Computer Simulation Study on Dynamic Recrystallization Mechanism of Magnesium Alloy during Compound Deformation

Lingyi Wang[1*], Zhongtang Wang[2]

[1]College of Information Technology, Shenyang Institute of Technology, Fushun, Liaoning 113122, China

[2]School of Materials Science and Engineering, Shenyang Ligong University, Shenyang, Liaoning 110159, China

Email*: 793539510@qq.com, ztwang@imr.ac.cn

Abstract: The evolution law of dynamic recrystallization structure in the process of indentation-flattening compound deformation technology (IFCDT) of AZ31 magnesium alloy was studied. A computer simulation method for dynamic recrystallization structure evolution process was proposed based on cellular automata theory (CA method). Firstly, the material model of cellular automata method is established. Secondly, the performance parameters and compound deformation parameters of AZ31 magnesium alloy were determined. Finally, the dynamic recrystallization process of AZ31 magnesium alloy during compound deformation was analyzed. During the compound deformation of AZ31 magnesium alloy, the dynamic recrystallization mechanism is initial state, nucleation of new grains, generation of new grains, growth of new grains, continuous growth of new grains, and covering of original large grains. Compared simulation results with experimental results, the maximum relative errors is 15.4%. It is proved that cellular automaton method may be used to predict the microstructure evolution of AZ31 magnesium alloy during indentation-flattening compound deformation.

1. INTRODUCTION

With the development of computer simulation technology, the visualization of material forming process has been realized. It can not only observe the changing rules of temperature field, strain field, stress field, velocity field, displacement field and force and energy parameters in the deformed zone, but also observe the evolution rules of microstructure in the deformed zone, including the changing rules of grain size and process of dynamic recrystallization process. Cellular Automata (CA) method is an important theory for computer simulation of microstructure evolution in material deformation process. It can be well applied to simulation analysis of dynamic recrystallization process in material deformation process.

Rappaz [1] had used CA method to simulate solidification structure. Goetz [2] had used CA method to simulate the dynamic recrystallization process for the first time. Zhou Sheng [3] combined the forming process with CA method to analyze the dynamic recrystallization process in blade forming. Cellular automata method has been applied to the simulation analysis of nucleation, recrystallization and phase transformation of solidification crystallization [4]. Li [5] had studied the dynamic recrystallization law of TA15 titanium alloy during the transformation of beta phase to alpha phase.

Based on the improved cellular automata model and flow field transmission model, the evolution process of equiaxed and columnar grains in magnesium alloys under convection was analyzed, and the growth laws of single, multi-dendrite and columnar grains in magnesium alloys under convection were analyzed [6]. Jin [7] had found that the distribution of dislocation density was highly inhomogeneous after dynamic recrystallization started, and presented typical dynamic recrystallization characteristics. Thermal processing parameters affected the nucleation and growth behavior of dynamic recrystallization by changing the cumulative velocity of dislocation density. The process of grain nucleation and growth during solidification of magnesium alloy cast-rolled strip was analyzed by cellular automata method. The influence of technological parameters (pouring temperature, casting-rolling speed, etc.) on grain size and orientation in solidification structure of magnesium alloy strip was analyzed [8]. WU [9] had established a three-dimensional numerical simulation model of dendrite growth of magnesium alloys based on cellular automata. The dendrite growth of magnesium alloys in basal plane was simulated with six-fold symmetry, and the dendrite growth law during directional solidification of magnesium alloys was obtained. The improved cellular automaton model is used to simulate the solidification process of AZ91D magnesium alloy. The grain size of magnesium alloy during dendrite growth was predicted accurately [10]. The improved cellular automaton method is used to simulate dendrite growth of dendrite magnesium alloy with dense hexagonal structure, and established dendrites along different grain orientations and crystal growth model [11]. Shingo [12] have proposed a new method to improve the microstructure property and plastic formability of AZ31 magnesium alloy. During deformation twinning of AZ31 magnesium alloy, twin nucleation is found to be mostly controlled by a combination of grain size, and bulk dislocation density while twin propagation is affected most by grain boundary length, angle from grain boundary plane to the RD plane, and grain boundary misorientation [13]. The microstructure and mechanical properties of AZ31 magnesium alloy sheet were improved significantly by severe plastic deformation (SPD) and short time post-annealing [14]. During thermal deformation of AZ31 magnesium alloy, two types of twin are identified: (1) slip-assisted twins that nucleate at grain boundaries with no apparent influence from nearby twins, and (2) twin-assisted twins that result from twins propagating across a grain boundary [15]. Chu [16] established recrystallization grain size model and dynamic recrystallization volume fraction model during magnesium alloy deformation. The dislocation density model, critical dislocation density model, nucleation rate model and grain growth model of magnesium alloys are derived. The recrystallization grain size model and the dynamic recrystallization volume fraction model are derived.

In this paper, the dynamic recrystallization evolution of AZ31 magnesium alloy was computer simulated by using cellular automata. The influence of compound deformation parameters on the dynamic recrystallization nucleation and grain growth of AZ31 magnesium alloy was analyzed.

2. Microstructure Evolution Model

The principle of indentation-flattening compound deformation process is shown in Fig.1a. Intense tangential deformation of Magnesium alloy sheet can be produced by indentation deformation (called primary deformation), which can aggravate the dynamic recrystallization of magnesium alloy, and more twin structures and more slip systems can be produced, which is conducive to refine grain size and weaken the texture of base plane, and significantly improve the formability of magnesium alloy sheet. The dynamic recrystallization of magnesium alloy can be further aggravated by the flattening deformation (called secondary deformation) of the magnesium alloy sheet after one-step deformation, which further refines the grain size and weakens the texture of the base plane, and significantly improves the formability and mechanical properties of the magnesium alloy sheet.

(a) Principle of IFCDT)   (b) Experimental Tools   (c) Experimental equipment

Figure 1 Principle of indentation-flattening compound deformation technology (IFCDT)

When the cellular automata method is used to simulate the process of dynamic recrystallization of magnesium alloy, the strain hardening parameter model of AZ31 magnesium alloy can be seen as equation (1), and the recovery parameter model can be seen as equation (2), the strain hardening rate model can be seen as equation (3), and the yield strength model can be seen as equation (4). Kinematic and dynamic models of dynamic recrystallization are shown in equation (5) - equation (8).

$$h = 10^{13} \dot{\varepsilon}^{m} \exp\left[\frac{0.17Q_b}{RT}\right] \tag{1}$$

$$r = 17.7\dot{\varepsilon}^{-0.17} \exp\left[-\frac{0.17Q_b}{RT}\right] \tag{2}$$

$$\dot{n} = \frac{\partial \sigma}{\partial \varepsilon} = 136\dot{\varepsilon}^{0.17} \exp\left[\frac{0.17Q_b}{RT}\right] \tag{3}$$

$$\sigma_s = \alpha Gb\sqrt{\frac{10^{13}}{17.7}}\dot{\varepsilon}^{0.17} \exp\left[\frac{0.17Q_b}{RT}\right] \tag{4}$$

$$X_{DRX} = 1 - \exp\left[-1.803\left(\frac{\varepsilon - \varepsilon_c}{\varepsilon_s - \varepsilon_c}\right)^{2.231}\right] \tag{5}$$

$$\varepsilon_c = 0.168 \times 10^{-2} Z^{0.083} \tag{6}$$

$$\varepsilon_s = 0.0027 Z^{0.118} \tag{7}$$

$$d^{1.683} = 20.08^{1.683} + 3766.978t^{1.03} \exp(-\frac{252218}{RT}) \tag{8}$$

In which, X_{dyn} is dynamic recrystallization integral,%; ε, strain; T, deformation temperature, K; t, heating time, min; n, strain hardening index; d, grain size of dynamic recrystallization, μm; ε_c is critical strain; ε_s is steady-state strain; $Z = \dot{\varepsilon}\exp[252218/(RT)]$.

The relationship between flow stress, deformation temperature and strain rate can be expressed as a function of some microscopic characteristics in the hot working process of metal materials. The flow stress model of AZ31 magnesium alloy is as follows:

$$\dot{\varepsilon} = 5.718 \times 10^{20} [\sinh(0.0081\sigma)]^{9.13} \exp\left(-\frac{252218}{\mathrm{R}T}\right) \tag{9}$$

In which, σ_s is material flow stress (MPa); $\dot{\varepsilon}$ is strain rate, 1/s; T is deformation temperature, K; R is gas constant, 8.314 J/(mol·K).
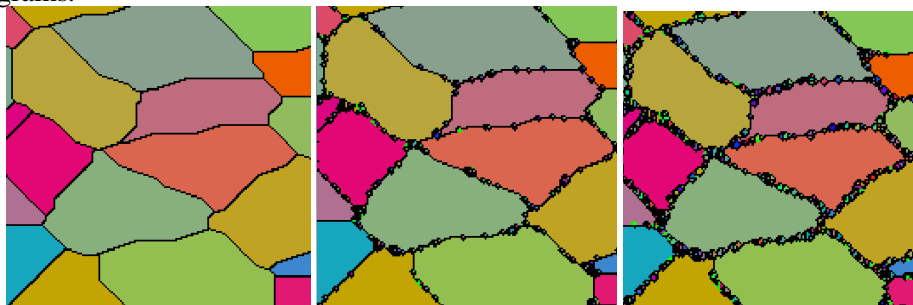
3. Computer simulation scheme

Finite element calculation software was used to simulate the microstructure evolution of AZ31 magnesium alloy during compound deformation. In the cellular automata (CA) module, 330×440 quadrilateral space was used, each cell size was 1 µm, and the simulated area represented the actual sample of 0.33 mm×0.44 mm. Moore neighbor was used for the neighbor type.

The process parameters of compound deformation are as follows: the tooth spacing (s) of waveform die being 6 mm, the initial thickness of sheet being 7 mm, the deformation temperature being 200°C - 400 °C, the preheating temperature of die being 25°C- 250 °C, the reduction (h) is 1.5 mm, 2 mm and 3 mm respectively, and the tooth spacing is 10 mm. The composite deformation coefficients are 0.15, 0.2 and 0.3. The reduction speed is 30 mm/min. The initial grain size of the numerical simulation is the same as that of the experimental measurement, that is, the average grain size is 49.5 µm. Properties of AZ31 magnesium alloy [17]: initial dislocation density $\rho_0 = 10^{10}$ m^{-2}, shear modulus of elasticity G=17000MPa, boundary activation energy Q_b=134000(J/mol), deformation activation energy Q=252218 (J/mol), constant K=6030, hardening constant h_0=10^{13} (m^{-2}), recovery constant r_0=17.7. The compound deformation process of AZ31 magnesium alloy was simulated by finite element software. The microstructural simulation function of the software was redeveloped by Fortran language. A UGRAIN subroutine was developed to predict the dynamic recrystallization process of AZ31 magnesium alloy.
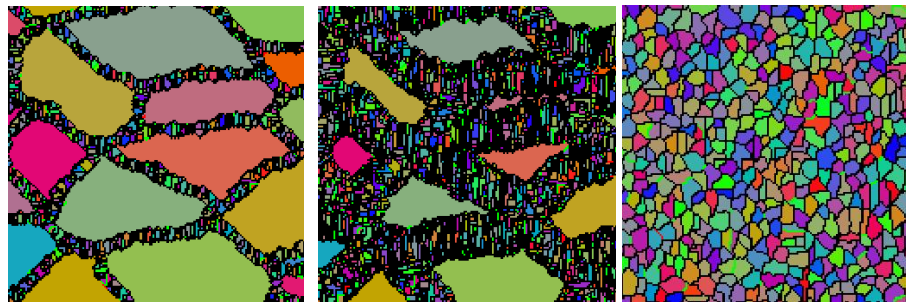
Fully dynamic recrystallization is defined when the dynamic recrystallization fraction is greater than 95%, the grain size is dynamic recrystallization grain size, and then the grain size grows. The average grain size d_{AV} is used to characterize the grain size of the non-complete recrystallization, $d_{AV} = d_0(1 - X_{dyn}) + d_{dyn} \cdot X_{dyn}$, where d_0 and d_{dyn} are original grain size and dynamic recrystallization grain size, respectively, and X_{dyn} is volume fraction of dynamic recrystallization.

4. Analysis of simulation results

The computer simulation results of dynamic recrystallization are shown in Fig.2. With the development of deformation process, small new grains are produced at the grain boundary at the beginning of deformation. These new grains grow up gradually and cover the original coarse grains. The complete dynamic recrystallization process is realized, and the material structure is refined. Mechanism of dynamic recrystallization process: initial state → nucleation of new grains → production of new grains → growth of new grains → continuous growth of new grains → covering of original large grains.
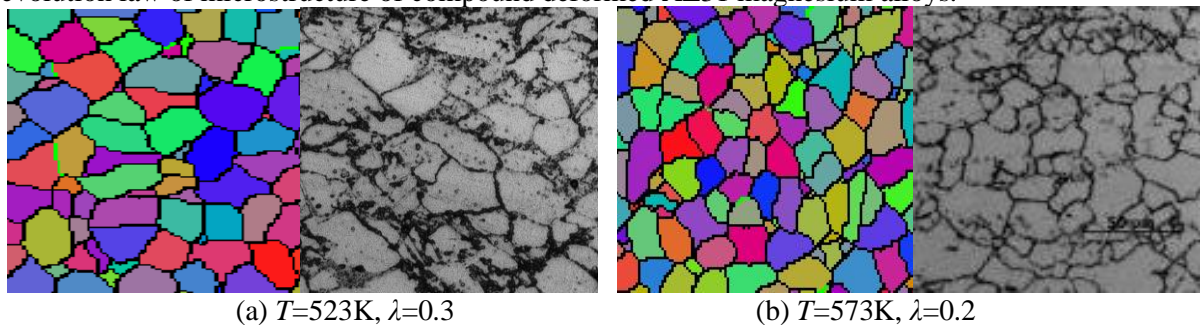

(a) initial state grains   (b) nucleation of new grains   (c) production of new grains

(d) growth of new grains   (e) continuous growth of new grains   (f) covered by new grain

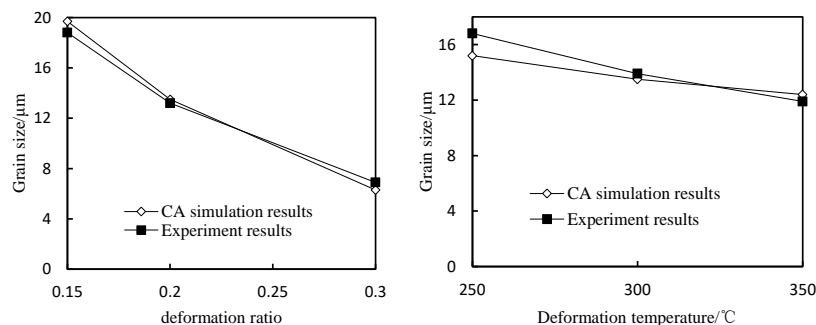Figure 2 Computer simulation results of dynamic recrystallization process

The results of microstructure simulation and experimental results of compound deformed magnesium alloys are shown as Fig.3. The numerical comparison between the grain size of compound deformed magnesium alloys obtained by simulation and experimental results are shown as Fig.4. The numerical simulation results are in good agreement with experimental results, and the relative errors is less than 15.4%. Experiments show that cellular automata (CA) method can be used to predict the evolution law of microstructure of compound deformed AZ31 magnesium alloys.

(a) T=523K, λ=0.3   (b) T=573K, λ=0.2

Figure 3 Microstructure simulation results and experimental results of magnesium alloy after composite deformation

(a) Deformation temperature 573K   (b) Compound deformation coefficient 0.2

Figure 4 Comparison of simulation results and experimental results

5. Conclusions

(1) The microstructure evolution of dynamic recrystallization during indentation-flattening compound deformation of AZ31 magnesium alloy was simulated by computer simulation. The structure evolution model of cellular automata theory was established, and the properties and compound deformation parameters of AZ31 magnesium alloy were determined.

(2) During the compound deformation of AZ31 magnesium alloy, the dynamic recrystallization mechanism is that: initial state → nucleation of new grains → production of new grains → growth of new grains → continuous growth of new grains → covering of original large grains.

(3) Cellular automata (CA) method was used to simulate the dynamic recrystallization structure evolution of AZ31 magnesium alloy during indentation-flattening compound deformation. The results were in good agreement with the experimental results, and the relative errors was less than 15.4%.

Acknowledgements

References

[1] Rappaz M, Gandin Ch A, 1993, *Acta Metallurgica et Materialia*, 41(2),pp.345-360.

[2] Goetz R L, Seetharaman V, 1998, *Scripta Materialia*, 38(3), pp. 405-413.

[3] ZHOU Sheng, FU Jian, WANG Tao, 2009, *Hot Working Technology*, 38(5), pp. 96-100.

[4] Guo Yong-guan, Li Shuang-ming, Liu Lin, 2008, *Acta Metallurgica Sinica,* 44(3), pp. 365-370.

[5] Li Ping, Gan Guoqiang, Xue Kemin, 2012, *Rare Metal Materials and Engineering*, 41(S2), pp. 343-347.

[6] YANG Man-hong, GUO Zhi-peng, XIONG Shou-mei, 2015), *The Chinese Journal of Nonferrous Metals*, 25(4), pp. 835-843.

[7] JIN Zhaoyang, LI Keyan WU Xintong, YAN Kai, 2015, *Journal of Yangzhou University (Natural Science Edition)*, 18(3), pp. 41-45.

[8] Huang Feng, Di Hong-Shuang, Wang Guang-Shan, 2009, *Acta Physica Sinica*, 58(S1), pp. 313-318.

[9] Mengwu WU, Shoumei XIONG, 2012, *Acta Metallurgica Sinica (Engl. Lett.)*, 25(3), pp. 169-178.

[10] HUO Liang, LI Bin, SHI Yufeng, XU Qingyan, HAN Zhiqiang, 2009, *Tsinghua Science and Technology*, 14(5), pp. 307-312.

[11] WU Meng-wu, XIONG Shou-mei, 2012, *Transactions of Nonferrous Metals Society of China*, 22(9), pp. 2212−2219.

[12] Shingo Kudo, Shouta Yokoyama, Kosei Shimoyama, Shinobu Kaneko, Fumio Fujita, 2017, *Materials Science & Engineering A*, 680, pp. 75-84.

[13] Andrew D. Orme, Isaac Chelladurai, Travis M. Rampton, David T. Fullwood, Ali Khosravani, Michael P. Miles, Raja K. Mishra, 2016, *Computational Materials Science*, 124, pp. 353-363.

[14] Kai Soon Fong, Atsushi Danno, Ming Jen Tan, Beng Wah Chua, 2017, *Journal of Materials Processing Technology,* 246, pp. 235-244.

[15] Khosravani, D.T.Fullwood, B.L.Adams, T.M.Rampton, M.P.Miles, R.K.Mishra, 2015, *Acta Materialia*, 100, pp. 202-214.

[16] Chu Zhibing, Zhang Duo, Jiang Lianyun, Ma Lifeng, Li Yugui, Huang Qingxue, 2018, *Rare Metal Materials and Engineering*, 47(3), pp. 884-894.

[17] Liu X, Li L X, He F Y, Zhou J, Zhu B W, Zhang L Q, 2013, *Transactions of Nonferrous Metals Society of China*, 23(9), pp. 2692-2699.