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Materials

Cellular automata modelling of austenite grain coarsening during reheating — I. Normal grain coarsening

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Abstract: A two-dimensional cellular automaton (CA) model has been developed for the description of the normal grain coarsening process. The probabilistic CA method incorporating Moore's definition of the neighbourhood is used to simulate the normal grain coarsening process with a new transition rule. The model simulates the grain coarsening process in as much detail that is possible, from the point of initial nucleation to subsequent coarsening with computational times. The unique result is that the grain coarsening speed can be controlled by the specific method, this result is vital to model the grain coarsening quantitatively. In order to make this model valid, experimental work has been done to provide solid evidence for this model. Comparison of the modelling result and the experimental result has been carried out.

Key words: computer simulation; grain growth; microstructure; reheating

1 Introduction

The thermomechanical rolling process can be briefly divided into the following general categories: reheating, rough rolling, finish rolling and runout table cooling. During each of these stages, a great deal of physical metallurgy related to the process occurs which influences the microstructure and subsequent mechanical properties of the final product. Grain coarsening represents one of these processes occurring during reheating and in the delay between the rolling passes after recrystallization. At present, the evolution of microstructure is oversimplified because only the mean grain size is considered, and therefore it is difficult to provide information on the dynamic evolution of the microstructure and its inhomogeneous distribution across a given cross-section.

Due to the difficulty of directly incorporating the topological features into the empirical models of grain coarsening, together with the difficulty of giving a space-time description of grain distributions, there has been increasing interest in using computer simulations to study the grain coarsening in single phase materials. A variety of models have therefore been put forward. These have included the continuum field model [1, 2], the Monte Carlo (MC) model [3-5], the Vertex model [6], and the cellular automaton (CA) model [7]. Although these methods can give graphical description of the dynamical microstructural evolution, different methods put forward different grain coarsening exponents. Among these, the Exxon group using the Monte Carlo method [3] predicted the grain coarsening kinetics to be 0.41±0.03. Fan and Chen [1] using the continuum field model put forward the n value of 0.5. Liu [7] using the CA method got the n value of 0.45. A common feature of all these models is that all of them describe grain kinetics as a single value or a range. However, Hu [8] presented a detailed study of isothermal grain coarsening in zone-refined iron in the temperature range of 550-850°C, which showed that n increases with temperature from approximately 0.25 to 0.5, meaning that n is temperature dependent.

Liu [7] applied the CA method to simulate normal grain coarsening using Von Neumann's definition of neighbouring cells with deterministic transformation rules. Raabe [9] showed some consecutive 2D sections from a 3D grain coarsening simulation of a recrystallized aluminum single crystal. All equations of motion were simultaneously integrated using a weighted stochastic sampling integration scheme.

Building on these, it has been tried to simulate the grain coarsening process during reheating using the CA method. This paper reports on the first stage of the work which is to simulate the normal grain coarsening behaviour of austenite [10, 11]. The model uses Moore's [12] definition of a neighbourhood to simulate the grain coarsening process with a new nuclea-

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tion method and a new transition rule for grain coarsening. The model simulates the grain coarsening process in as much detail that is possible from the point of initial nucleation to subsequent coarsening with computational times. In this model, the unique result is that grain coarsening exponents are different under different conditions, which means that the grain coarsening speed can be controlled. This result is quite different from any other reported results that always give the grain coarsening exponent as a single value or a range. It has been found that the grain coarsening exponent 0.5 is not a limitation for grain coarsening from a topological viewpoint. Based on these results, a relationship has been built to compare the experimental result and the modelling one with a fair accuracy.

2 CA modelling of normal grain coarsening

In consideration of the normal grain coarsening of austenite, a probabilistic CA model has been designed to meet three requirements. First, the outcome of the model has to be independent of the CA network. Second, the model has to reflect the topological grain coarsening process, and third, the grain coarsening kinetics has to be properly taken into account. This is achieved in the manner described below.

In order to simulate normal grain coarsening, a network of cells is laid out according to a regular lattice arrangement and the distance between two neighbouring cells is assumed to be 1 unit. In this model, the number of lattice cells can be selected. In general, the lattice is divided into a 300×300 regular network of cells with a periodic boundary condition. At the same time, grain orientation is represented by a state index which is plotted by a specific colour. Lattice cells which are adjacent to neighbouring cells with different grain orientations are regarded as being part of the grain boundary, while a cell surrounded by cells with the same grain orientation is in the grain interior. Similar to the MC method, the unit of time is defined as 1 cellular automaton step (CAS), which corresponds to one loop re-orientation attempt. This means that for all cells, at every CAS, the state index of each cell is updated simultaneously. At the beginning of the simulation, each cell is given the same initial state with an index zero, after which the time-stepping calculation is initiated. Austenite begins to nucleate at random locations, followed by grain coarsening. These aspects are detailed below.

Details about the modelling of nucleation process have been given elsewhere [19]. The initial state of each discrete cell is taken from the nucleation stage, and subsequently updates with time. The state of a cell at time t_{n+1} is determined only by the state of all its neighbouring cells at time t_n. If Moore's definition of a neighbourhood is used, represented by **figure 1**, then the transition process can be written as:

$$G(i,j,t+\mathrm{d}t)=F\left(\sum_{i=i-1}^{i=i+1}\sum_{j=j-1}^{j=j+1}G(i,j,t)\right) \quad (1)$$

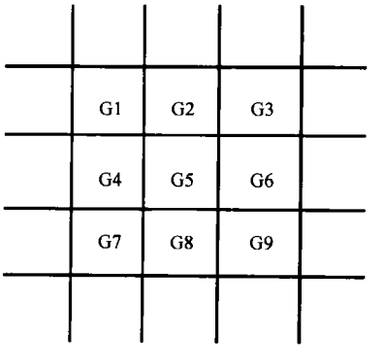

Figure 1 Moore's definition of a neighbourhood.

At each time step, every cell is scanned, and its state will change according to the following integrated rules (see figure 1).

(1) If all 8 cells around G5 have the same state as G5, then G5 will keep its state at the next time step.

(2) (a) If any three of states G2, G4, G6, G8 are the same integer, for example equal to integer A, then G5 →A. Similarly, if (a) does not hold, then (b) if any three of states G1, G3, G7, G9 are the same, for example equal to an integer B, then G5→B.

The distribution of grain boundary energy is homogeneous. A cell must overcome an energy barrier to change its state: if any of the eight surrounding cells have a different state from G5, then G5 has the possibility to change its state. In this case, the probability is the same for all grains and is set to be *P*. In the model, energy is referred as the energy barrier for the cells on the boundary to change the state.

When a cell is selected, its checking process is (1)→(2a) → (2b) → (3). If its state can meet any one of the conditions and change or maintain according to this condition, then the following conditions will be ignored. For example, condition (1) is actually to judge if this cell is in the grain interior or on the boundary. If it is in the grain interior, it must maintain its state and the following conditions do not need consideration any more and the next cell will be checked subsequently; if not, this cell must be on the boundary and then the computer will check if its state can meet condition (2a) and so on. In the present model, the triple point is not explicitly considered, but the final result shows that 120°C dihedral angle tends to form between the grain boundaries under the integrated

transition rules.

Of the integrated rules given above, the first is quite easy to understand because the activation energy for grain boundary diffusion is much lower than that for volume diffusion [15], so the diffusion is easier along grain boundaries than in the grain interior, this condition is set to reflect that a cell on grain boundary can change its state to the neighbouring state while a cell in the grain interior will maintain its state. The second rule is to simulate the grain curvature effect: the grain boundary would tend to form a straight line because of the surface tension requirement. The reason to select the Moore configuration considering both the nearest and next-nearest neighbors is to make a boundary form in any direction. Although the third rule may seem unnecessary, it is to simulate the effect of grain boundary energy, which is vital to keep the boundaries move and make small grains vanish. Grain coarsening belongs to a self-diffusion process that can be explained by vacancies. In order for an atom to jump into a hole from a lattice position bordering the hole, it must overcome the net attractive force of its neighbours on the side opposite to the hole. Thermal vibration of the crystal lattice provides the atom enough energy to overcome the barrier. Conditions (1) and (2) are deterministic, while condition (3) is probabilistic. P is selected in the range [0, 0.02]. It is quite interesting to find that P is related to the grain coarsening kinetics, which will be discussed later.

Liu [7] adopted the CA to model the normal grain coarsening with Von Neumann's definition of neighbourhood. Although both belong to the first level neighbourhood, the Von Neumann neighbourhood is relatively simple in comparison with the Moore neighbourhood. As explained above, it is found that the Moore neighbourhood is helpful in making the boundary form in any direction and the whole microstructure is independent of the CA lattice. By the way, he assumed that temperature was high enough for all cells on the boundary to overcome the energy barrier to reach its new state, *i.e.* the probability for such a transformation is 1. This is not true from the metallurgical theory and experimental observation [15]. This condition of course makes his model to be a deterministic rather than a probabilistic one. Raabe [9] showed some consecutive two-dimensional sections from a three-dimensional grain coarsening simulation of a recrystallized aluminum single crystal. All equations of motion are simultaneously integrated using a weighted stochastic sampling integration scheme. He also adopted Von Neumann's definition of the neighbourhood. It is obvious that his model is different from the present method.

3 Experimental

The composition of the microalloyed steel investigated in the paper is (wt%) C, 0.1; Mn, 1.5; Si, 0.4; P, 0.01, Nb, 0.03; and N, 0.008. This material was obtained in the form of steel plate from Corus Research, Development and Technology (Swinden Technology Centre). The cubic samples (8 mm×8 mm×8 mm) were cut from the as-rolled steel and were heated at temperatures between 1200 and 1300°C. According to the solubility of Nb in austenite for the steels [16]:

$$\log[\mathrm{Nb}][\mathrm{C}] = 2.06 - 6700/T \qquad (2)$$

When [Nb]=0.03 and [C]=0.1, the precipitate dissolution temperature T_{Diss} can be calculated to be 1189°C, and the abnormal grain coarsening temperature (T_{GC}) is 1064°C. The reason for the temperature of 1200°C and 1300°C is that below this temperature, complete solubility in austenite occurs for a Nb monocarbide, mononitride, and carbonitride, so normal grain coarsening can be demonstrated. Prior to each austenitising treatment, the samples were sealed in an evacuated quartz tube backfilled with dry argon (99.9 % in purity).

The experimental procedure is as follows.

- When the specific temperatures were reached, the samples were put in. The holding time at respective reheat temperature varied from 30 min to 12 h, followed by quenching in an iced-brine solution.

- Temper treatment: 500°C for 24 h to allow for phosphorus segregation along prior-austenite grain boundaries.

- Quantitative metallographic analysis for the determination of both grain size and grain size distribution was shown as a function of reheating temperature. Heyn intercept method was used to calculate the average grain size and every grain size, thus the grain size distribution and error bars with 95% confident limits could be established.

4 Results and discussion

4.1 Validation of the CA model

Grain boundaries are associated with a positive boundary energy and surface tension. Diffusion of atoms across the boundary results in boundary motion towards the centre of the curvature. It is generally believed that a circular boundary shrinks under its own curvature, which is characteristic of the surface-driven process. This is true, but this is not the only reason to explain why grain coarsening happens. Grain coarsening is also driven by the grain boundary energy. In steels for example, at high temperatures, grain

coarsening can happen by the diffusion of atoms across the boundary because of thermal effect, while at room temperature with little or no energy input, nothing happens no matter wherever there is curvature or not. This is direct evidence of the effect of energy. It is believed that above explanation gives a relatively complete picture of grain coarsening. From the transition rule of this model, it can be seen that this model has considered both factors. In order to prove it, we let this model run in the 2D ideal grain coarsening condition.

In order to validate the present CA model, two cases have been considered, one is circle, which shows the equal curvature along the boundary. Another is square, where curvatures at the corner and edge are different. Results of both cases can be used to analyse any other geometry.

For this simple model, instead of the nucleation space-filling process, all cells in the lattice are just assigned one of two states: within the circle, the cells are assigned with state 1; outside the circle, the cells are assigned with the different state 2. The P value is the same for all cells. Then we can observe the circle evolution under the transition rule of normal grain coarsening.

Figure 2 shows the circle evolution at a specific P value. It can be seen that the circle briefly maintains the circle shape, shrinking towards the centre under its own curvature. The reason for the zigzag boundary is due to a statistical perturbation. This process has been repeated more than 10 times, and all results are same.

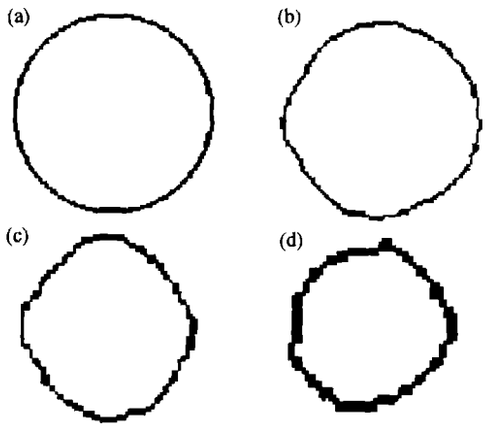

Figure 2 Circle evolution: (a) at beginning; (b) 12773 CAS; (c) 52731 CAS; (d) 69177 CAS.

It is also quite interesting to see that the higher the P value, the more frequently the cells along the boundary to change the state, and the more quickly the circle shrinks. It takes about 78×10^3 CAS for the circle to shrink completely when P=0.0045, while it only needs about 15×10^3 CAS to finish the process when P=0.01. This actually validates the present work on the grain coarsening exponent, which will be introduced later, in which the grain coarsening exponent is different at different P, and illustrates the importance of the energy effect in grain boundary migration.

We also have interest to see how square evolves under the same condition. **Figure 3** shows this process. At the initial stage, the cells on the corners shrink more quickly than that at the centre of the square, while the cells on the edge remain relatively static. Gradually, the square turns to look like a circle, after which the behaviour is exactly the same as that of a circle. This proves the curvature effect in this model. This result is in agreement with our general understanding of boundary curvature. The grain boundary moves faster at higher curvatures, which is driven by the higher surface tension.

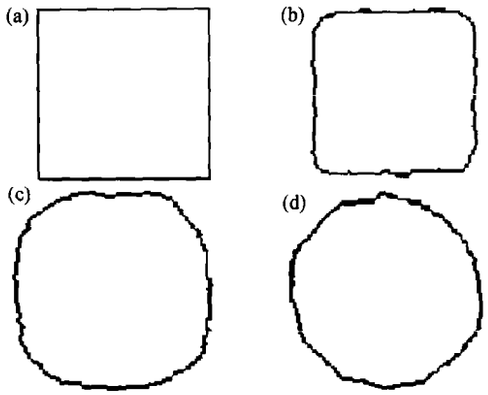

Figure 3 Square evolution: (a) at beginning; (b) 634 CAS; (c) 2200 CAS; (d) 6125 CAS.

Although the above cases never exist in reality, a demonstration of the two cases helps in understanding how the present model works and how grain coarsening occurs in reality. This model has actually coupled the grain boundary migration driven by both curvature and energy. In reality, it is suggested from this 2D model that grain coarsening is also driven at least by both factors.

4.2 CA modelling results

The results from the CA model for normal grain coarsening are shown in **figure 4**. Simulations were performed for up to 22000 steps. Many features of normal grain coarsening can be seen. Beginning from nucleation, where the individual nuclei are randomly distributed, a variety of grain shapes are allowed to develop until impingement between neighbouring grains along shared boundaries. It takes about 200 CAS to finish the nucleation stage. Because the nucleation process is not the focus of the present work, we do not provide any further analysis about the nucleation process. In the grain coarsening process,

within a given area, such irregular grain structures might rapidly adjust as the time increases, which is in conformity with surface energy and tension considerations.

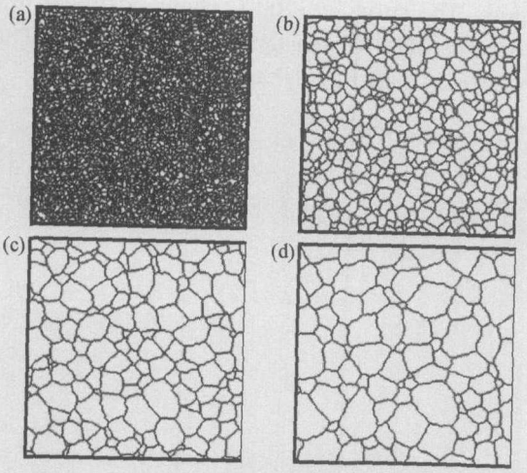

Figure 4 Representative fields of simulated microstructures: (a) After nucleation; (b) 4000 CAS; (c) 12000 CAS; (d) 20000 CAS.

Figure 5 shows the frequency distribution in the number of sides of individual grains, which is plotted based on the modelling pictures at different CAS. The grain with three sides is always unstable and disappears gradually, replaced by grains that have the highest probability (and the highest stability) with 5-6 sides. At the other extreme, grains with more than 9 sides are almost nonexistent in the pictures. It can be observed from the simulated microstructures that there may exist some curved boundaries, but the boundary always tends to form a straight line with increasing computation times. When four grains meet at one point, they are always unstable and tend to separate. It is also quite interesting to observe that 120° dihedral angles tend to form between grain boundaries. While these geometries are not explicitly imposed on the model, the final results show they are the best choice for grain coarsening under the integrated conditions. These characteristics fit the general topological requirement of the grain size distribution.

This CA model can automatically output the average grain size, grain size distribution, normalized grain size distribution, n and microstructural pictures at any time step if required. Because it is a probabilistic model, this model can never offer the exact same result when repeated, but it indeed outputs the close result under the same condition due to the statistical reason. Over a statistically significant number of trials, it is obtained that the standard deviation of the average grain size is 2%, the standard deviation of n value is 4.5%. This proves that this model is reliable and accurate.

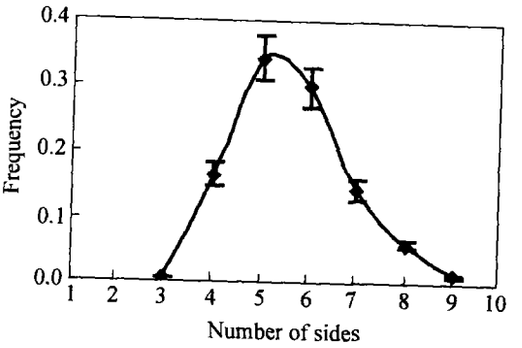

Figure 5 Distribution of grain sides under normal grain coarsening.

Figure 6 plots the grain size distribution normalized by the mean diameter. The grain size distribution is relatively stable and is invariant of CAS. This distribution is not completely Log-Normal and quite like the experimental results. The experimental normalized grain size distribution at 1200°C and the Log-Normal distribution are also plotted. It can be seen that the simulation results agree reasonably well with the experimental data. Both the experimental data and the simulation data are asymmetric and have a cut-off at the large size region.

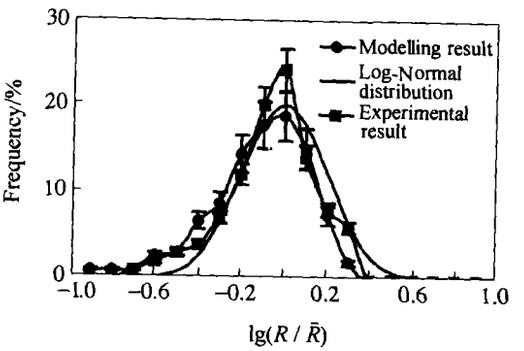

Figure 6 Comparison of modelling grain size distribution with the experimental result and Log-Normal result.

The average diameter increases with computational time, it is also found that the grain coarsening exponent (n) can be controlled by a proper choice of P, more than 20 trials give the similar results. These results are completely different from any other reported simulation results which always give grain coarsening kinetics as a single value or a range. We arbitrarily set the P value to be 0, which means that condition (3) is ignored, and the CA program becomes a deterministic method, not a probabilistic one. The curve with P=0 shows that the grain size only has a slight growth after nucleation. It reflects the fact that at relatively low temperatures, such as iron at room temperature, not enough energy is input to make atoms jump over the boundary, and also the grain size can maintain stability. This completely fits the natural phenomena. Then

a different P is selected to observe the grain size evolution with the calculation time. It can be seen that grain coarsening can briefly meet the general relation $R_t = kt^n$, where the n increases correspondingly with P. This is not difficult to be explained: the higher the probability, the more chances that the cell can change its state, so the faster the grain grows. This is a quite useful result. If it is known what the n value should be for a material at a specific temperature, then a corresponding P value can be selected to simulate the material. **Figure 7** shows how the grain coarsening exponent (n) changes with P. The regression relation between n and P is:

$$n = 0.07319 + \frac{0.5161P}{0.002376 + P} \quad (3)$$

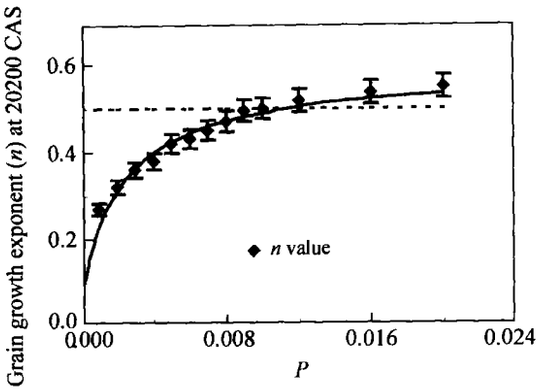

Figure 7 Grain growth exponent (n) changes with P.

In general, the grain coarsening exponent should be in the range [0.06, 0.5] if the P value is selected to be in the range [0, 0.01] in this model. It is also seen that n=0.5 is not a limitation for grain coarsening from a topological point of view, the grain coarsening exponent can be over 0.5 if we select a large P.

4.3 Experimental results

The austenite microstructural pictures at 1300°C are shown in **figure 8**. At temperatures around 1200 and 1300°C, the situation is relatively stabilized as indicated by flattening of the curve of the mean grain size which shows normal grain coarsening. Reheating at 1300°C would be expected to ensure the dissolution of nearly all precipitate, so that, only a small volume fraction of precipitate remains to retard grain coarsening. These remaining particles, however, are ineffective because they are coarse. The reheating time is 30 min, 1 h, 2 h, 7 h, and 12 h, respectively. The initial rapid grain coarsening occurs at 30 min and 1 h, but the growth rate decreases gradually with the increase of the reheating time. This is understandable because at the moment, the grain size becomes very large, which needs a relatively long time to consume other small grains. It is speculated that abnormal grain coarsening occurs during the 30 min after the sample was put in, after that, the grain coarsening in this temperature and reheating time region can, therefore, be considered as normal grain coarsening at high temperature. The curve at 1200°C shows a similar trend with one at 1300°C, but the grain size at 1200°C on the whole is smaller than that at 1300°C.

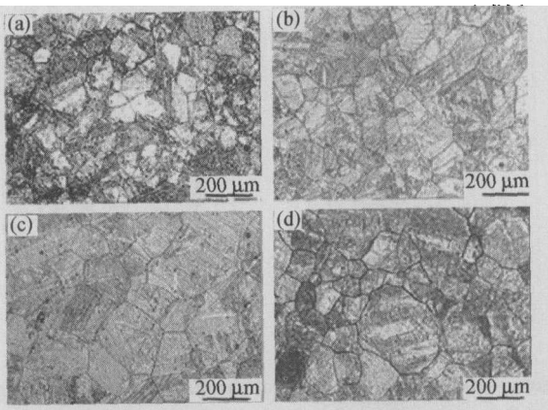

Figure 8 Isothermal grain size evolution with the reheating time at 1300°C: (a) 30 min; (b) 1 h; (c) 7 h; (d) 12 h.

Regression equations need to be drawn to reflect the grain coarsening and its kinetics at different temperatures, which provide the basis for the following process.

4.4 Comparison of the experimental result and the modelling result

Although the present CA modelling of normal grain coarsening looks like a real grain coarsening process in every detail, it can not compare with the real microstructure because the time scale and grain size scale are different. In order to analyse the grain coarsening process quantitatively, it is necessary to build the relationship between the CA parameters and real material parameters such as temperature, time scale and grain size scale. Based on the experimental results and simulation ones, a methodology used for achieving the above aim is put forward [11, 19].

Figure 9 shows a comparison of the experimental curve and the simulation one. It can be seen that the simulation curve can give a reasonable representation of the experimental one. It is seen that the CA technique, in conjunction with the methodology used for obtaining the correlation between CA and real parameters, can be satisfactorily used to simulate the isothermal grain coarsening data for the observed steel, because the CA method and experimental result show a similar trend with the reheating time.

Because of the difficulty of direct measurement and observation of the physical system, the CA method can help us understand and predict what happens in real system. From the present work, it can be seen that

CA is a quite good tool to model microstructure evolution. The experimental work is indispensable to the present model, but the experimental results are always discontinuous. The advantage of the present model is that it can output continuous curve of microstructure evolution by coupling of the experimental results.

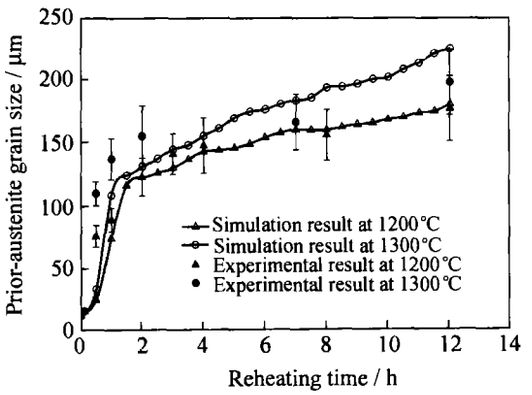

Figure 9 Comparison of the experimental result and the modelling result.

5 Conclusions

(1) A two-dimensional cellular automata model has been developed to describe the normal grain coarsening with a nucleation condition and a new transition rule. The output pictures look quite like the experimental pictures from a topological viewpoint. The grain size distribution and grain side distribution are time invariant with the calculation time step.

(2) The model reflects the fact that grain coarsening kinetics gradually increases with P, and temperature can be coupled in the program. It is shown that grain coarsening kinetics increases with temperature which is close to the experimental observation. This result paves the way for modelling the normal grain coarsening quantitatively.

(3) The experimental research on austenite grain coarsening behaviour of microalloyed steel has been carried out. The grain size evolutions with the temperature and reheating time have been plotted. This provided the basis for the modelling work.

(4) Because the modelling result and experimental one show similar trends with time, the methodology used for obtaining a correlation between CA and physical parameters has been put forward, which is believed to have the potential to simulate the grain coarsening process on a physical time scale.

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