Two dimensional cellular automata simulation of grain growth during solidification and recrystallization

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Abstract. A two dimensional cellular automata model has been developed to simulate and to study grain growth behavior during solidification and recrystallization processes, including predicting mechanical properties of metallic materials or investigating mechanical defects. Using the algorithm implemented, grain growth in model materials (nickel-based and titanium alloys) has been calculated in different thermal fields.

1. Introduction

Microstructure is known to play a key role in prediction of material thermo-mechanical behavior by a number of manufacturing processes such as casting, welding or additive manufacturing. In order to examine solidification and recrystallization microstructures, a variety of experimental methods can be successfully used but the dynamic evolution of microstructures in these processes is hard to be observed. In order to study grain growth behavior and predict material properties, numerical simulations of evolving microstructures have been performed quite a while and various models based on phenomenological, analytical or statistical approaches which take into account mechanisms of grain nucleation and growth have been developed in order to do it.

The paper [1] gives an overview of advances in solidification science and technology including numerical techniques. Cellular automata (CA) technique is one of the most successful methods allowing to investigate numerically microstructure features from about 1 µm to several centimeters, due to its adaptivity, low computational costs, etc. (see, e.g., [1-8]). In 1993 Rappaz and Gandin [2] proposed an approach to the simulation of grain structure formation during solidification process. Their model includes the mechanisms of heterogeneous nucleation and grain growth. Using this model they simulated two dimensional (2D) [4] and then, in 1997 [5], three dimensional (3D) grain structures by coupling CA model with finite element method for heat flow calculations. Using the combined CA finite difference (FD) model Lee et al. [6-8] simulated evolving microstructures of binary alloys during solidification. Pavlyk and Dilthey [4] proposed an original algorithm to determine interface curvature and orientation of growing grains as well as transition rules for cells.

Grain growth during recrystallization is also successfully simulated using CA models. In describing this process it is important to pay careful attention to grain boundary mobility. Humphreys and
Hatherly have written a monograph [9] on the subject of recrystallization emphasizing the theoretical description of the various phenomena taking place during recrystallization. Raabe [10] reviewed the fundamentals and some CA applications, for example, recrystallization simulation by use of a probabilistic CA model or by coupling CA with crystal plasticity FE model. Raghavan and Sahay [11, 12] developed 2D CA model for the grain growth in order to study grain growth kinetics. Gruber [13] simulated grain growth in 2 and 3 dimensions using Monte-Carlo method.

In this work the 2D grain growth model is developed using the CA method. The implemented algorithm of grain growth is based on the approach of Rappaz and Gandin [2]. Using this algorithm, grain growth in model materials has been calculated in different thermal fields. In this work we have chosen nickel-based and titanium alloys as model materials.

2. Model description
The implemented algorithm includes the following procedures: (i) calculation of the temperature field, (ii) calculation of the number of grains nucleated at each time step, (iii) nucleation of grains with randomly chosen crystallographic orientations, satisfying certain conditions and (iv) calculation of the solid fraction increment using grain growth algorithm developed by Rappaz and Gandin [2]. In order to calculate the temperature field, the heat transfer equation with Robin boundary conditions (BCs) is solved using the finite difference method [14, 15]. Let us dwell briefly on the main stages.

2.1. Grain nucleation
Grain nucleation is based on the approach of Rappaz and Gandin [2], Dong and Lee [8]. According to the approach of Oldfield [16] a continuous nucleation distribution \( dn/d(\Delta T) \) can be used in order to describe the grain density increase \( dn \) induced by an increase in the effective undercooling \( d(\Delta T) \). In order to describe the grain nucleation at the mould wall and in the bulk of the liquid Rappaz and Gandin [2], Dong and Lee [8] have used Gaussian functions which are characterized by mean undercooling \( \Delta T_N \) and standard deviation \( \Delta T_\sigma \). In this work, a continuous Gaussian nucleation distribution [8] is used to describe the grain nucleation in the bulk of the melt

\[
n(\Delta T) = \frac{N_{\text{max}}}{\Delta T_\sigma \sqrt{2\pi}} \int_{0}^{\Delta T} \exp \left( -\frac{(\Delta T - \Delta T_N)^2}{2(\Delta T_\sigma)^2} \right) d(\Delta T),
\]

(1)

where \( N_{\text{max}} \) is the maximum nucleation density. The undercooling within the volume is determined by the following formula

\[
\Delta T = T_L + m_L \left( C_L - C_0 \right) - T_b
\]

[17]. Here \( T_L \) is liquidus temperature, the \( m_L \) is the liquidus slope, \( \langle C_L \rangle \) is the intrinsic volume-averaged liquid concentration, \( C_0 \) is the initial melt concentration, and \( T_b \) is the bulk temperature defined as the average temperature in the volume.

The calculated number of nuclei \( n(\Delta T) \) is randomly distributed among cells. A grain nucleates in the \( i \)-th cell only if i) the cell has one of the randomly distributed nuclei within it; ii) the total undercooling in the cell \( \Delta T_i > \Delta T_N \), where \( \Delta T_N = T_L - T_b \). After nucleation, the cell state changes into “solid”, and the neighboring cells are considered as “growing” cells.

2.2. Calculation of the solid fraction increment
The concept of CA method is that a simulation object is considered as a set of interacting elements which dynamics is defined by rules of their relationships. In this work the simulated area is discretized by a regular rectangular mesh. At certain time each cell can have one of three states: liquid, solid and growing (i.e. a mixture of solid and liquid).

Grain orientation is defined by \( \theta \) randomly where \( \theta \) is the orientation angle of a principal crystallographic direction. Angle \( \theta \) changes from 0° to 45°. Every nucleus has four growth directions perpendicular to each other and four vectors are associated with these directions. The first growth
direction aligns with the preferential <10> direction. At each time step the ends of the vectors are connected by straight line and the centers of adjacent cells are checked to be within the area of the growing grain. Schematic representation of 2D CA algorithm of crystallite growth is shown in Figure 1. New growing cells develop by the similar algorithm. When the nucleus has taken all the neighboring cells, it stops growing. Growth rate for all grains is the same.

2.3. Simulation of recrystallization

Grain boundaries move driven by temperature gradient at a velocity established by the formulae

\[ v = \frac{M(\theta, T) \gamma(\theta)}{M_{\text{max}} \gamma_{\text{max}}} \]  \[\text{[11, 13]}\].

Constants \( M_{\text{max}} \) and \( \gamma_{\text{max}} \) are the grain boundary mobility and grain boundary energy, respectively, when the boundary becomes a high angle grain boundary. In the calculations these constants are chosen to be equal to 1 \[\text{[14]}\]. The grain boundary energy can be calculated \[\text{[18]}\] by

\[ \gamma = 3 \gamma_{\text{bound}} \Delta D / D_1 D_2, \]  \[\text{(2)}\]

Where \( \Delta D = D_1 - D_2 \), \( D_1 \) and \( D_2 \) are the diameters of neighbouring grains, and \( \gamma_{\text{bound}} = \frac{\theta}{\theta_{\text{max}}} \left[ 1 - \ln \left( \frac{\theta}{\theta_{\text{max}}} \right) \right] \) \[\text{[13]}\]. Within the numerical implementation the grain diameter is calculated as the diameter of a circle of the same area:

\[ D = \frac{4S_c}{\pi} \approx h \sqrt{\frac{4n_c}{\pi}}, \]  \[\text{(3)}\]

where \( S_c \) is the area of a circle and \( n_c \) is the number of cells within the grain.

The grain boundary mobility is a function of misorientation between the two grains, which is given as \[\text{[11, 13]}\):

\[ M(\theta, T) = M_m \frac{\theta}{\theta_{\text{max}}} \left[ 1 - \ln \left( \frac{\theta}{\theta_{\text{max}}} \right) \right], \]  \[\text{(4)}\]

\[ M_m = M_0 \exp \left( - \frac{Q}{RT} \right), \]  \[\text{(5)}\]

where \( R \) is the universal gas constant, the constant \( M_0 \) and the activation energy for migration \( Q \) are chosen according to the data \[\text{[9]}\] for titanium alloy: \( M_0 = 0.45 \text{ m/s}, Q = 25 \text{ kJ/mol} \).

3. Results

In order to demonstrate capabilities of the implemented algorithm based on the model mentioned above the simulations of grain growth of a nickel-based superalloy \[\text{[6, 19, 20]}\] and a titanium alloy \[\text{[21, 22]}\] during solidification process under different temperature conditions are performed.
3.1. Evolution of growing polycrystalline structure in a nickel-based superalloy

The computational domain is divided into 2000 × 500 regular square cells with a cell size of 50 µm. The time step in all calculations is 1 ms. The initial bulk temperature is 1609 K. Cooling is set at the boundaries of the computational domain, the temperatures are given in Table 1. Material properties and model parameters used in the simulations are listed in Table 1 [6, 19, 20]. Figure 2 shows the calculated temperature field at the beginning (5 ms) and at the end (35 ms) of solidification process. The corresponding solidification process is demonstrated in Figure 3, where different colours represent different crystallographic orientations of grains.

Table 1. Material properties and model parameters used in the simulations [7, 19, 20].

| Property                        | Variable | Value       |
|---------------------------------|----------|-------------|
| Density                         | ρ        | 7950 kg/m³  |
| Heat capacity                   | cₚ       | 668 J/(kg·K) |
| Thermal conductivity            | λ        | 30.3 W/(m·K) |
| Convection heat transfer coefficient | κᵢ   | 1000 W/(m²·K) |
| Environment temperature at the left boundary | Tₑˡ   | 1550 K |
| Environment temperature at the right, top and bottom boundaries | Tₑʳ = Tₑᵗ = Tₑₛ | 1605 K |
| Liquidus temperature            | Tₗ      | 1609 K      |
| Liquidus slope                  | m       | -10.9 K/wt% |
| Initial concentration           | C₀      | 4.85 wt%    |

Figure 2. Temperature field evolution: τ = 5 (a) and 35 ms (b).

Figure 3. Numerical simulation for evolution of nickel-based superalloy microstructure: τ = 5 (a), 10 (b), 20 (c) and 35 ms (d).
Figure 3a illustrates that the grains initially nucleate and grow at the left boundary in the area of the most intensive cooling and then at the other boundaries where the temperature is higher than at the left boundary but lower than in the center. Due to a high temperature area in the middle of the specimen, the probability of grain nucleation decreases towards the center of the ingot and growth of near-boundary grains primarily occurs (Figure 3d). Figure 3c illustrates the final microstructure. The shape and size of grains are irregular. While an equiaxed grain structure is observed at the left size, the most part of the ingot has a columnar microstructure.

3.2. Recrystallization of a titanium alloy under temperature gradient

Using the implemented algorithm we generated the initial microstructure. A titanium alloy was chosen as a model material. A detailed description of the thermo-mechanical properties of titanium specimens is given in [21, 22].

The computational domain is divided into $1200 \times 400$ regular square cells with a cell size of 50 $\mu$m. The time step is 1 ms. The 2D polycrystal is subjected to the temperature gradient so that $T_{\text{max}} = 800$ K on the right boundary, $T_{\text{min}} = 400$ K on the left boundary (Figure 4).

Figure 5a demonstrates the initial microstructure. Typical example of the microstructural evolution with time is shown in Figure 5. At the right side the growth of larger grains at the expense of smaller grains can be observed, which is a typical recrystallization feature [9, 11].

![Temperature gradient](image)

**Figure 4.** Temperature gradient.

![Initial microstructure evolution](image)

**Figure 5.** Initial calculated polycrystalline microstructure (a) and its evolution during recrystallization: 11 (b), 21 (c), and 33 ms (d).
4. Conclusions
The CA model realized enables us to describe the microstructure evolution during solidification and recrystallization processes. The grain growth model implemented offers various opportunities as, for example, to predict mechanical properties of metallic materials or to investigate mechanical defects arising during solidification and/or recrystallization such as e.g. hot cracks.

It should be mentioned that the results obtained have not been compared with concrete experimental data (grain size, shape, grain distribution within the mesovolume etc) which should be done to improve simulation results. Future work will be focused on the development of a 3D finite element and CA multiscale coupled model.

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