achieved than grain boundary wetting. For example, when the second phase wets the grain boundary, the dihedral angle has to be zero for the grain boundary wetting but it only has to be less than 60° for the triple junction wetting.

## 4. Conclusion

By comparing the Monte Carlo simulation between effects of anisotropic grain boundary mobility and energy, we showed that anisotropic energy induces AGG under a more realistic condition than anisotropic mobility. The experimentally observed realistic microstructure of AGG with high frequency of island grains is reproduced by growth by wetting combined with the pinning effect of the grain boundary. Based on these results, a new concept of the triple junction wetting is introduced as a possible mechanism of AGG.


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