Consideration of pinning and dissolution with dividing sites in Monte Carlo simulation of grain growth

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Abstract
Various distributions of particle size are considered in the present work to study the effect of pinning by a bimodal distribution of particles on grain growth simulation in comparison with that of the real distribution of MnS (30-50 nm) and AlN (5-8 nm) in a Fe3%Si alloy grade HiB. A dividing site technique is used to make easy consideration of different size of particles together without increasing matrix size for calculation. The dissolution of precipitates introduced after the stagnation stage allows grain growth to start again. The dividing sites technique allows the consideration of particle dissolution by gradual vanishing of peripheral layers of particles, in agreement with the experimental evolution.

1. Introduction
The second phase particles which act on the grain boundary migration rate permit to control the grain size and orientation during normal growth. So, it is possible to seek the most appropriate matrix for the abnormal growth of a given orientation such as the Goss grains in Fe-3%Si steels. The grain boundary dragging by a second phase depends on its shape, size, distribution and volume fraction. Zener [1] was the first to propose a model permitting to calculate this dragging force, then, several models were proposed to explain the effect of a homogeneous distribution of particles on recrystallization and grain growth [2-5]. Simulations of materials containing particles generally take into account only one particle size [6-14]; the introduction of several particle sizes was performed in an analytical way [15,16]. The case of bimodal distribution was considered by simulation of interactions between grain boundary migration and precipitates [17]. The aim of the present work concerns the influence of the bimodal distribution of MnS (30-50 nm) and AlN (5-8 nm) inhibitors on normal grain growth of Fe-3%Si alloy, grade Hi-B that presents an inhomogeneous microstructure, where the size factor is not required condition for grain growth.

2. Dragging force in simulations procedures
As mentioned, Zener [1] was the first to propose a relation between the dragging force and grain size, volume fraction of the particles and the grain boundary energy, i.e.:

\[ P_z = \frac{3}{2} \frac{\gamma f}{r} \]  \\

Pz is the pinning force, \( \gamma \) is the grain boundary energy, \( f \) is the volume fraction of the particles and \( r \) is their average radius. The introduction of particles is performed by randomly allocating them in the matrix [6-8]. The pinning study is performed by introducing the Zener dragging force \( P_z \) [18]. In the present work, the initial matrix used in the simulation is the microstructure of a Fe-3%Si sheet grade Hi-B after primary recrystallization. This microstructure was characterized by EBSD on a grid 200x230 sites with a step scanning equal to 2 \( \mu \)m, (figure 1-a).

Figure 1: Initial matrix used in the simulation (a), grain size distribution (b) and \{100\} pole figure (c).
A deterministic approach of a Monte Carlo simulation technique was adopted from analysis of the experimental parameter evolution. Inside a grain each site of the studied zone is characterized by an orientation given by the three Euler angles ($\phi_1$, $\phi_2$, $\phi_3$). An orientation number different from all the orientations present in the matrix is assigned to precipitates: (-1) for the precipitates inside the grains and (-2) for those at grain boundaries. Four particle sizes (1, 7, 13, and 19 sites) have been considered. This choice corresponds to a node (1 site) with its first (7 sites), second (13 sites) and third (19 sites) neighbors, in a hexagonal grid of simulation. The use of grid with low resolution (200x200) [6] by allocating one site by particle does not allow to simultaneously consider particles with different sizes. Figure 2 shows the random distribution of a 2% volume fraction of particles with 1, 7, and 19 sites by particle. Fig.2 reveals the presence of grains whose size is similar to that of precipitates having 7 sites; the grain size distribution of the initial matrix is presented figure 1-b. The first size class shows an abnormality: the particles are bigger than many grains of the matrix. The effect is obviously more pronounced with 13 or 19 site particles. Then, consideration of these precipitates in the calculation of the pinning effect does not have any more sense; it is rather two-phase microstructure, in which one can not consider pinning effect.

3. Simulation procedure with dividing sites

Generally, the real microstructures used in simulation are characterized by EBSD [19]. The precipitates whose size is less than 1 $\mu$m are difficult to characterize because of the low resolution of W filament-SEM, a technique of dividing sites was used in the simulation to bypass the difficulty [17]. At the particle scale, each site is divided in a given number of sites permitting the introduction of different size of particles while respecting the ratios between particle and grain sizes. Double-grid method was also used for modeling stressed grain growth related to grain boundary migration [20]. The choice of initial matrix size and that of dividing coefficient $G$ must be in agreement with the experimental values of the ratio between biggest precipitate sizes and smallest grain sizes. In the present matrix (HiB Fe3%Si with MnS and AlN inhibitors), that ratio is about 5%. With the initial matrix (200x230 sites) 4 sites are attributed to the smallest grains (5$\mu$m), therefore it is impossible to reasonably consider particle effect in simulation by assigning them an entire site. With a dividing site coefficient $G=64$, one site is treated as 64 sub-sites, a matrix with (1600x1840) sites is used instead of the initial matrix (figure 3). The introduction of different sizes of particles becomes easy, one sub-site is attributed to AlN particle and 13 sub-sites are attributed to MnS particle.

With that dividing technique, a finer grid is locally used without increasing the calculation time, since the memory is not occupied by big matrixes. The dividing procedure is only performed during computation; the calculation time is practically the same as that with 1 site/particle and a matrix 240X240. To achieve the same effect of growth with adequate size reports for (largest particle/smallest grain) and (smallest particle/largest particle) it would be necessary to start the simulation with initial matrixes with a minimal size $10^5 \times 10^5$. After dividing sites, the first class is equal to about 200 sites instead of 10 sites in the initial matrix (Fig.1 b) without dividing; this smaller size among the grains of the matrix is clearly higher than that of the biggest precipitates (13 sub-sites) considered in the present work.

The grain boundary energy was firstly considered as isotropic i.e. $\gamma = J = 1$. With anisotropy of the grain boundary energy, $J$ involves different values in the simulation [21]. The initial microstructure was drawn with a step size equal to 2 $\mu$m. After dividing sites the grid parameter becomes equal to

Figure 2
Microstructure 200x200 with random distribution of 2% particles affecting: 1 site (a), 7 sites (b) and 19 sites (c). (by particle)
0.25 µm. The particle diameter for a hexagonal grid is given by 
\[ d = \left( \frac{4A}{\pi} \right)^{1/2}, \text{ where } A = \frac{na^2 \sqrt{3}}{2}, \text{ n is the site number of the particle and ‘a’ is the grid parameter [10]}. \]

Table 1 presents the values used in the simulation. The figure 3 shows the dragging force for different implicit values of \( P_z = 0, 1, 3, 5 \).

| Particle size (sites) | Particle diameter d (µm) |
|-----------------------|-------------------------|
| 1 site                | 0.2625                  |
| 7 sites               | 0.6946                  |
| 13 sites              | 0.9465                  |
| 19 sites              | 1.1443                  |

**Table 1:**
Values of pinning force used in simulation.

The figure 4 shows that when the dividing coefficient \( G \) increases the pinning effect is more marked and the maximal size of particles to stabilize pinning effect increases; one changes from 5 sites for \( G=0 \) to ~ 30 sites for \( G = 64 \). The technique permits to consider different size of particles with a bimodal distribution and different layers of dissolution without increasing calculation matrices.

4. Bimodal distribution
The choice of the site number allocated to particles is based on the neighbor number for the grid; for a hexagonal grid 1, 7 and 19 sites [10, 12, 13, 16] are generally considered. The second neighbors being constituted of 6 sites, it was chosen to work with 1, 7, 13 sites because this distribution is more in agreement with the experimental matrix. The bimodal distribution of MnS (30-50 nm) and AlN (8-9 nm) precipitates in the Fe-3%Si Hi-B gives a size ratio of about 3.5 between the two types of precipitates [22]. To study the effect of the bimodal distribution of these precipitates on the normal grain growth, the average size of each population was taken into consideration, that is: 1 sub-site (d=0.26) for AlN and 13 sub-sites (d=0.94) for MnS, respecting together the experimental diameter ratio and the true neighborhood of the hexagonal grid. The two populations of particles have been identically allocated in the microstructure, the volume fraction of the two populations of precipitates was equal 2 and 1% respectively, the dragging force is calculated with values of table 1.

6. Simulation of the precipitate dissolution
The dissolution of the precipitates begins by the diffusion of the peripheral atoms. In first approximation, that behavior can be described in simulation procedure by gradual vanishing of precipitate volume, the peripheral sites become sites of the matrix. The dissolution of precipitate occurs by successive layers; the sites initially allocated to particles (that is not submitted to reorientation) are gradually submitted to reorientation, layer after layer. Figure 5 shows the isotropic case with 2% particles in the initial matrix. In a first approach the precipitates dissolution was considered at the end of stagnation, about after 1300 MCS. The dividing sites technique allows the
consideration of particle dissolution by gradual vanishing of peripheral layers of particles, the results are most in agreement the experimental evolution.

Figure 5
Dissolution with and without dividing site in isotropic case of grain growth with 2% particles.

Conclusion
This work was focused on the introduction of a bimodal distribution of precipitates similar to the experimental one that control normal growth in a Fe-3%Si Hi-B. The study was performed in a determinist way from the evolution parameter analysis obtained experimentally. A high resolution matrix (1600x1840) coupled to a technique of dividing sites of the experimental matrix was used to respect the ratio between the size of biggest particles and that of smallest grains. The dissolution of the precipitates at the end of growth is an important step because the purification of the matrix by precipitate dissolution enables to get a secondary matrix without residual primary matrix. In the procedure simulation, the dividing sites technique allows the consideration of particle dissolution by gradual vanishing of peripheral layers of particles, in agreement with the experimental evolution.

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