MATEC Web of Conferences **67**, 06088 (2016) DOI: 10.1051/matecconf/20166706088
SMAE 2016

Comparative Research on Nanometer and Micrometer Grain Growth of Polycrystalline AZ31 Magnesium by Phase Field Models

Yan WU[1,a,*] and Si XIA[2, b]
[1,] School of Mechanical Engineering, Wuhan Polytechnic University,P. R. China
[2.] Special Vehicle Techology Center, The fourth Academy of China Aerospace Science & Inoustry Corp, P. R. China
[a] wuy611@163.com[*] [b]xiasi_85@163.com

Abstract. Nanometer scale and micron scale grain growth of polycrystalline AZ31 Magnesium alloy have been comparatively studied by phase field simulation, and the models are established under realistic spatial-temporal scales. The expression of local free energy density function is modified due to the different initial state of grain growth process at nano scale. The term of grain boundary range is to explain the physical backgrounds of the order parameter gradients at grain boundary and the diffusion grain boundary, and it is related to the correct gradient and coupling parameters. The simulated results are compared in nano scale and micron scale, they are also compared with experimental results in the literature, in order to find out the mechanisms for nano-structural evolution. It is shown that the grain boundary range will cover two adjacent grains in nano scale polycrystalline while the range should be a constant big value of about 1.2μm for grains in micron scale. It is found that the grain growth rate at nano scale is slower than that at the micron scale, and these simulated results can be proved by the experimental results in the literature. It is found that the grain size fluctuation is more intensely in nano-sized grains than that in micron-sized grains by the quantitative analysis of the mixed degree of grains size in nano-structure and micron-structure in the models.

1.Introduction

As we know, the mechanical properties of materials are determined by the microstructure. So it is an important way to improve the mechanical performance of Mg alloys by control their microstructure evolution. On the other hand, prediction and controlling the microstructure evolution by the methods of experiments and simulation have increasingly become a focus of current research[1-4]. Generally, First Principle calculation, Molecular Dynamics simulation are thought to be suitable for the analysis of nano-structure and properties since these models are all the typical simulation methods for material behaviors at atom and molecular scales, but the simulated scale is too small, the simulated time is picosecond and cannot finish the evolution of microstructure.

* Corresponding author:wuy611@163.com

Recently, our previous work has already achieved a phase field model to simulate the grain growth process during recrystallization of AZ31 alloy in the real time and space, and the simulated results were agreed well with the experiments [1-4] by introducing a new concept of the grain boundary range. It is believed that the model is the first time to accomplish grain growth simulation of realistic spatiotemporal evolution of microstructure in industrial scale. However, as far as the authors know, there is no phase field model has been reported on nano scale grain growth process in a real alloy.

In this paper, a modification phase field model is reported to comparative study nano-grain and micro--grain growth of polycrystalline AZ31 Mg alloy in the realistic spatiotemporal process. The driving force is re-discussed and the parameters are varied systematically to find the possibilities to form the expected structure Comparisons of the simulated results with the experiments at different temperatures are made to explain the mechanisms of the grain growth especially in nano-structure to establish references for the development of the nanocrystalline materials.

2. Model Description

Phase field methods are based on thermodynamics and kinetics. The temporal evolution of microstructure can be determined by solving the time-dependent Allen-Cahn equation and Cahn-Hilliard diffusion equation as below,

$$\frac{\partial \eta_j(\mathbf{r},t)}{\partial t} = -L\frac{\delta F}{\delta \eta_j(\mathbf{r},t)}, (j = 1,2,...,n)$$

$$\frac{\partial c(\mathbf{r},t)}{\partial t} = M\nabla^2 \frac{\delta F}{\delta c(\mathbf{r},t)} \tag{1}$$

where L and M are the structural relaxation and chemical mobility parameters, respectively, η_j ($\mathbf{r}$, t) is the long-rang orientation parameters, c ($\mathbf{r}$, t) is a concentration field variable, F is the free energy of the system, and its expression in isotropic single phase system is seen as follows,

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

where K_2 is the gradient energy coefficient, f_0 is the local free energy density function.

The local free energy density function f_0 represents the figuration of a phase field model and the basic requirement for it is that f_0 has p degenerate minima located at (η_1, η_2, …η_p) = (1, 0, …, 0), (0, l, …, 0),…,(0, 0, …, 1). We adapt an expression to describe the local free energy density function as follows [5],

$$f_0 = A + A_1(c(\mathbf{r},t) - c_l)^2 + \frac{A_2}{4}(c(\mathbf{r},t) - c_l)^4$$
$$-\frac{B_1}{2}(c(\mathbf{r},t) - c_l)^2\sum_{i=1}^{p}\eta_i^2(\mathbf{r},t) + \frac{B_2}{4}(\sum_{i=1}^{p}\eta_i^2)^2 + \frac{K_1}{2}\sum_{i=1}^{p}\sum_{j\neq i}^{p}\eta_i^2(\mathbf{r},t)\eta_j^2(\mathbf{r},t) \tag{3}$$

where c_l is the concentration at the lowest point of the free energy curve as a function of concentration at a certain temperature, K_1 is the coefficient of coupling item between η_i and η_j, p is the possible number of the grain orientations in the system, and it is taken as 32 as suggested in reference [5].

A wrought AZ31 Mg alloy plate is chosen in the model, and the alloy composition is w(Al)=3%, w(Zn)=1% with rest of Mg. The parameters in the model are already decided by preliminary work of this study that c_l equals to 0.2, A=-25.01 kJ/mol, A_1=22.02 kJ/mol, A_2=18.30 kJ/mol, B_1=3.54 kJ/mol, B_2=92.86 kJ/mol, K_1=141.24J/mol, K_2=35.37×10^{-13}J·m2/mol in micro-grain structure [5]. A=-25.57 kJ/mol, A_1=99.14 kJ/mol, A_2=18.30 kJ/mol, B_1=80.33 kJ/mol, B_2=2321.51 kJ/mol, K_1=2090.16J/mol, K_2=0.21×10^{-13}J·m2/mol in nano-structure [8].

The nucleation process of crystallization is simplified by a phenomenological method, and the well-defined microstructure is formed after a short time. The initial state is given as the 4dx × 4dx unit grids distributing evenly in the simulated area, and the radius of the nucleus is a random value between 0 to 2 grids. There are 512×512 of two dimensional uniform grids in the simulations. The overall size of the simulation cell is 1.5 μm×1.5 μm in nano-structure with each grid size of 2.93 nm, whereas for the micro-grain model, the unit grid size is 0.293 μm and the entire simulation area is 150 μm ×150 μm. The local initial composition is considered as 0.03. The value of the time-step has to be relatively small in order to obtain the convergence results; however, an extremely small value of time-step will require more steps for solving the kinetic equations. The values of 0.6 seconds in the nano scale model and 0.3 seconds in the micron scale model for time-steps are chosen to balance the two factors. The boundary condition of the differential equations is defined as the periodic boundary, in order to minimize the boundary effect on the grain growth kinetics.

3. Grain Boundary Range

A new concept called “grain boundary range” [5-8] have been proposed to define the distance of gradient variation of the long-rang orientation parameters across an interface. The range has a physical concept of the region around an interface which the interface affects in ways of interface energy and interfacial element segregation. The position of the interface defined in our model is the geometric center of symmetry of the grain boundary range. The variation of η across a flat boundary was calculated by present multiscale model in micron grains and it is shown in Fig.1 (a). The grain boundary range r in the microstructure can be measured from Fig.1 (a), and it is indicated by the scale bar in the figure and is about 1.2 μm wide.

The value of grain boundary range 1.2 μm is too large for grains in nano scales whose grain size is less than 1μm and the grain boundary range will have no physical meaning if it covers more than two grains. The volume fraction of grain boundaries increases dramatically when the grain size decreases and reference [9] showed that the nanocrystalline materials might consist of over 50% of geometric boundary regions (interface component) depending on the average grain size. Therefore, we suggest that the nanocrystalline materials will have a grain boundary range which covers up to nearly whole two adjacent grains as is seen in Fig.1 (b). In the simulation ,the average grain size is from 24 nm to 85 nm in nano scale, so the grain boundary range is chosen as 47 nm. The simulated results based on such range model of variation of η across a flat boundary are shown in Fig.1 (b) in nano-structure by our present multiscale phase field model.

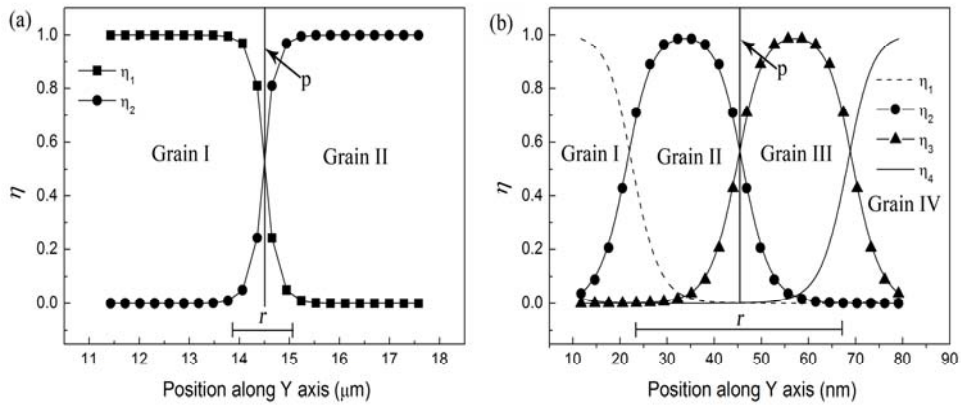
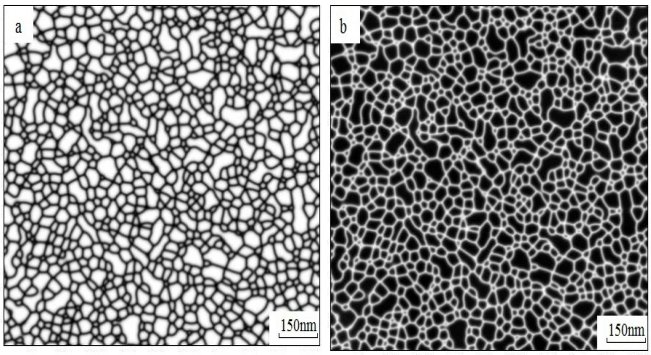


Fig.1. Characteristics of grain boundary in orientation parameters by simulations. (a) for micron scale model; (b) for nano scale model. p — grain boundary position; *r* — the grain boundary range.

It is also seen from Fig.1 (a) that, the values of η_j (j represents a certain orientation of the grains) vary in one grain from 1 to 0 into another grain gradually across the grain boundary range. However, the grain boundary range covers its adjacent two grains in nano scale in Fig.1 (b), which means that the attribution of the orientation of a grain may be influenced not only by itself but also by its nearest neighbors. It is the size and the physical character of the boundary range that makes the key difference in our present model for different scale applications.

4. Simulated Results and Discussion

The morphology and evolution of the polycrystalline structure in the AZ31 alloy were simulated by our phase field model during annealing time and the results are showed in Fig.2. The values of all simulated parameters were obtained from physical analysis or experiments in our model so the results in Fig.2 are all in real time and real scale. Therefore, the grain size can be compared with the actually measured results by experiments directly.



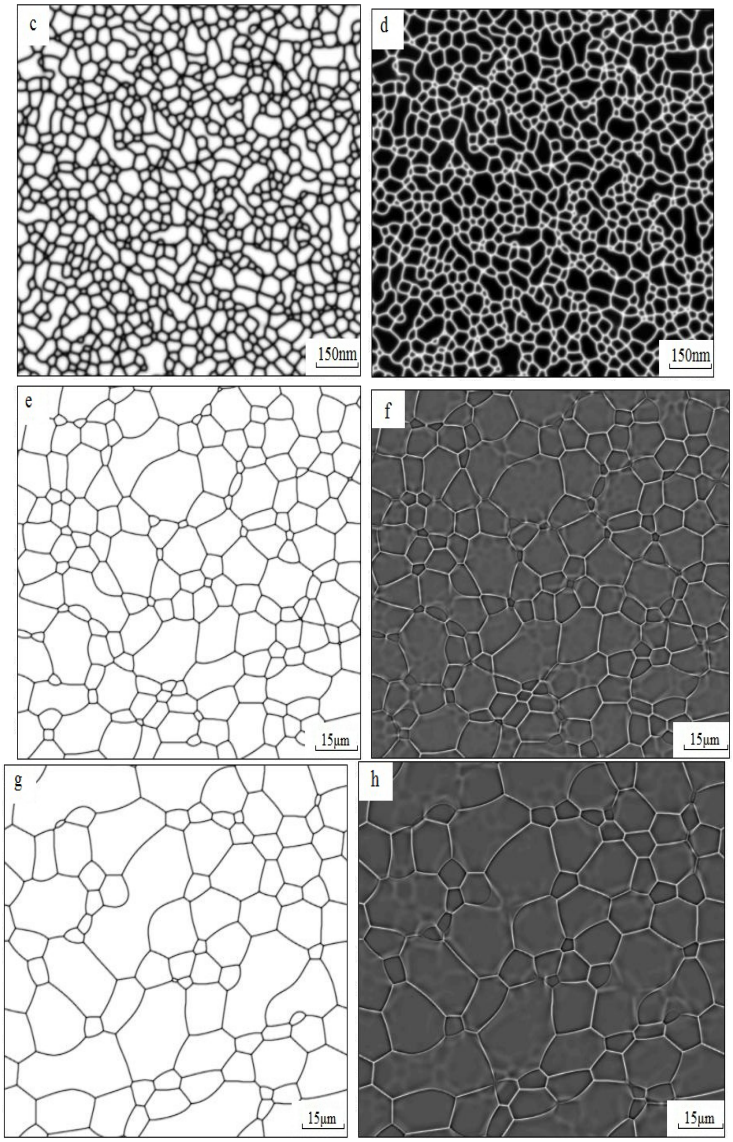


Fig.2. Simulation results of grain growth both in nano scale (a, b, c, d) and micron scale (e, f, g, h) when t=200 min (a, b), 300 min, (c, d), 10min (e, f), and 60 min (g, h), respectively at 350^{o}C. (a), (c), (e) and (g) in orientation field; (b), (d), (f) and (h) in concentration field.

It is seen in Fig.2 that, the grain structure based on the orientation field and the concentration field at the same time are identical both in nano-structure and micron-structure, which is a proof of the validity of our phase field model. However, the concentration field shows a variation pattern in large grains in Fig.2 (h) for example and this suggests that a grain only big enough to 10 m in diameter can have a character that the boundary energy may vary significantly with different crystal orientation neighbors. There are some great elongated grains in nano scale as is seen in Fig.2 (a) and (c) showed in circles, and they are the proof of a grain coalescence mechanism of coupling grain rotation during grain boundary migration. On the other hand, the grains in micron scale always show the round polygonal shape, which exposes some differences of grain growth mechanisms in nano scale compared with micron scale. Several large grains can be seen in

the fine grains in Fig.2 (a) and (c) in nano-structure, and these grains imply a tendency of easy abnormal grain growth in nano-structure.

In order to examine the reliability of the simulated results, the simulated results in nano scale and micron scale are compared with the experiments, as is seen in Fig.3.

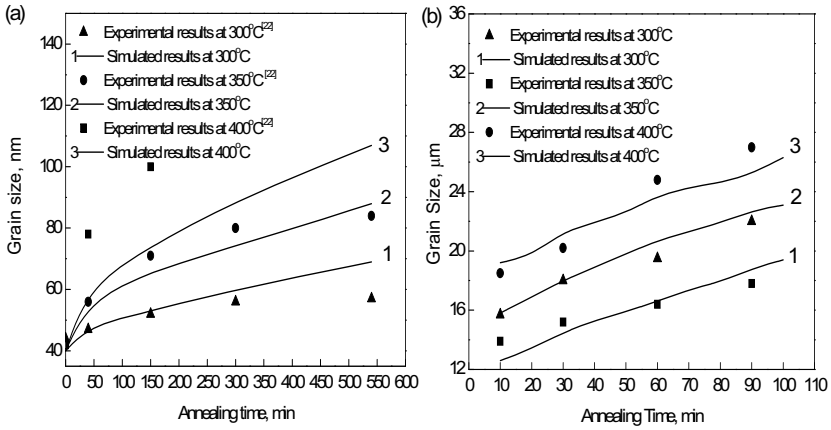


Fig.3 The simulated average grain size evolution in nano scale (a) and micron scale (b) as a function of annealing time compared with the experiments in ref. [10, 11]for AZ31 Mg alloy at different temperatures.

The simulated results are well matched with experiments at 300 °C and 350 °C in nano scale, however it is not matched at 400°C. the reason is that the nano-grains at high temperature is not grow up continuously, grains may coupling together to grow up saltantly. Hillert theory is chosen to explain the grain rrowth: $d^n-d_0^n=kt$， where d is the average grain size, d_0 is the initial grain size, n is the time exponent, k is the parameter. It is found that n=5 in nano scale and n=2 in micron scale, which prove that the nano-grain growth speed is lower than micro-grains[10, 11]。

Large Grains and little grains are mixed as is showed in Fig.2, so the equation $\Delta d=(d_{\max}-d_{\min})/d_{ave}$ are used to calculate the valuation of grain size, Δd is the valuation of grain size, $d_{\max}$ is 5% of maxim grain size, $d_{\min}$ is 5% of minimum grain size d_{ave} is the average grain size, and the simulated results are showed in Fig4.

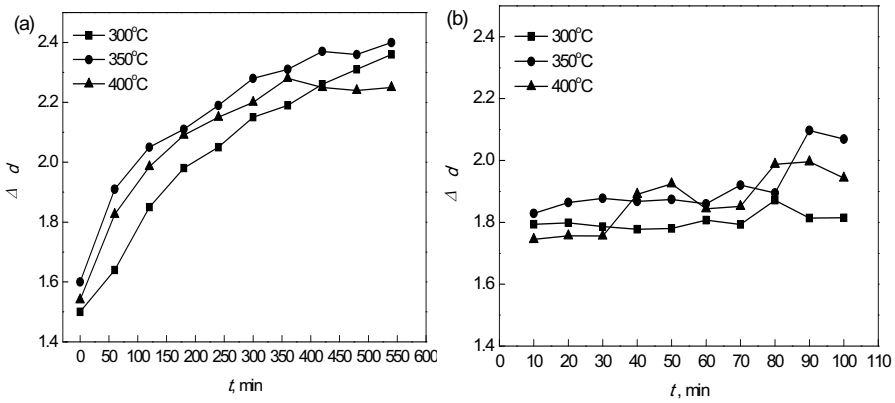


Fig.4 Grain size fluctuation in nano-structure (a) and micron-structure (b)

It is shown from Fig. 8 that, the variation of grain size is largest at 350 ^{o}C at the same annealing time in nano scale and the variation of grain size increase at first and then decrease with the lapse of time at 400^{o}C. In micron scale, the variation of grain size changed very little as the time going on at 300 ^{o}C, however, it is increased with the lapse of annealing time at 350 ^{o}C and 400 ^{o}C. The increase amplitude of it in nano scale is larger than that in micron scale, so it is suggested to use of the unique grain size fluctuation by introducing a few of abnormal grains into nanostructure to improve the ductility of materials but maintain their strength. The suggestion need further simulation and experiments to study.

5.Conclusions

1. Simulated results show that the grain boundary range for grains in nano-scales covers no more than two adjacent grains, while the range should be a constant big value of about 1.2μm for grains in micron scale.

2. It is found that the grain growth rate in nano-scales is much slower in an order of magnitude than that in micron scale, and it is in consistent with the experimental results. The lower grain boundary mobility and lower grain boundary energy in nano-structure are suggested being the reasons.

3. It is found that the grain size fluctuation is more intensely in nano-sized grains than that in micron-sized grains by the quantitative analysis of the mixed degree of grains size in nano-structure and micron-structure in the models.

6.Acknowledgments

Authors would like to acknowledge the National Nature Science Foundation of China by the grant 51171040 and the High Technology Research and Development Program of China by the grant 2013AA031601 for the financial support to this study.

References

1. J. Liu, P. Yao, N. Zhao, etc, Effect of minor Sc and Zr on recrystallization behavior and mechanical properties of novel Al-Zn-Mg-Cu alloys, J. Alloys Comp. 657 (2016) 717-725.
2. L. Zhong, J. Peng, M. Li, etc, Effect of Ce addition on the microstructure, thermal conductivity and mechanical properties of Mg-0.5Mn alloys, J. Alloys Comp. 661 (2016) 402-410.
3. J. She, F. Pan, J. Zhang, etc, Microstructure and mechanical properties of Mg-Al-Sn extruded alloys, J. Alloys Comp. 657 (2016) 893-905.
4. L. Chen, J. Chen, R. A. Lebensohn, etc, An integrated fast Fourier transform-based phase-field and crystal plasticity approach to model recrystallization of three dimensional polycrystals, Comput. Methods Appl. Mech. Eng. 285 (2015) 829-848.
5. M. Wang, B.Y. Zong and G. Wang, Grain growth in AZ31 Mg alloy during recrystallization at different temperatures by phase field simulation, Comput. Mater. Sci. 45 (2009) 217-222.
6. Y. Wu, B. Y. Zong, X. G. Zhang, M. T. Wang, Grain growth in multiple scales of polycrystalline AZ31 Magnesium alloy by phae-field simulation, Metall. Mater. Trans. A. 4 (2013) 1599-1610.

7. X.G. Zhang, Y.P. Zong, M.T. Wang and Y. Wu, A physical model to express grain bounaries in grain growth simulation by phase-field method, Acta. Phys. Sin-Chinese Ed. 60 (2011) 755-763.
8. X.G. Zhang, Y.P. Zong, Y. Wu, A model for releasing of stored energy and microstructure evolution during recrystallization by phase-field simulation, Acta. Phys. Sin-Chinese Ed. 21 (2012) 88104-088104.
9. C. Shek, J. Lai, G. Lin, Investigation of interface defects in nanocrystalline SnO_2 by positron annihilation, Nanostruct. Mater. 11 (1999) 887
10. C. Deng, Fabrication of ultra-fine grain magnesium alloy by powder metallurgy and research on the microstructure and property, Master Thesis, Harbin Institute of Technology, 2009
11. R. Liu, L.Wang, G. Huang, etc. Study on annealing technique for wrought magnesium alloy plate and modeling research on the changing law of its grain size, Light Alloy Fabric. Technol, 32 (2004) 22-25.