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Comparison of Analytical Models with Cellular Automata Simulation of Recrystallization in Two Dimensions

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Cellular automata simulation of recrystallization in two dimensions is carried out. The simulated microstrutural evolution is compared in detail with the predictions from mathematically exact analytical theories considering both kinetic and geometrical aspects. Very good agreement is observed between the cellular automata simulation and the theoretical results. Moreover, the simulated data is used to test new expressions recently derived to describe the evolution of the interfaces between recrystallized grains. This work focuses on recrystallization but its results are applicable to any nucleation and growth transformation.

Keywords: *microstructure, kinetics, recrystallization, computer simulation, cellular automata*

1. Introduction

Recent years have witnessed a large increase in computer simulation of microstructural evolution. For example, there are many papers on computer simulation of grain growth evolution using a wide range of simulation techniques. Not so much attention has been given to recrystallization. One promising technique is that of cellular automata. Hesselbarth and Göbel[1] applied it for recrystallization in an early work. Other papers have also applied this technique[2-8].

An important issue that arises when a computer model is chosen is whether it is able to forecast the process results. In other words, to what extent one can trust that it actually simulates the intended process or phenomenon. Although the ultimate test of any model is to accurately represent reality, its first test is to determine its ability to describe the phenomenon in simple cases for which there are mathematically exact analytical solutions. A "good" model should be able to agree closely with the mathematically exact analytical solutions. Moreover, if valid, the simulation can assist the development of the analytical theory itself. The simulation can provide accurate data for situations in which there are no analytical results.

The basis of analytical modeling of recrystallization are the mathematically exact results of Johnson and Mehl[9], Avrami[10-12] and Kolmogorov[13], the JMAK theory, extended by DeHoff's[14] concept of microstructural path. Vandermeer and coworkers have successfully used this approach and developed it in recent years[15-17]. Detailed description of this theory has been recently given by Rios and Padilha[18]. In this theory, nucleation is assumed to take place in sites randomly located in the strained matrix. The simplest assumption is that all nucleation occurs at the beginning of recrystallization. This is normally called site-saturation and has been experimentally found to be a reasonable assumption for recrystallization[19]. When, in addition to that, a constant interface velocity is also assumed, a number of exact theoretical expressions are obtained. However, even for the simplest assumptions there are gaps in the theory. For instance, only recently analytical expression were developed[20] to quantitatively describe the time evolution of the interface area between recrystallized grains.

In this work, a cellular automata(CA) simulation of recrystallization is carried out. The simulated microstrutural evolution is compared in detail with the predictions from mathematically exact analytical theories considering both kinetic and geometrical aspects. Moreover, the simulated data is used to test new expressions derived to describe the evolution of the interfaces between recrystallized grains. It is worthy of note that although this work focuses on recrystallization its results are applicable to any nucleation and growth transformation.

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2. Cellular Automata Simulation

2.1. Description of the simulation

Cellular automata methodology was used to simulate recrystallization. The implementation followed that of Hesselbarth and Göbel[1,7,8] using the von Neumann neighborhood criterion. The matrix consisted of a square lattice with 812 x 812 cells and 784 nuclei. One cell was considered to have a unit area and consequently the side of a single cell had unit length. The units of all quantities reported here follow from this. The number of nuclei per unit of area, N_A, was equal to 1/841. The matrix size and number of nuclei were chosen for reasons described in a previous work[7,8]. The nuclei were randomly dispersed on the matrix. The nucleation was site-saturated: all nuclei appeared at $t = 0$. The simulation produced a sequence of matrices as a function of time. Time is discrete in CA, it takes integer values starting from $t = 0$. One time unit corresponds to the interval between two consecutive matrix updates[1,8]. From the simulated matrices, all the desired quantities could be extracted. Hesselbarth and Göbel give a more detailed account of two-dimensional cellular automata in general. Oliveira[8] gives further details of the present simulation.

2.2. Geometry and kinetics of the evolution of a single grain in CA

When a single grain grows in isolation, alone in a strained matrix, it is possible to find analytical expressions for its geometric and kinetic evolution. The following expressions are specific for the von Neumann neighborhood criterion adopted in this simulation. The time origin, $t = 0$, corresponds to an area fraction equal to zero, $A_A = 0$.

All nucleation takes place at $t = 0$ but at that instant the sizes of all nuclei are equal to zero. Therefore, the area of a single grain, a, and its perimeter, l, at $t = 0$ are equal to:

$$a(0) = 0 \tag{1a}$$

$$l(0) = 0 \tag{1b}$$

For $t \geq 1$ the area of a single grain as a function of time is[8]:

$$a(t) = 2t^2 - 2t + 1 \tag{2}$$

This equation is not valid for $t = 0$. Neglecting the lower order powers of time:

$$a(t) \cong 2t^2 \text{ area units} \tag{3}$$

Equation 3 is in error at the very beginning but will be used in what follows. Equation 3 suggests that for better results with CA it is better to use a large matrix with a small number of nuclei.

The perimeter of a single grain, l, for $t \geq 1$ is[8]:

$$l(t) = 8t - 4 \tag{4}$$

Again, neglecting early time behavior:

$$l(t) \cong 8t \text{ length units} \tag{5}$$

The interface velocity, v, can be calculated with the help of Cahn-Hagel[21] equation for 2d:

$$v = \frac{da}{ldt} \tag{6}$$

Inserting Equations 3 and 5 gives:

$$v = 0.5 \text{ units of length/unit of time} \tag{7}$$

The units will be omitted from now on.

The interface velocity is a constant. Therefore, for a single grain the simulation was able to produce constant growth rate.

The integral of the curvature of any closed figure along its perimeter is 2π, so the average interface curvature of a single grain is, for $t \geq 1$:

$$k = \frac{2\pi}{l(t)} \tag{8}$$

or

$$k = \frac{\pi}{4(t - 1/2)} \cong \frac{\pi}{4t} \tag{9}$$

If one considers the set of all grains growing as if they were isolated, it is common to refer to this set as the "extended space" and to the geometric properties of this set as "extended quantities". For example, the sum of the area of all grains growing as if they were isolated divided by the total volume is normally called "extended area fraction". This terminology will be used in what follows.

3. Results and Discussion

Figures 1-7 show the results obtained from the simulation compared with the theoretical expressions.

In this section, the expressions derived in the previous section for single grain evolution are used to obtain expressions containing "global" measurements, that is, average measurements such as area fraction and interface length per unit of area. The calculated expressions are compared with the results from the simulation. Section 3.1 mainly deals with quantities related to the mobile interface: the interface between recrystallized and nonrecrystallized regions. Section 3.2 compares simulations results with new expressions derived for the evolution of the interfaces between recrystallized and nonrecrystallized regions.

3.1. Area fraction, interface length per unit of area, microstructural path, grain boundary velocity and grain boundary curvature

The extended area fraction, A_{AE}, is the sum of the area of all individual grains supposing that they grow without impingement. The subscript "E" is reserved for "extended quantities" defined in a manner similar to the extended area fraction.

$$A_{AE} = N_A a = 2N_A t^2 \tag{10}$$

For randomly located nuclei, extended area fraction, A_{AE}, and real area fraction, A_A, are related by the JMAK[9-13] expression:

$$A_A = 1 - \exp(-2N_A t^2) \tag{11}$$

Figure 1 shows a comparison between A_A calculated from the analytical solution and obtained from the CA simulation. The agreement is very good.

The extended interface length between transformed and untransformed regions, L_{AE} is the sum of the interface length of all individual grains supposing that they grow without impingement:

$$L_{AE} = N_A l = 8N_A t \tag{12}$$

For randomly located nuclei, extended interface length and real interface length, L_A, are related by the DeHoff's[14] expression:

$$L_A = L_{AE}(1 - A_A) = 8N_A t \exp(-2N_A t^2) \tag{13}$$

Figure 2 shows a comparison between the L_A calculated from the analytical solution and obtained from the CA simulation. The agreement is very good.

In two dimensions the microstructural path can be seen as a curve on the (A_A, L_A) plane. From Equations 3 and 5:

$$l = 4\sqrt{2}\sqrt{a} \tag{14}$$

Multiplying both sides by N_A and using the above:

$$L_A = \sqrt{32N_A}(1 - A_A)\sqrt{\ln\left(\frac{1}{1 - A_A}\right)} \tag{15}$$

Figure 3 shows a comparison between the values calculated using the theoretical expression for the microstructural path obtained above and those obtained from the simulation. The agreement is very good.

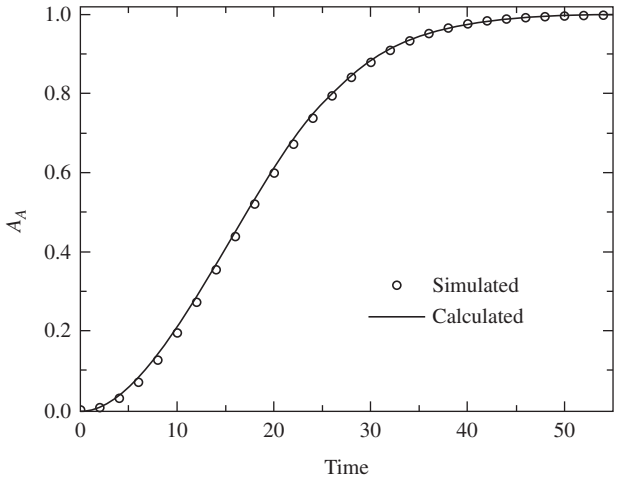

Figure 1. Area fraction, A_A, against time. Simulation results are in agreement with those calculated from the kinetics of a single grain, Equation 11.

The grain boundary velocity is given by[21]:

$$v = \frac{da}{ldt} = \frac{1}{L_{AE}}\frac{dA_{AE}}{dt} = \frac{1}{L_A}\frac{dA_A}{dt} = 0.5 \quad (16)$$

The grain boundary velocity calculated from the simulated values was 0.51 ± 0.01, very close to the theoretical prediction. This means that the interface velocity in real space is the same as that in extended space, as expected.

The average curvature of the interface between transformed and untransformed region can be measured by DeHoff's[22] sweeping tangent method:

$$k = \frac{\pi T_A}{L_A} \quad (17)$$

T_A is the number of points of tangency between a sweeping test line and a grain boundary per unit test area. Also by multiplying and dividing Equation 8 by N_A and using Equation 13:

$$k = \frac{\pi}{4t} = \frac{2\pi N_A(1 - A_A)}{L_A} \quad (18)$$

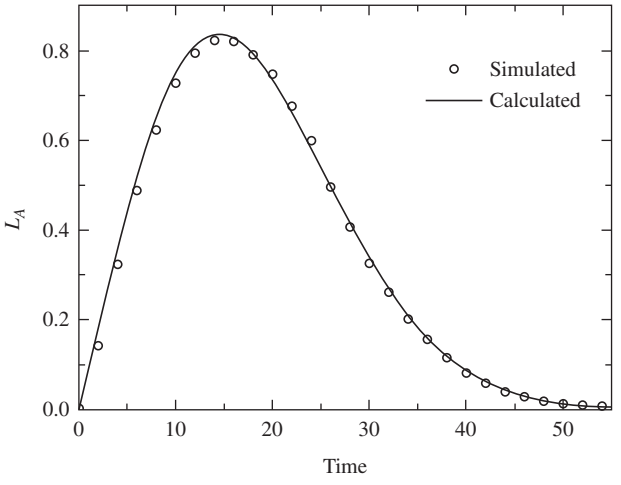

Figure 2. Length of the interface between transformed and untransformed region per unit of area, L_A, against time. Simulation results are in agreement with those calculated from the kinetics of a single grain, Equation 13.

JMAK assumes that the interface shape remains unchanged after impingement. For example, the interface between transformed and untransformed region of a circular grain after impingement remains the arc of a circle of the same radius of the radius of the circle that it would have if it were growing as an isolated grain. This implies that the average curvature of the interface between transformed and untransformed region, Equation 17, is equal to the average curvature of a single grain, Equation 18.

Figure 4 shows a comparison between the values calculated using the theoretical expression, Equations 9 or 18, obtained from a single grain, for the average curvature of the interface between transformed and untransformed region per unit of area, k, and the values obtained from the simulation, by means of the sweeping tangent method, Equation 17. The agreement is very good. This means that the moving interface shape remains the same after impingement, as supposed in the JMAK theory.

It is important to stress that the calculated curves in Figures 1-4 were not fitted but obtained from the kinetics of a single grain using nothing but the JMAK correction for impingement.

3.2. New expressions for the impinged interface length per unit of area, total interface length per unit of area and the contiguity

There are two kinds of interface during recrystallization: mobile and immobile. The mobile interface is the interface between the recrystallized region and the deformed matrix. This interface migrates and its migration determines the recrystallization progress. The immobile interface is a consequence of impingement of recrystallized grains. The recrystallized grain size is a function of the interface area between recrystallized grains when the recrystallization reaches 100%.

Traditionally, recrystallization studies focus on the mobile interface. This could be seen in the previous section. All equations involve only L_A. However, the amount of interface between recrystallized grains is an important quantity and contains valuable information about the evolution of recrystallization. The CA simulation is able to provide accurate data on these interfaces and so gives a good basis for comparison with analytical models. In what follows, recently obtained[20] analytical expressions are shown for the interface length of the interface between recrystallized regions per unit of area, L_R, and for the total interface area per unit of area, L_T, defined as:

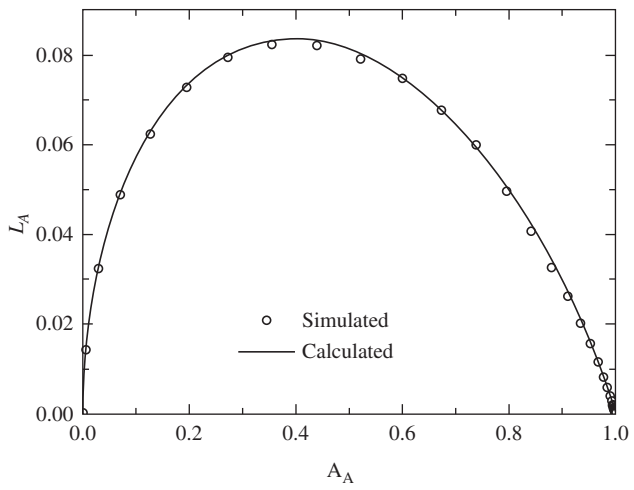

Figure 3. Microstructural path: length of the interface between transformed and untransformed region per unit of area, L_A, against Area fraction, A_A. Simulation results are in agreement with those calculated from the kinetics of a single grain, Equation 15.

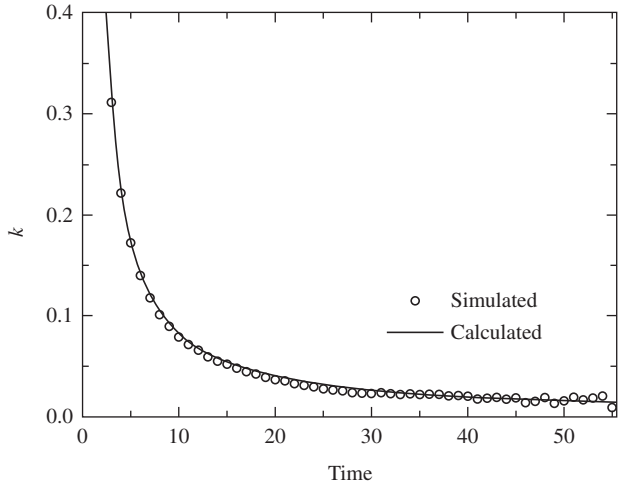

Figure 4. Average curvature of the interface between transformed and untransformed region, mobile interfaces, per unit of area, k, against time. Simulation results are in agreement with those calculated from the kinetics of a single grain, Equation 9.

$$L_T = L_A + 2L_R \tag{19}$$

Another important quantity, derived from those is the contiguity parameter, C_R. The contiguity is the ratio of immobile interface length to the total interface length and is quite sensitive to deviations of nuclei location from randomness, as recently shown by Vandermeer and Jensen[23]. It can be defined as[23]:

$$C_R = \frac{2L_R}{L_A + 2L_R} \tag{20}$$

The expressions for the interface length of the interface between recrystallized regions per unit of area, L_R, as a function of time is given by[20]:

$$L_R(t) = L_{RF}\left(-4\sqrt{\frac{N_A}{2\pi}}\,t\exp(-2N_At^2) + erf(\sqrt{2N_A}\,t)\right) \tag{21}$$

The total interface length per unit of area is:

$$L_T(t) = 8N_At\exp(-2N_At^2) + \tag{22}$$

$$2L_{RF}\left(-4\sqrt{\frac{N_A}{2\pi}}\,t\exp(-2N_At^2) + erf(\sqrt{2N_A}\,t)\right)$$

The contiguity, C_R, then becomes:

$$C_R(t) = 1 - \tag{23}$$

$$\frac{8N_At\exp(-2N_At^2)}{8N_At\exp(-2N_At^2) + 2L_{RF}\left(-4\sqrt{\frac{N_A}{2\pi}}\,t\exp(-2N_At^2) + erf(\sqrt{2N_A}\,t)\right)}$$

It is more common to plot C_R as a function of area fraction than of time. Combining Equation 11 and Equation 23 gives:

$$C_R = 1 - \tag{24}$$

$$\frac{\sqrt{32N_A}(1-A_A)\sqrt{\ln\left(\frac{1}{1-A_A}\right)}}{\sqrt{32N_A}(1-A_A)\sqrt{\ln\left(\frac{1}{1-A_A}\right)} + 2L_{RF}\left(-\frac{2}{\sqrt{\pi}}(1-A_A)\sqrt{\ln\left(\frac{1}{1-A_A}\right)} + erf\left(\sqrt{\ln\left(\frac{1}{1-A_A}\right)}\right)\right)}$$

Notice that the above expressions are specific for the CA simulation carried out here. More detailed discussion and derivations of Equations 21-24 are the subject of a paper now in preparation[20].

Figures 5-7 show the comparison of the values calculated by means of Equations 21-24 and those obtained from the simulation. The agreement is very good. For L_R and L_T, Figures 5 and 6, the normalized quantities L_R/L_{RF} and $L_T/2L_{RF}$ were plotted.

The agreement between the new expressions and the simulation was very good.

It is important to mention that no adjustable parameters were used in this work. Only exact analytical solutions were compared with the simulations. The good agreement between theory and simulation shows that CA is a good model for recrystallization. It is able to reproduce exactly the situations for which there are mathematically exact solutions. This good agreement suggests that CA can be confidently applied to situations in which there are no analytical solutions. This will be done in future papers.

4. Summary and Conclusions

The very good agreement between the cellular automata(CA) simulation and the theoretical expressions shows that CA is a good model for recrystallization. CA is able to reproduce exactly the site-saturated, constant velocity situation for which there are exact solutions.

Moreover, the simulation results were useful to test new expressions recently developed[20] for the evolution of length per unit of area

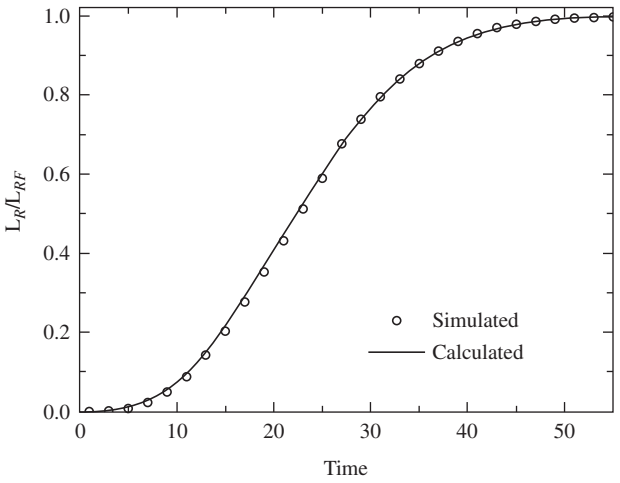

Figure 5. Length of the interface between transformed and transformed region per unit of area, L_R/L_{RF}, against time. Simulation results are in agreement with those calculated from the kinetics of a single grain, Equation 21.

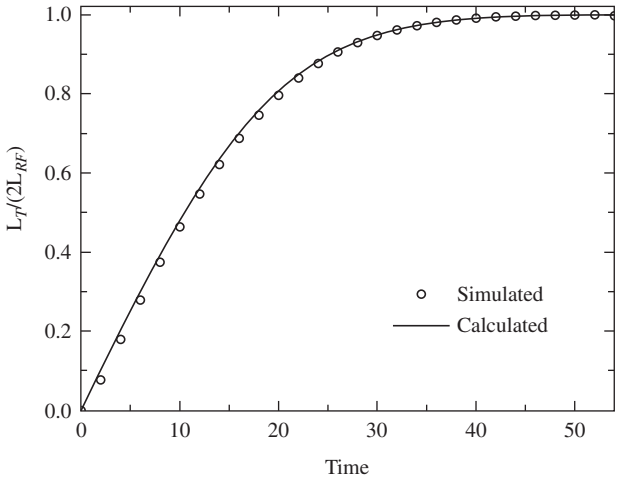

Figure 6. Total interface length per unit of area, $L_T/(2L_{RF})$ against time. Simulation results are in agreement with those calculated from the kinetics of a single grain, Equation 22.

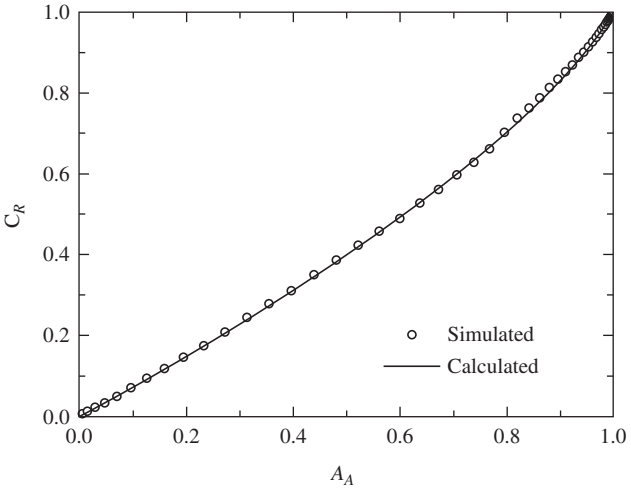

Figure 7. Contiguity, C_R, against area fraction. Simulation results are in agreement with those calculated from the kinetics of a single grain, Equation 24. The contiguity is the ratio of immobile interface length to the total interface length.

of the interface between the recrystallized regions. The new expressions showed very good agreement with the simulated results. It is worth pointing out that no adjustable parameters were used throughout this work. The present work has emphasized recrystallization but its results are general and may be applied to any nucleation and growth transformation.

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