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Simulation of crystallographic changes during recrystallization by one-dimensional cellular automaton

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Abstract. Cellular automata are one of the most frequently used methods to simulate the recrystallization process. The cellular automata give the complex nature of this process with a simple implementation. One of the greatest effort in this field is to calculate the changes in crystallographic texture. One-dimensional cellular automata are introduced to calculate the kinetics of recrystallization. This study introduces a simple method which makes it possible to incorporate the texture components to the calculations.

1. Introduction

Cellular automaton is a widely used mathematical method [1], due to the simple implementation and complex behavior [2]. The method is originated to famous Hungarian mathematician John von Neumann [3]. The first application in physical metallurgy was made by Hesselbarth and Göbel [4]. The aim of this study was the simulation of recrystallization process. This solution was a two-dimensional deterministic automaton. Davies developed this method with the incorporation of the stochastic rules into the grain growth process [5, 6]. Schönfish studied further the stochastic nature of the stochastic, asynchronous and random-grid automata [7]. After Davies' work the main efforts were to couple the automata with crystal plasticity computations [8], simulate the dynamic recrystallization [9] and incorporate the solute drag to the simulations. In parallel during the research the effort to simulate crystallographic changes are clearly visible [10].

In this field there are two main directions: the study of local changes during nucleation and growth, and measuring and evaluating the texture of the metals in relation to the given technological parameters [11]. These two directions divided the simulations also into two groups. In one case the simulations handle few grains, and for example orientation imaging microscopy (OIM) gives the initial state of the calculations. The other methods take into consideration the local changes in higher abstraction level, and calculate the macroscopic texture, the variation of the mechanical parameters. The aim of the two group is the same: to get a deeper understanding about the crystallographic changes.

The cellular automaton is a discrete dynamic system. The examined space (universe) is divided into identical volume elements, called cells. The size, the properties and the behavior of the cells are totally the same. The properties of the cells are called states, which have a finite number of possibilities. The states are determined mostly by physical values, for example, the dislocation density. This is a continuous measure, but it clearly describes that the cell is either deformed or recrystallized. The physical interactions are described by local rules, these are discrete functions. The input parameters are the states of the given cells and the states of its neighbors. The output of these functions are the new states of the cells. The automaton tries to change the state of each cells, it builds a new universe. When every cell has been updated, one simulation step is finished. This covers the main problem of the cellular



automata. The time and the characteristic distance is measured by discrete values, the number of steps and the number of cells.

It is necessary to determine the real time interval and distance during the simulation. This method is called scaling. There are several ways of scaling an automaton. The easiest way is scaling with global optimization methods [12].

The complexity of the automaton increases the computation time of scaling. One of the parameter which increase the complexity is the dimensionality. There are large differences between one- and two-dimensional automata [13].

The one-dimensional automata have been studied and classified by Wolfram [14]. Wolfram showed that even the simplest automaton has a complex behavior. According to this idea, one-dimensional cellular automata were developed to simulate recrystallization, allotropic phase transition and grain coarsening [15]. All automata are studied and scaled. It was found that the scaling of a one-dimensional automaton is a fast process, and it can be automatized.

The one-dimensional automata have several limitations, of course. But the calculations are fast, the automata are scaleable, and the calculations with a given resolution (number of cells) are robust. If the aim is the simulation of the effect of technological parameters on the crystallographic changes, the one-dimensional automata could be an ideal method. In this report a possible solution is introduced for the calculation of these changes.

2. Method

One-dimensional simulation of recrystallization [12] extends with the simulation of crystallographic changes. The main question is the description of the texture of the metals. Several ways can be used, like pole figures, orientation distribution functions (ODF) or the volume fraction of the main crystallographic components [16]. The one-dimensional cellular automaton can prove to be a fast calculation if it concerns a few 10s to 100s of grains. This amount of grains does not provide enough data to plot a valuable pole figure or ODF if it has an exact crystallographic orientation described by the Euler angles. The aim of this study is to calculate the changes of the crystallographic orientations during recrystallization. The scaling is performed based on the changes of the volume fractions of main texture components. Based on the texture measurement the volume fraction of the main components can be calculated. In case of EN-AW-3003 aluminum alloy in rolled (86% reduction) and annealed (280°C, 5h) state figure 1 shows the volume fractions. The exact results and methods are introduced in [19].

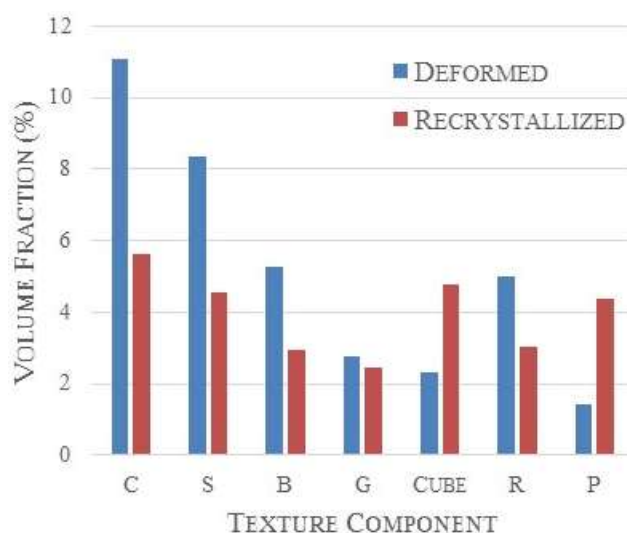


Figure 1. The volume fractions of the EN-AW-3003 aluminum alloy in deformed (86%) and annealed state (280°C, 5h) measured and published by Pethő [19].

First a deformed grain structure is needed with the measured volume fraction. The volume fraction determines the probability of the existence of a main crystallographic component in the given volume element. A recrystallization like automaton is developed to evolve the deformed grain structure. The crystallographic orientation of the different grains are determined at the nucleation process. A scale was built up by the volume fraction which was extended with the random component to 100%, and the texture component is determined with a simple Monte-Carlo algorithm [18].

In a one-dimensional automaton it is impossible to include all of the rules of nucleation process [17]. So, the similar scheme can be followed during simulation, but the scale of probability is calculated based on the recrystallized volume fractions. But in this case the simulation can be scaled by a measured kinetic function.

In the one-dimensional simulation the activation energy of the nucleation and growth are the two main kinetic parameters. In both cases (deformed structure generation and the simulation) the activation energies are constant values independent of the crystallographic orientations. Of course, these values can depend on the local orientation differences, but in this consideration this simple assumption gives a useful solution.

The disadvantage of this method is the number of grains. Because if only a few grains build up the universe the accuracy of the computation is small. Enough nuclei have to be formed to get the necessary result in case of all texture components. So, in this case a larger universe is needed as in a normal kinetic simulation. But this means a slower computation. However, the introduced method is faster than a two-dimensional computation, and easily take into account the partial annealing and the dynamic recrystallization too if enough measured data exist.

3. Results

The measured volume fraction of the main texture components is shown on Figure 1. Values of the deformed and the annealed states (4 and 5 hours) are used in the computation. The sequence of the volume fractions with the random component build a probability function. The sum of the volume fractions is extended by the random component to 100%. The probabilities of the deformed state are used in the computation of the deformed grain structure. The probabilities of the annealed state are used in the simulation of recrystallization. Based on the probability functions the deformed structure is calculated. The parameters of the simulation are: activation energy of nucleation: 71kJ/mol, activation energy of growth: 49kJ/mol, number of cells: 10000, temperature: 553K. The dataset comes from a kinetic analysis and scaling of the automaton of EN-AW-3003 aluminum alloy. The results are shown by figure 2.

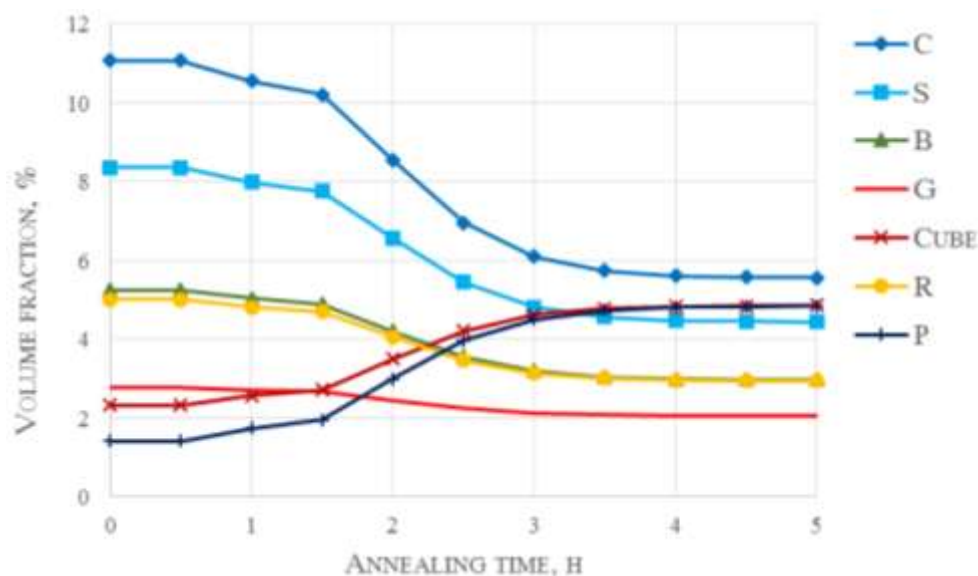


Figure 2. The calculated changes of volume fraction of the main texture component based on cellular automaton.

Figure 2 shows that it is possible to calculate the changes of the volume fractions based on one-dimensional cellular automaton. The approximation is not as sophisticated as in case of deep researches in this field, but it can be applied to calculate the effect of technological parameters on the crystallographic orientations.

4. Summary

One main task of the cellular automata simulations of recrystallization is to calculate the crystallographic changes during the phase transformation. One possible solution of the mentioned simulation is the one-dimensional cellular automaton. One-dimensional automata provide fast computation but have some restrictions. The calculation of the crystallographic changes is one aspect which seems to be lost in one-dimension. But in high abstraction level a possible solution can be found.

The volume fractions of main texture components can be calculated based on texture measurements. This is a discrete description of the crystallographic texture which fits with the nature of the cellular automata. The changes of the main texture components during recrystallization can be calculated based on the nucleation probabilities of different texture components. The probability of nucleation of a given texture component is equal to its volume fraction in the annealed state if a constant rate of growth is considered. These assumptions are proved by the one-dimensional cellular automata.

The calculation requires a larger number of nuclei than a simple kinetic calculation, which means a larger universe. A larger universe makes the calculation slower of course, but the one-dimensional automata remain faster than a sophisticated two-dimensional calculation. In the study of the effect of technological parameters the one-dimensional automata are a competitive solution.

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