Prediction of recrystallized grain size during hot deformation of AZ31 magnesium alloy by monte carlo method

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Abstract. Magnesium alloy is an important engineering metal material, which has a series of excellent mechanical, chemical and physical properties. It is widely used in aerospace, advanced manufacturing, biomedical and other fields. In the processing and preparation of magnesium alloy, high temperature and large deformation treatment are usually introduced. The introduction of temperature and strain rate will lead to grain coarsening and dynamic recrystallization. Therefore, it is necessary to study the effects of high temperature and deformation on the grain evolution of magnesium alloys. Based on the Monte Carlo simulation method, the microstructure evolution of AZ31 magnesium alloy at different temperatures and strain rates was simulated and analyzed. The results show that high temperature is the main reason for grain growth, and increasing strain rate can promote recrystallization and refine grain size.

1. Introduction

Magnesium alloy which can suffer high impact and resist high corrosion is also the lightest metal material in industrial applications. Magnesium alloy has properties of low density, high strength, large elastic modulus, high thermal conductivity, good shock absorption and so on. Therefore, the magnesium alloy is widely used in aerospace, transportation, chemical and other fields [1]. And it is considered as one of most important engineering metal materials. High temperature and deformation are often employed in the process of producing the magnesium alloy. Equal channel angular pressing, friction stir processing, laser additive manufacturing and other processes all have influences in the magnesium with high temperature and deformation. Magnesium is a polycrystalline material which initial grains or recrystallized grains will have a phenomenon of grain growth with high temperature and strain rates. That grain size has a relatively large impact on mechanical properties of magnesium alloy shows the coefficient value of the grain size is higher in Hall-Petch equation of the relationship between the grain size and strength. Thus, it is crucial to study and research the grain growth of magnesium alloy in hot working processes. However, it is difficult to observe the actual processes of the grain growth. The experimental research has a complex procedures and quite high cost. Thus, it is effective to utilize the numerical methods to study the dynamic grain growth process of magnesium alloy under high temperature and deformation.

Many researchers have conducted the researches by using the numerical simulation methods in order to observe the evolution of microstructure of alloys. Mishra and DebRoy [2] used a Monte carlo method combined with experimental measurements to study the heat-affected zone microstructure evolutions in welds. Huang et al. [3] studied the grain growth phenomenon of polycrystalline materials. Francis et al. [4] simulated the grain growth process in thin platinum films, and conducted experiments to verify the results. Choudhury and Jayaganthan [5] used both 2D and 3D MC models to investigate
the mobile and immobile impurities in polycrystalline materials. Wei et al. [6] conducted a detail 3D MC simulation of grain evolutions in GTAW process of stainless steels. Yu et al. [7] studied the anisotropic boundary effect on the grain evolutions of single-phase systems by MC models. Ko et al. [8] used a modified MC model to simulate the abnormal grain growth phenomenon in Fe-3% Si steel. Sabeti [9] applied the MC model to the grain growth process with nanocrystalline and studied the detail influence of the nanocrystalline. Liu et al. [10] combined the MC model with finite element methods and studied the microstructure evolutions of polycrystalline materials. Grujicic et al. [11] predicted the grain size and its microstructure evolutions in a friction stir welds via MC methods. Rodgers et al. [12] simulated the metal additive manufacturing process via a kinetic monte carlo method. Alzate-Cardona et al. [13] applied the MC method to the study of microstructure evolutions in presence of time dependent magnetic fields.

According to the current engineering applications which are in urgent need to quickly determine the grain size of magnesium after hot working, in this paper, a fast algorithm for grain evolution of AZ31 magnesium alloy based on Monte Carlo algorithm is proposed. On the basis of this work, the grain growth and evolution process of AZ31 magnesium alloy under different temperature and strain rate conditions were simulated, and the effects of temperature and deformation on grain growth were analyzed in detail, as well as the variation rule of micro-morphology, which provided reference for engineering application.

2. Model description
In this context, 2-dimension Monte Carlo method is used to analyze the evolution of the grain size of magnesium alloy. At the first, the region of simulating magnesium alloy is meshed by \( n \times n \) square grid. Each lattice point is assigned to a random grain orientation value. And all these values are positive integers and have \( 1 - q \) distributing range. If using Moore neighbor Model, then each central grid point will correspond 8 neighbor grids. Use the equation below to calculate energy of the system:

\[
E = \sum_{i=1}^{k} (1-8q_i q_j)
\]  \( (1) \)

While the MC model begins iterating, each step of iteration selects random lattice points with \( n^2 \) times in the system. During each selection, we randomly change the grain orientation value of selected grid points and calculate the energy of the system again. If the value of recalculating energy increases, then discard this change, otherwise accept the change. Using the theory that the energy tends to decrease during the grain growth drives the simulation of grain growth. According to the influence of the temperature, the iteration step in our model relates as an exponential function with temperature. It means that the higher temperature is, the larger number of iterations will be. This simulates the impact of the temperature:

\[
MCS = aT^\beta
\]  \( (2) \)

In this equation, \( a \) and \( \beta \) are selected material parameters.

In regard to the impact in strain rate, our model introduces the probability of nucleation and recrystallization below by adding recrystallized grains to the system to refine grains and simulate the effect of deformation on grain growth.

\[
\eta = e^e - \frac{q}{E}
\]  \( (3) \)

In equation (3) \( e \) is the strain rate, \( Q \) is the material activation energy. \( R \) is the gas constant. \( T \) is the absolute temperature. The detail model algorithm can also be found in the literatures [14].

The above model is programmed in Fortran language for calculation. The calculation flowchart of the MC model in this work is shown in Figure 1, and the parameters in formula 2 and formula 3 are shown in Table 1.
Figure 1. Flowchart of MC method.

Table 1. Parameters of Materials.

| Parameters | values       | Ref.    |
|------------|--------------|---------|
| Q          | 70 kJ·mol⁻¹  | [14]    |
| R          | 8.31         | constant|
| C          | 7.58         | chosen  |
| q          | 100          | model Constant |

3. Results and discussion

In this article, the 300 × 300 grid model is employed to simulate the grain growth of AZ31 magnesium alloy in 2-dimension square area. The side length of grid of the mesh is set to 1 µm. The temperatures of simulating growth are 100°C, 200°C, 300°C and 400°C. Under each temperature, it simulates three working conditions of strain rates, 0.1s⁻¹, 1s⁻¹ and 10s⁻¹.

According to equation 2, the times of iterated MCS of MC model are calculated with different temperature of working conditions. With temperature during 100°C to 400°C, each times of iterations are 285, 676, 1123 and 1610. It is obvious that the times of iterated MCS are increasing with increasing temperature, and it is a rapid non-linear growth trend. The probability of changing orientations of center grid points will significantly increase with increasing the times of iterated MCS of MC model so that it also increases the probabilities of the grain growth.

In formula 3, the probability of recrystallization nucleation is proportional to the strain rate value experienced by the material. As the strain rate increases, the probability of recrystallized grains nucleating at the grain boundary increases, and the probability of generating new fine grains increases.
in order to refine the grain. Additionally, there is a relation between the probability of recrystallization nucleation with temperature. With the increasing temperature, the rate of nucleation will be enlarged. It represents the combined effect of temperature and deformation. In our article, the minimum rate of nucleation approaches to zero, and the maximum rate of nucleation tends to be 2.72%.

According to the outcomes of the times of iterated MCS and the probability of recrystallization nucleation by calculations, conducting model calculations are able to predict the final grain sizes at the different thermal conditions.

The simulation results are shown in Figure 2. By comparing the figures, with the increase of temperature, the grain size shows an increasing trend under different strain rate conditions. In the range from 100°C to 300°C, the growth rate is relatively large. As the temperature continues to rise, the average crystal grain growth rate tends to be down. With the comparison of different strain rate curves, it can be clearly observed that as the strain rate increases, the grain size decreases greatly. This reflects the effect of deformed grain refinement, which is consistent with results of the nucleation rate analysis. When the strain rate becomes 10 s^{-1}, it is difficult for the grain size to grow, which is caused by the large recrystallization nucleation rate. The smallest grain size appears under the lowest temperature and highest strain rate conditions, which is only 2.56 μm, and the largest grain size appears at 400°C with the minimum strain rate conditions, which reaches 14.9 μm.

![Figure 2](image)

**Figure 2.** Relation of grain size and strain rates at different temperatures.

A simulated grain morphology map can be obtained from the calculated grain data value by assigning a random color to each grain orientation degree. Take the grain morphology at different temperatures at a strain rate of 1.0 s^{-1} as an example shown in Figure 3, it shows that as the heat treatment temperature continuously increases, the grain size rapidly coarsens. The morphology of the most of grain is hexagonal equiaxed grains, which is consistent with many theoretical analyses and experimental observations [15-17]. Under higher temperature conditions, a small amount of fine-sized grains appear at the boundaries of larger grains, which is caused by the growth of new grains generated by dynamic recrystallization nucleation. By comparing Figure 4 with the grain morphology with the same temperature (400°C) and different strain rates, it can be discovered that at the same temperature of 400°C, the working condition with larger strain rate finally produces dense equiaxed grain morphology. However, in the working condition with a small strain rate, the number of newly nucleated recrystallized grains is too smaller to refine the grains. And there are not widely distributed small sized grains around the large grains. When the strain rate increases from 0.1 s^{-1} to 10 s^{-1}, the value of grain size decreases from 14.9 μm to 6.7 μm, and the size is refined by 55%.
4. Conclusion
The two-dimensional MC algorithm with the minimum energy rule can be considered as the criterion to predict the process of grain coarsening for AZ31 magnesium alloy with high temperature and deformation. The predicted results show that when the temperature increases, the microstructure grains of the magnesium alloy will rapidly coarsen, and there is a fine and compact recrystallized grain structure being formed on the boundaries of the large grain. As the strain rate increases, the rate of
recrystallization nucleation increases greatly, which will refine the overall grain size. The experimental results show that under higher temperature conditions, the grains can be refined indirectly by controlling the strain rate, and it also controls the microstructure evolution of AZ31.

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