Effect of Strain Restored Energy on Abnormal Grain Growth in Mg Alloy Simulated by Phase Field Methods

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Abstract. Abnormal grain growth of single phase AZ31 Mg alloy in the spatio-temporal process has been simulated by phase field models, and the influencing factors of abnormal grain growth are studied in order to find the ways to control secondary recrystallization in the microstructure. The study aims to find out the mechanisms for abnormal grain growth in real alloys. It is shown from the simulated results that the abnormal grain growth can be controlled by the strain restored energy. Secondary recrystallization after an annealing treatment can be induced if there are grains of a certain orientation in the microstructure with local high restored energy. However, if the value of the local restored energy at a certain grain orientation is not greater than $1.1E_0$, there may be no abnormal grain growth in the microstructure.

1. Introduction

Abnormal grain growth phenomena are also know as secondary recrystallization, and they are the phenomenon that growth of most of grains during the annealing process is blocked due to various reasons and a few grains grow rapidly away from the normal grain growth [1-2]. Since the abnormal grain growth usually results in very large grain size, the grain size is sometimes even on the order of centimeters. It is known that the matrix grains away from the expanded grains should keep their size stable basically, so that the abnormal grain growth can continue [3]. So, key theoretical problem on studding abnormal grain growth is to investigate grains which are likely to be secondary grain to grow abnormally and the reason the matrix grain size maintain stable. For this reason, abnormal grain growth and the influencing factors have been researched in the scientific literature and reports, during the past years [4-7].

Reference [4] has studied the abnormal grain growth mechanism of austenite in high-strength welded steel Q1030 at different heating temperatures and showed that in a certain heating temperature range, parts of austenite grains in Q1030 steel grow abnormally, leading to mixed grain phenomena. Reference [5] also found that abnormal grain growth can occur when the composite material with the pinning particles Al_2O_3 was annealed at 530^{o}C for Friction Stir-Processed Al 6061, but completely prevented at 470^{o}C . On the other hand, Monte Carlo Potts model has been used in reference[6] to prove that the inhomogeneity of interface migration is the reason of abnormal grain growth . Reference [7] has puttd forward a new concept of sub-boundary-enhanced solid-state wetting,according to the authors, gains with sub-boundaries have growth advantage and may have

abnormal growth , the results are obtained by a phase field mode simulation. However, there is no systematic study on the mechanism of abnormal grain growth in alloys.

AZ31 Magnesium alloy is selected as the research object in this paper. Phase-field models are established to simulate the abnormal grain growth phenomena of AZ31 Mg alloy, in order to seek the influences resulting in abnormal grain growth, and explore the possibility of obtaining the ideal mixed grain microstructure containing dispersed large grains in AZ31 Mg alloy. AS we know, grain size is a critical issue for the application of advanced materials, researches about influencing factors on abnormal grain growth is important to control the properties of materials so that use them effectively.

2. Model description

Grain growth simulations in 2D and 3D were performed using the phase field methods successfully [8,9], where the thermodynamic variable such as concentration, the orientation state of grains and the temperature are represented as the field [10-11]. In this paper, η indicates a series of long-range orientation field variables, describe the instantaneous spatial orientations of grains, such as: $\eta_1(\mathbf{r}, t)$, $\eta_2(\mathbf{r}, t)$, ...$\eta_p(\mathbf{r}, t)$, p is the number of η in the system. It is showed in reference[11] that the influence of the number of p on grain size distributions is much small when p>10. The larger the value of p, the closer to the real grain growth process. So, p is taken as 512 in order to be closer to the actual situation. If η_1=1 and $\eta_i(_{i\neq 1})$=0, it means in the grain, if $0\eta_1<1$,it means in the grain boundaries.

Total free energy F in the single phase system with multi-orientation parameters can be expressed as [12]:

$$F = \int [f_0(c, \eta_1(\mathbf{r}, t), \eta_2(\mathbf{r}, t), ..., \eta_p(\mathbf{r}, t)) + \frac{K_2}{2} \sum_{i=1}^{p} (\nabla \eta_j(\mathbf{r}, t))^2] d^3\mathbf{r} \tag{1}$$

Where K_2 is the gradient item parameters, f_0 represses the function of the local free energy density. f_0 is described by the expression as follows[12]:

$$f_0 = A + A_1(c(\mathbf{r}, t) - c_i)^2 + \frac{A_2}{4}(c(\mathbf{r}, t) - c_i)^4$$
$$-\frac{B_1}{2}(c(\mathbf{r}, t) - c_i)^2 \sum_{i=1}^{p} \eta_i^2(\mathbf{r}, t) + \frac{B_2}{4}(\sum_{i=1}^{p} \eta_i^2)^2 + \frac{K_1}{2} \sum_{i=1}^{p} \sum_{j \neq i}^{p} \eta_i^2(\mathbf{r}, t) \eta_j^2(\mathbf{r}, t) \tag{2}$$

where $c(\mathbf{r}, t)$ is the variable of concentration field, c_l is the lowest concentration point of the free energy and concentration curve, K_1 is the coupling item parameters between η_i and η_j.

The time-dependent instantaneous microstructure evolution can be governed by the Allen-Cahn equation and Cahn-Hilliard diffusion equations as follows below[13, 14]:

$$\frac{\partial \eta_i(\mathbf{r}, t)}{\partial t} = -L \frac{\delta F}{\delta \eta_i(\mathbf{r}, t)}, \quad (i=1, 2, 3, \ldots, p)$$

$$\frac{\partial c(\mathbf{r}, t)}{\partial t} = M \nabla^2 \frac{\delta F}{\delta c(\mathbf{r}, t)} \tag{3}$$

where L is the interface mobility coefficient and M is the diffusion mobility coefficient.

The nucleation process is simplified to be phenomenal nucleation by putting a predetermined initial microstructure in the models. The initial state is that $4dx \times 4dx$ unit grid averagely scattered in the simulation area, which means the radius of the nucleation is a random value from 0 to 2 grids. 512×512 two dimensional grids are selected in the paper, each grid size is 0.29μm. The time step Δt must be selected to prevent the calculation results from being inaccurate or inefficient, and is chosen as 0.3s[15].The boundary is the periodic boundary, so as to reducing the boundary effect. The temperature is set as 300 ^{o}C in the models, the other parameters are selected by ref. [12] that c_l = 0.2, A

= -22.1 kJ·mol^{-1}, A_1 = 21.1 kJ·mol^{-1}, A_2 = 13.0 kJ·mol^{-1}, B_1 = 1.79 kJ·mol^{-1}, B_2 = 51.2 J·mol^{-1}, K_1 = 141.2 J·mol^{-1}, K_2 = 3.54×10^{-12} J·m^2·mol^{-1}, L = 1.0×10^{-7} m^3·(J·s)$^{-1}$ in the models.

3. Influencing factors of abnormal grain growth

The strained restored energy is controlled by the value of B_1 and B_2, which means the the local value at a certain orientation of free energy in the system can be different if the local strained restored energy is different. Since the energy of the system has to be minimum in the gains, the derivative of Eq. (2) for η is 0 when η=1, so it is obtained that:

$$B_1(c\text{-}c_1)^2=B_2 \tag{4}$$

On the other hand, it is defined that when η_i^2=1 and $\sum_{j\neq i}^{p}\eta_j^2=0$ in Eq. (2), f_0 represents the free energy of the system after recrystallization, but $\sum_{i=1}^{p}\eta_i^2=0$ represents the deformed system before recrystallization [12] . So E_0 released can be obtained as below:

$$E_0 = f_0(\sum_{i=1}^{p}\eta_i^2=0) - f(\eta_i^2=1,\sum_{j\neq i}^{p}\eta_j^2=0) \tag{5}$$

where E_0 is the form of defects energy in the system, and it will be the driving force for recrystallzation[16]. It is studied from reference[17] that the greater the prestrain, the greater the stored energy, and the value of the stored energy will become a constant when the perstain is larger than 0.2 [17]. In this paper,the restored energy is selected to be 0.54 J/g, through conversion, it is obtained E_0=12.8 J·mol^{-1}[17] and the prestrain in the system is taken as 0.25. Then the values of B_1 and B_2 can be obtained by solving Eqs. (4) and (5).

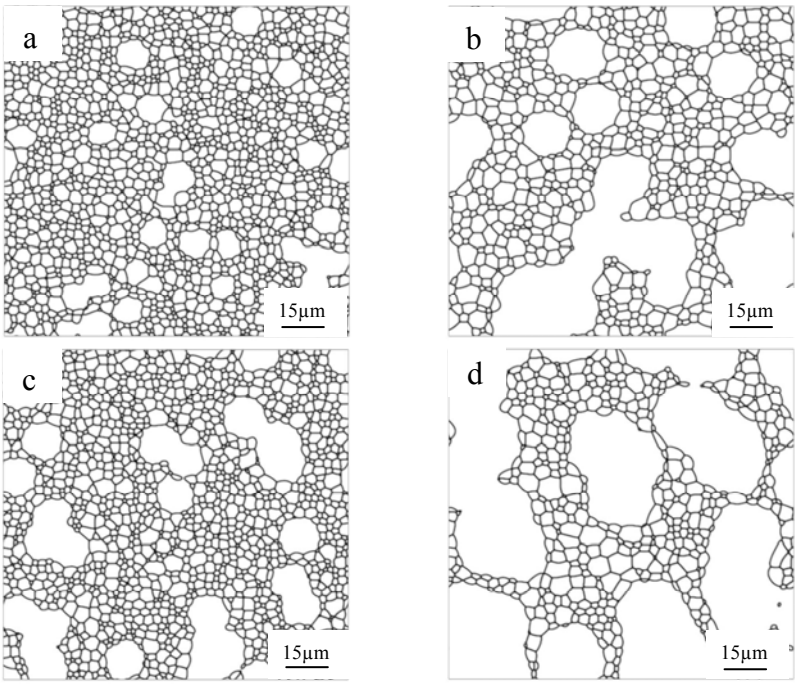

Fig. 1 The simulated results with the local E_0' are 1.2E_0 and 1.3E_0 respectively in a certain grain orientation at different annealing time t: **a** E_0' is 1.2E_0 and t = 10 min; **b** E_0' is 1.2E_0 and t = 20 min; **c** E_0' is 1.3E_0 and t = 10 min; **d** E_0' is 1.3E_0 and t = 20min

From the simulation results of Fig.1, it can be seen that there are several very big grains in the microstructure, this is because there are some grains with high restored energy in a proper orientation which is due to plastic deformation, as is seen in Fig.1. where E_0' is the local high strain restored energy, and can be obtained by change the local parameters B_1' and B_2'. In Fig. , the value of local B_1' and B_2' are enlarged to be 1.2 and 1.3 times as much as B_1 and B_2 respectively, then E_0' is changed to be $1.2E_0$ and $1.3E_0$.

Quantitatively analyze the average grain size changes over the annealing time, and the simulated results are seen in Fig. 2.

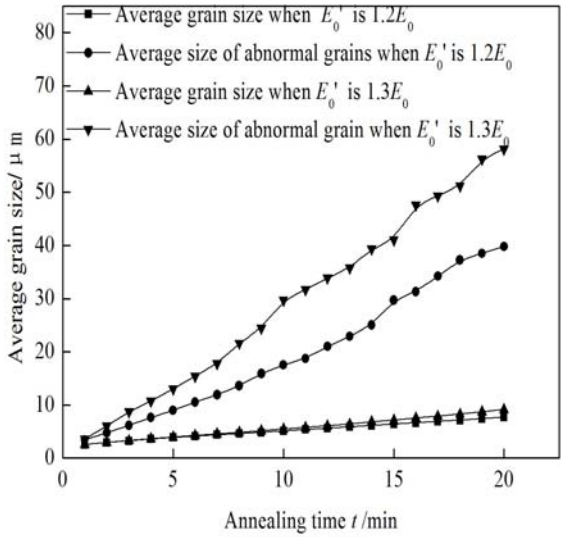

Fig.2 The average grain size of the microstructure along the annealing time if local E_0' in proper grain orientation is $1.2E_0$ and $1.3E_0$, where E_0' is the local restored energy, E_0 is the restored energy in the matrix grains

It is found from Fig. 2 that, the grains growth velocity for the total microstructure is very slow, it is about 8 μm at 20 min, however, the other much big grains grow very fast and their grain size is increasing along the annealing time. It may be the reason that the the uneven plastic deformation of the Mg alloy will result in uneven distribution of restored energy. If the several local grains of a certain orientation contain higher restored energy, the enormous grains will be appeared in the simulated microstructure. E_0' may be the driving force for grain growth, and it is the reason for some big separate grains in the microstructure. However, If the local restored energy is too much high, there may be all enormous grains without normal grains left after annealing. So the plastic pre-strain should be carefully controlled.

When local strain restored energy in a certain grain orientation is changed to be $1.1E_0$, the phenomenon of abnormal grain growth is not obvious, as is shown in Fig. 3.

From the simulated results of Fig.3, it is found that, if E_0' is $1.1E_0$ while the matrix restored energy is E_0, the phenomena of abnormal grain growth is not obvious. However, there are a few large grains with abnormal growth trend when the annealing time is 20 min, and if the local restored energy is further increased, significant secondary recrystallization may be occurred.

Quantitatively study the evolution of the grains with the annealing time and the simulated results are shown in Fig 4.

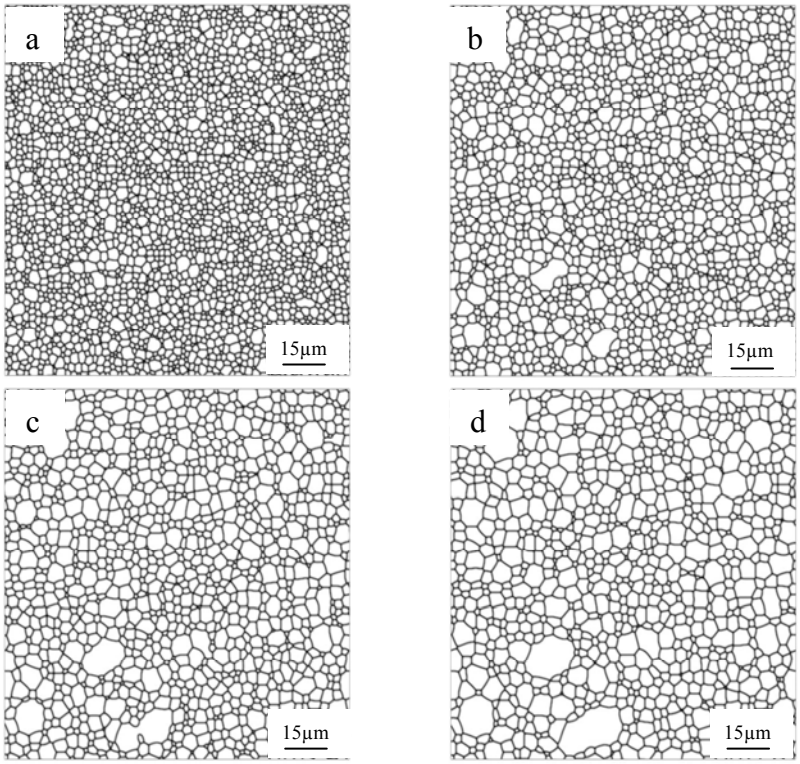

Fig. 3 Simulated results of grain growth when the local $E_0^{'}$ in a certain grain orientation is $1.1E_0$: **a** t = 5 min; **b** t = 10 min; **c** t = 15 min; **d** t =20 min

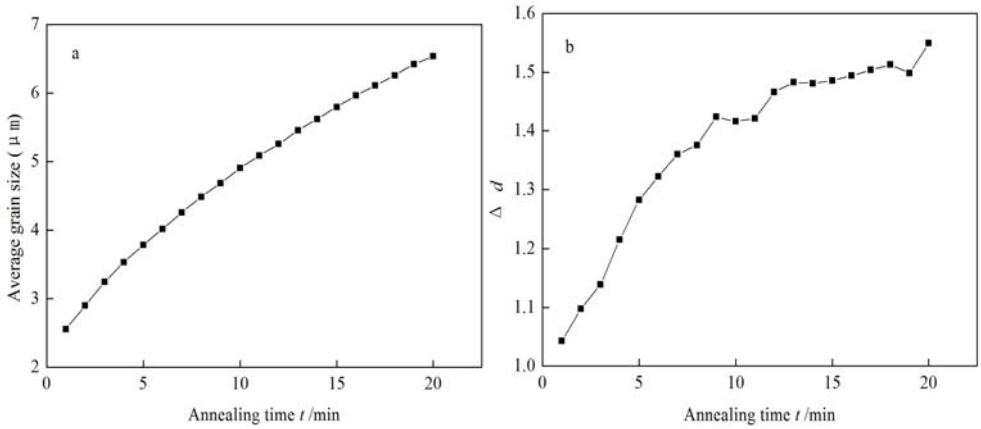

Fig. 4 Average grain size changing with the annealing time and grain size fluctuation when the local $E_0^{'}$ is 1.1 E_0 in a certain grain orientation: **a** average grain size evolution; **b** grain size fluctuation.

As is seen from Fig. 4 (a), the average grain size is increased smoothly with the annealing time, without sudden changes. Further study the grain size fluctuation of the microstructure by the function $\Delta d = (d_{\max}\text{-}d_{\min}) / d_{ave}$, where Δd is the mixed grain degree, $d_{\max}$ is the average grain size of maximum grains of total content of 5%, $d_{\min}$ is the average grain size of minimum grains with total content of 5%，d_{ave} is the average grain size of total microstructure[12]. It is shown that $\Delta d < 2$ in Fig. 4 (b), which indicate that the size difference between large and little grains is small, so there may be no secondary recrystallization when $E_0^{'}$ is 1.1 E_0.

4. Conclusion

If several local grains of a certain orientation contain higher restored energy, the enormous grains will be appeared in the simulated microstructure, the the uneven plastic deformation of the Mg alloy will

result in uneven distribution of restored energy. However, if the local restored energy in a certain grain orientation is not greater than $1.1E_0$, there may be no secondary recrystallization.

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