Research of Monte-Carlo Simulation in Grain Growth

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Abstract. This paper is produced after writing code for doing Monte Carlo simulations of a single type and use the model to study the self-assembly of co-polymers confined to a surface. A great interest has been aroused in the field of Monte Carlo simulation in material science since then. The Monte Carlo algorithm for single-phase normal grain growth is realized which can simulate and observe the current development of the microstructure of large grains in three dimensions. And this study will go through both two- and three-dimension Monte Carlo simulation in grain growth with a brief introduction of the methodology about this. At last, an enormous potential of the Monte Carlo simulation could be spotted in material field and the future material analysis will rely more on computational science due to the powerful computing power.

1. Introduction
Grain size is an important feature for evaluating material performance, especially when we need to balance different materials. [1] In fact, it is one of the most important issues in microstructure control. This kind of research is often carried out through accurate analysis and comparison of microstructures with the help of image analysis software such as Fiji. However, with the improvement of computer operational capability, computer simulation of grain growth has become possible. Monte Carlo simulation is a simulation method that relies on repeated random sampling and statistical analysis to calculate the results. This method is related to random experiments, and unknown results of random experiments in advance. A relationship between the conceptual basis of the Monte Carlo method and the physical properties of grain growth has been found since they both rely on statistics and randomness. Monte Carlo simulation seems to represent this phenomenon well.

In the context of magnetic domain evolution, the application of Monte Carlo method in the simulation of grain growth originated from the Potts model. Potts proposed to extend the 2-state spin-up or spin-down ferromagnetic Ising model to systems with arbitrary spin degeneracy. The Potts model was introduced into the simulation of grain growth to simulate the effects of grain growth kinetics, grain size distribution and topology and anisotropic grain growth.[2][3][4]

This paper was motivated by the observation of abnormal grain growth in several superalloys at high temperature produced by some certain metallurgy techniques. The study contains the methodology part and several examples of use of Monte Carlo simulation about grain growth in two and three dimensions respectively.

2. Methodology
For polycrystalline materials, after the nucleus is formed, the grain growth phenomenon is divided into two different types which are normal grain growth and abnormal grain growth respectively.
Firstly, during normal grain growth, the grain size shows a consistent growth trend. The main characteristics are the grain size $F (R/R_{\text{th}})$ and topology. The distribution function $P (Nc)$ does not change over time. Among them, $R$ is the grain radius, $R_{\text{th}}$ is the average grain radius, and $Nc$ is the number of grain sides.

Under isothermal conditions, the grain growth of normal grains can be derived from the parabolic kinetic equation below:

\[ R = k t^n \quad (1) \]
\[ R_{\text{th}}^{m} - R_{\text{th}}^{m}(t=0) = B t \quad (2) \]

In equation 1, parameter $t$ represents the time while $k$ is the growth rate constant and $n$ is the grain growth index. Due to derivation of time by formula (1) and theoretical prediction after transformation, the steady-state grain growth coefficient $n$ should be equal to 0.5. However, the experimental and simulation results show that the value of $n$ should always be less than 0.5 due to the difference between actual material and ideal materials without ignoring the influence of the crystal topological structure. At the condition that the value of $R$ is incredibly larger than the value of $R_0$ which is referred as the original radius of the grain, the two equations are equivalent. ($m=\frac{1}{n}$, $b$ is a constant)

Then the difference between $R_{\text{th}}^{m} - R_{\text{th}}^{m}(t=0)$ is directly proportional to time.

Secondly, for abnormal grain growth, the size of some grains increases rapidly in the recrystallized microstructure. The maximum size of the crystal grains grows at a rate much greater than the arithmetic average rate. The kinetic equation of abnormal grain growth can be expressed as below:

\[ X = 1 - \exp \left[-g(t)\right] \quad (3) \]

Above all, $b$ and $p$ are constants, and most of the measured values of $p$ are about 1.8±0.3 at present.

It is generally believed that the direct cause of the change in grain growth is the change in driving force. The driving force of grain growth mainly comes from the reduction of total grain boundary energy. But due to complexity of growth, mobility, surface energy, and curvature in the sheet, abnormal grain growth took place. Through the growth kinetic theory of the above grains, the simulation of the normal grain could be carried out.

Firstly, the planar topological structure of the crystal with a network grid point is labelled. In the actual structure, the crystal lattice microstructure is divided into discontinuous lattices. The cell geometry diffusion method is used to generate the initial figure. Several lattice points were randomly sprinkled with different crystal orientations on the plane. In such a model, we can determine the boundary between each nucleus point and other nucleus points after isokinetic diffusion and growth through geometric calculations, which are called grain boundaries. An then we could use Monte Carlo method to simulate the later grain growth of grain growth.

The evolution of the microstructure of the grain growth changes can be achieved by changing the orientation number of each crystal lattice (the spin number is reversed), where the spin number is the number of sprinkle dots above. Among the grids we have constructed, randomly select one point and then calculate the interaction between the grid point and all the neighboring grid points which could be expressed below:

\[ E = -J \sum_{ij}^{MN} \left( \delta_{s_i s_j} - 1 \right) \quad (4) \]

Among them, $S_i$ is the number of crystal orientations of lattice point $i$, and its value is one of $Q$ orientations, and $S_j$ is the number of crystal orientation of the adjacent lattice points of lattice point $i$. $\delta_{s_i s_j}$ is the delta function, and $M$ and $N$ are the number of grid points. $E$ represents the boundary energy of this lattice point.

The crystal orientation changes of each lattice point could be simulated using MC method as below.

(1) Randomly select a test grid point, its lattice orientation is $a_1$ and calculate its lattice point grain boundary energy $E$.

(2) Carry out random orientation test and choose one of the other $Q-1$ lattice direction value.

Then the lattice parameter is changed to $a_2$ ($a_2 \neq a_1$) and the changed grain boundary energy $E_2$ is obtained.
(3) Calculate the corresponding energy change $\Delta E$ after the orientation change.

Determine whether the orientation change can be achieved by calculating the probability $W$ of the crystal orientation change of the grains from the formula below.

$$W = \begin{cases} \exp(-\Delta E / K_B T) & \Delta E > 0 \\ 1 & \Delta E \leq 0 \end{cases}$$

(5)

If $\Delta E \leq 0$, it is considered that the orientation change is allowed.

If $\Delta E > 0$, the orientation probability is $\exp \left( -\frac{\Delta E}{k_B T} \right)$. At this time, a uniformly distributed random number $\eta$ is generated between $[0, 1]$.

If $\exp \left( -\frac{\Delta E}{k_B T} \right) > \eta$, the orientation change is allowed, otherwise it is not allowed.

In the simulation, we will consider the number of $N$ orientation experiments as a time unit which is called Monte Carlo time step, where $N$ is the total number of grid points [5-10].

3. Examples of application of Monte Carlo in grain growth

3.1. Examples of two dimensions

The view of the irregular grain growth of particles in a second phase state has been found. The Monte Carlo simulation of two dimensions could be used for the certain situation. Aggregates of grains with similar axes are thought to own permanent energy of grain boundary and maneuverability. The most important driving force comes from the curvature of the boundaries. The growth process of irregular grains is learned as a two control parameters function, namely the initial pinning degree of the particles to the matrix grains and the initial size advantage of the abnormal grains. Then the steady growth will be achieved, and its specific characteristics will be discussed based on available models. The results show that, violent grain growth can be obtained by using thermally motivated grain boundaries from the origin particles.

3.2. Example of three dimensions

A three-dimensional Monte Carlo program could be used to measure the degree of the interaction of grain growth and development of texture at thermal treatment. The program includes unique software that can transform the original grain structure into the input of the program. What’s more, the characterization of the orientation dependence of the boundary mobility could also be included into the input which increases the accuracy of the result prediction. The output of the program quantifies the expanded texture based on the pole figure or crystallite orientation distribution function and the statistical data of the structure of the grain such as the distribution of the grain size. Based on the initial condition and types of materials, grain growth could be predicted by the system.

Another example of three dimensions is the grain growth in polycrystalline materials. The growth of grains occurs due to the migration of grain boundaries, and the driving force for grain growth is the reduction of the free energy of these grain boundaries. It has been observed that the curved boundary usually migrates towards its curvature centre. As the smaller grains disappear, the mobility increases more. The grain growth simulation is carried out with a $Q$ value of 36. The choice of $Q$ state is very important because it determines the optimality of the simulation conditions and thus affects the simulation. A snapshot of the grain growth kinetics is shown in Figure 1 [11].
4. Discussion
The normal grain growth phenomenon could be modelled with the Monte Carlo simulation both in two and three dimensions. Results could be compared with experimental and real samples to verify the accuracy of the simulation. In these simulations, various lattice models with different grain boundary energy anisotropy characteristics were examined to check the generality of the results. The microstructure predicted depends on the artificial parameter $Tr$ in each a random single lattice where $Tr$ represents the temperature required and decides the energy fluctuation of the grain boundary movement. With $Tr$ increases, characterizing the boundary energy anisotropy of the single lattice could not be the dominant factor that affecting the expansion of the microstructure. Overall, the difference in grain size distribution between different lattice structure is quite important for low value of parameter $Tr$ and increases as $Tr$ decreases. The distribution is produced at a sufficiently large $Tr$ and is quite similar to the normal distribution at the moment of the weighting procedure is produced by using the weight of the square of the radius of the certain grain. The difference between the in-plane particle size distribution of normal and experimental samples with results from three-dimension system shows that the simulation reproduces the distributions observed in normal samples very well. Therefore, the grain size distribution predicted from this simulation is to characterize the general form of true normal grain growth and the driving force is mainly to reduce grain boundary energy through grain boundary migration[12].

5. Conclusion
After the analysis of two examples of the application of Monte Carlo simulation in two and three dimensions respectively presented above, several conclusions could be obtained. Firstly, if a certain material that includes several components has some significant original texture while other orientation decides the mobility of the grain boundary, the behavior could be predicted changing the value of cycles of the grain growth. Secondly, with boundary energy element included in the computational calculation, the 3D MC simulation could be used to predict the dependence between the energy of the grain boundary and degree of orientation.

Above all, the Monte Carlo simulation used in both two and three-dimensions could offer useful information for the analysis of microstructure and grain growth for different materials. With the fast development of technology nowadays, Monte Carlo simulation could come in handy in all kinds of fields such as economy, engineering, supply chain and science. In the future, computational material science will become the mainstay in material characterization with the help of Python.

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