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Research on recursive statistical measurement of grain size based on MC simulation method

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ABSTRACT

As it is difficult to measure grain size due to the migration of lattice points at grain boundaries, a new method of accurate and rapid grain size determination using Monte Carlo(MC) method, recursive statistical method, was proposed, and then recursive statistical method was used to measure grain size. The results show that the grain size measured by recursive statistical method is more accurate than that by intercept method, and the measurement accuracy is not affected by the grid type of the model and the size and shape of the grain, and the measurement speed is faster than other statistical methods.

KEYWORDS

recursive statistics; Grain size; Monte Carlo method; microstructure

In pure metals, alloys, ceramics and other polycrystalline materials, grain growth is the most common phenomenon, which has a very important effect on the properties of materials. At present, the most widely used and mature method to simulate grain growth is the MC method[1-2], because MC simulation can reveal the topological and dynamic characteristics during the evolution of material microstructure, and can simulate the evolution of material microstructure.

In the study of MC simulation of grain growth and analysis of simulation results, the statistical grain size is an essential link. At present, there are intercept method[3], fast labeling algorithm[4] and image tracking technology for grain number statistics. Zhang J X *et al.*[5] calculated the grain size using an approximate quantitative metallographic method, namely the cut-off method. Mo C L *et al.*[4] used the cursor to mark and correct the model point by point, that is, the fast marking algorithm, to calculate the grain size.

These methods can not give full play to the advantages of computer simulation experiment, and the calculation amount of fast labeling algorithm is greatly increased. Therefore, this paper presents an efficient and fast accurate statistical algorithm, namely recursive statistical method. It uses the number of lattice points in the statistical model to accurately calculate the grain size of the simulation process, and measures the grain size by recursive walking, which does not need to modify the calculation and greatly reduces the calculation amount.

1 Monte Carlo algorithm

The selected two-dimensional plane region is discretized into a number of tiny regular polygon elements. For each element, one of Q(Q>1) integers is randomly selected as its microscopic orientation. The adjacent small elements with the same orientation form a grain, and the grain boundary is formed between the adjacent elements with different orientations. The implementation process of the algorithm is as follows:

1) Determine the structure of the unit and divide the calculated two-dimensional area into units.

2) Map the region to a two-dimensional matrix and initialize the matrix (each element of the matrix is randomly assigned an integer from 1 to Q, which represents the orientation of its corresponding unit).

3) Randomly select a unit and calculate the free energy E_0 of the unit.

4) Randomly select one of the other Q~1 possible orientations to assign to the unit and calculate its free energy E_1.

5) Compare the energy difference $\Delta E(\Delta E=E_1-E_0)$ before and after the orientation change of the unit. When $\Delta E\leqslant 0$, the new orientation is accepted.

6) The shift of orientation of a series of units at the grain boundary constitutes the migration of the grain boundary.

2 Grain statistics

In the process of simulation, the grain size should be counted at any time. However, due to the random growth of grains in the simulation process, the size, shape and distribution of grains are irregular, and the grains are embedded with each other, which brings difficulties to the grain statistics. In order to facilitate the statistics, the model should be graded before the recursive statistical method used in this paper is used to calculate the grain size.

2.1 Model classification

To measure grain size, the essence is to count the number of lattice points accounted for by each unit grain. Recursive statistics method is to first divide all the lattice points occupied by unit grains into first-order grid points, second-order grid points, third-order grid points, and N-order grid points according to the order of statistics. The classification of the model is to make the statistical steps form a recursive relationship during statistics. Taking two-dimensional cellular grid points as an example, the graded grid points form the relationship shown in Figure 1, and the encircling circle from small to large is formed according to their level.

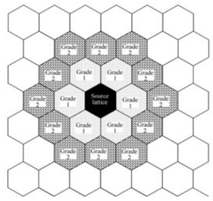

Figure 1 Classification of model

2.2 Recursive Statistics

The recursive statistics method is used for grain statistics analysis. By using the cursor to move through the numerical array points of the simulation results, a recursive relationship is formed. Then, this recursive relationship is implemented by a computer to count the number of array points. The specific steps of grain recursive statistics are as follows.

(a)First, any lattice point in the grain is defined as the central source lattice point. All the lattice points occupied by the grain are classified based on this point. First, all the lattice points occupied by the grain are classified, and then it is stipulated that each path of the statistics walk starts from a higher-level lattice point and continues to the lowest-level lattice point until reaching the boundary of the grain to end the statistics.

(b)The statistical process is illustrated using a honeycomb model as an example. First, the model lattice points are classified. Assuming that the second-level lattice points are the terminal-level lattice points, the walking paths of the statistics process are as follows:

1) Start walking from the central source grid point to the first level-1 grid point;

2) Determine if this grid point is a terminal grid point. If it is, proceed to step 3), otherwise proceed to step 4);

3) Walk to the next level-1 grid point and execute step 2);

4) Walk to the first level-2 grid point;

5) Determine the nature of this grid point. If it is a terminal grid point, proceed to step 6), otherwise continue walking to lower-level grid points;

6) If there are still level-2 grid points that have not been counted, walk to the next level-2 grid point and execute step 5), otherwise proceed to step 3).

c. The counting process forms a recursive relationship. The loop process of steps 2) and 3) is called the level-1 grid point loop process; the loop process of steps 5) and 6) is called the level-2 grid point loop process. And so on.

3 Simulation Results

A 600×600 Potts lattice was adopted. Each lattice point was assigned an orientation Q (ranging from 1 to 64), and periodic boundary conditions were introduced. The simulation results of the continuous growth and evolution of the grain structure over time are shown in Figure 2. It can be seen that as the simulation time increases, the average grain size significantly increases, and the grain growth is the result of large grains swallowing small ones; most of the grain boundary junctions are three-grain boundary intersections, and the intersection angles are basically equal to 120°.

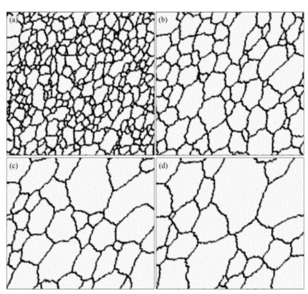

Figure 2 Simulation images (a) 500MCS; (b) 2000MCS; (c) 5000MCS; (d) 10000 MCS

Figure 3 shows the comparison of the grain size measurement results obtained by the recursive statistical method and the intercept method. It can be seen from the figure that for the same simulation result, the value measured by the intercept method is larger than that measured by the recursive statistical method. From the overall measurement results, the measured n value obtained by the intercept method is 0.4886, which is much larger than the actual value of the simulation result. However, the new calculation method adopted in this paper is to obtain the grain size by using the total number of unit cells occupied by each grain in the lattice in the statistical simulation results, so the measured n value is closer to the actual simulation value.

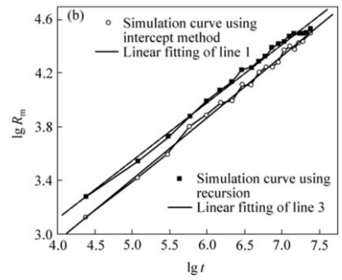

Figure 3 The simulated curve and its fitting line

4 Conclusion

1) Combining the characteristics of boundary migration in MC simulation of grain growth and the characteristics of the applied model, a new method of grain size measurement, recursive statistical method, is proposed.

2) The method can measure grain size more accurately than the intercept method, and the measurement speed is faster than the intercept method; It is not limited by the model lattice type, and the tetragonal, hexagonal and triangular lattice are applicable.

3) The method can still obtain accurate statistical results for grains with irregular shapes, and is suitable for two-dimensional and three-dimensional lattice models; The number and size of grains can be calculated accurately with or without periodic boundary conditions.

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