# ORIENTATION DEPENDENCE OF RECRYSTALLIZATION IN ALUMINUM – SIMULATION AND EXPERIMENT

**MAX-PLANCK PROJECT REPORT**

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***KEYWORDS**: recrystallization, cellular automaton, simulation, orientation dependence, nucleation, aluminium, columnar grains, electron backscattering diffraction*

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# PROJECT ABSTRACT

In this project the orientation dependence of recrystallization in aluminum (99.99%) was studied by means of experimental methods and computer simulation. Samples with columnar grain morphology were deformed in plane strain compression in a channel die setup up to a technical thickness reduction of 50% in several defined steps. After the last deformation step the samples were recrystallized at different temperatures. After each of the deformation steps and each of the recrystallization steps the samples were analyzed by means of electron backscattering diffraction technique. With the orientation data gained from the last deformation step an input file was generated for a recrystallization simulation based on a probabilistic cellular automaton.

# INTRODUCTION

**The probabilistic cellular automaton.** The recrystallization is simulated by means of a probabilistic cellular automaton with the independent variables time *t* and space $x=x_1,x_2,x_3$ [1,2,3]. Space is discretized into an array of equally shaped quadratic cells, each characterized in terms of the dependent variables. These are scalar (mechanical, electromagnetic) and configurational (interfacial) contributions to the driving force and the crystal orientation g=g ($\varphi_1,\phi,\varphi_2$) where g is the rotation matrix and $\varphi_1,\phi,\varphi_2$ are the Euler angles. The driving force is the negative change in Gibbs enthalpy $G_t$ per transformed cell. The starting data for the simulation is the crystal orientation map of the deformed sample obtained from an EBSD measurement.

The kinetics of the cellular automaton result from changes in the state of the cells (cell switches) occurring in accord with a switching rule, which determines the individual switching probability of each cell as a function of its previous state and the state of its neighbouring cells. The switching rule is cast in form of a probabilistic analog of the linearized symmetric rate equation from Turnbull (1951):

$$\dot{x} \approx n \nu_D \lambda_{gb} c \left\{ \exp\left( -\frac{\Delta G + \Delta G_t / 2}{k_B T} \right) - \exp\left( -\frac{\Delta G - \Delta G_t / 2}{k_B T} \right) \right\} \qquad (1)$$

where $\dot{x}$ is the grain boundary velocity, $\nu_D$ the Debye frequency, $\lambda_{gb}$ is the jump width through the boundary, $c$ is the intrinsic concentration of grain boundary vacancies of shuffle sources, $n$ is the normal of the grain boundary segment, $\Delta G$ is the Gibbs enthalpy of motion through in the interface, $\Delta G_t$ is the Gibbs enthalpy associated with the transformation, $k_B$ is the Boltzmann constant, and $T$ is the absolute temperature. Replacing the jump width by the Burgers vector and the Gibbs enthalpy terms by the local entropy, $\Delta S$, and total enthalpy, $\Delta H$, leads to a linearized form of equation (1):

$$\dot{x} \approx n \nu_D b \exp\left( -\frac{\Delta S}{k_B} \right) \left( \frac{pV}{k_B T} \right) \exp\left( \frac{\Delta H}{k_B T} \right) \qquad (2)$$

where $p$ is the driving force and $V$ is the atomic volume which is of the order $b^3$, where $b$ is the magnitude of the Burgers vector. Summarizing these terms reproduces Turnbull's expression

$$\dot{x} = nmp = nm_0 \exp\left(-\frac{Q_{gb}}{k_B T}\right) p \tag{3}$$

where $m$ is the mobility.

For dealing with competing switches affecting the same cell, the deterministic rate equation (3) can be replaced by a probabilistic analog that allows one to calculate switching probabilities. First, equation (3) is separated into a deterministic part, which depends weakly on temperature, and a probabilistic part, $\omega$, which depends strongly on temperature:

$$\dot{x} = \dot{x}_0 \, \omega = n \frac{k_B T m_0}{V} \frac{pV}{k_B T} \exp\left(-\frac{Q_{gb}}{k_B T}\right)$$

with

$$\dot{x}_0 = n \frac{k_B T m_0}{V} \qquad \text{and} \qquad \omega = \frac{pV}{k_B T} \exp\left(-\frac{Q_{gb}}{k_B T}\right) \tag{4}$$

The automaton considers the first- and second- (2D) neighbor shells for the calculation of the total driving force acting on a cell. The local value of switching probability depends on the crystallographic character of the boundary segment between such unlike cells. Details of the method are given in [1,2,3].

# RESULTS

**Experiments.** The sample material was a 4 mm sheet of commercially pure aluminum (99.99%). The material was rolled to a technical thickness reduction of 25% and then recrystallized 3h at 600°C. After recrystallization samples of 15 x 24 mm were cut out of the sheet and then plane strain deformed in a channel die setup with a technical thickness reduction of 50%. For the EBSD meas-

urement the samples were grinded, polished and etched with Al-M4 (containing hydrochloric acid, nitric acid and hydrofluoric acid). Figure 1 shows the EBSD mapping of the channel die deformed sample, which is also used as starting data set for the subsequent recrystallization simulation.

For comparing the data obtained from simulation and experiment, the samples were recrystallized at certain temperature and times. After each recrystallization step the orientations of the samples were measured by means of the EBSD-technique. In Fig. 1-3 the results of the EBSD measurements at different states of recrystallization are shown with the different orientations in different colours. The texture development during recrystallization shows that some orientations cause significant grain growth, whereas other orientations nearly disappear.

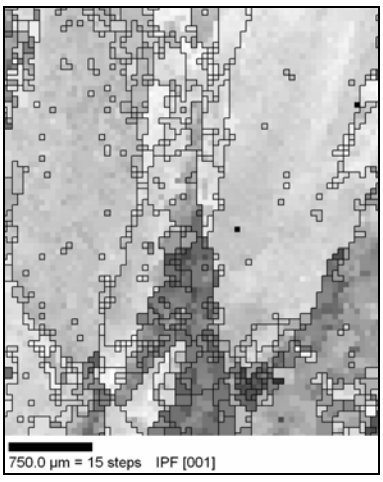



Fig.1a) Initial state, 50% deformed, experimental

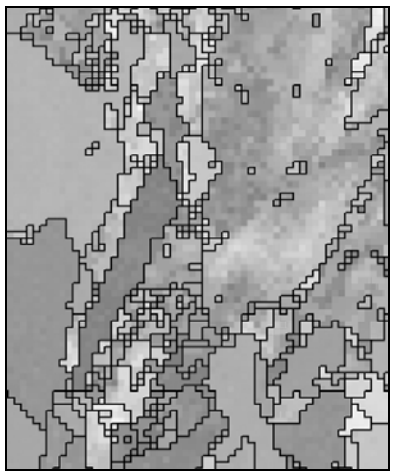


Fig.1b) after 10 min (250° C) , experimental

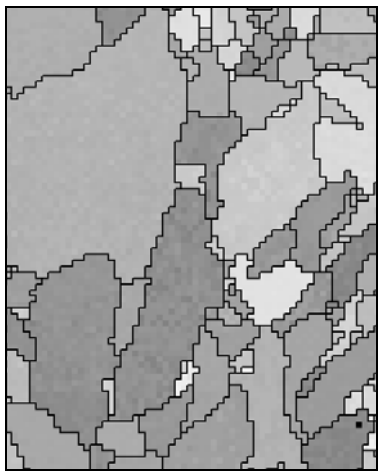
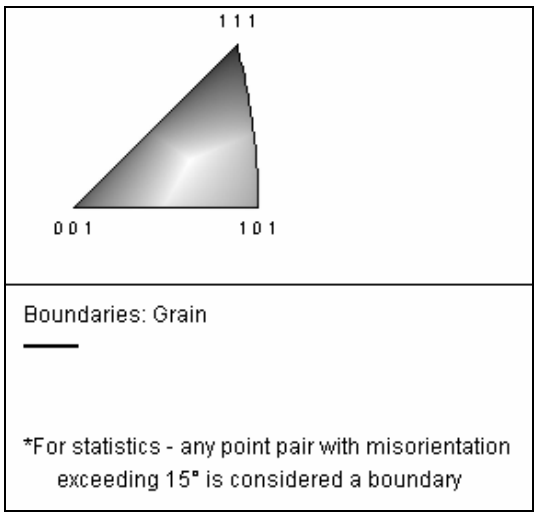


Fig.1c) after 35 min at 250° C and 25 min at 400° C, experimental



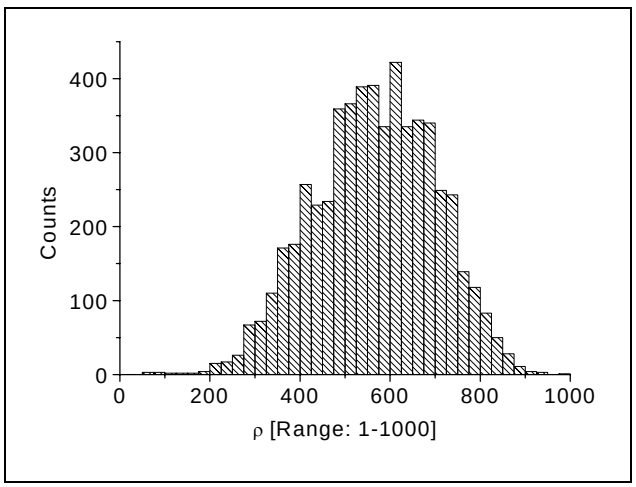




Fig. 2: Dislocation Density Distribution

**Simulations.** The dislocation density is the most important parameter for simulations with the cellular automaton. The pattern quality obtained from the EBSD measurement was used as a relative indicator for the dislocation density. This method is reasonable because with increasing dislocation density the pattern quality decreases. Of course the pattern quality cannot serve as an absolute value for the dislocation density. The pattern quality is dependent not only on the dislocation density but is also strongly dependent on the surface quality of the sample. Unevenness of the surface also causes poor pattern quality. Therefore a good sample preparation before the EBSD measurement was indispensable. Assuming that the disturbing influences on the pattern quality caused by the sample surface unevenness and also the measuring technique are statistically distributed over the entire measurement the resulting error affects only the absolute value of the pattern quality. Therefore the pattern quality can be used for relative comparison between the different states during recrystallization.

In Fig. 2 the dislocation distribution density of the initial state is presented as a histogram. On the basis of the dislocation density distribution the nucleation parameters were determined. A critical dislocation density was taken as a criterion for the spontaneous nucleation of isolated cells, below which, by definition, nucleation does not take place. Different simulations were performed with various critical dislocation densities. Here the simulations with the critical dislocation densities of $\rho_{krit}$=700 (Simulation I), $\rho_{krit}$=800 (Simulation II) and $\rho_{krit}$=900 (Simulation III) are described.

The simulation with $\rho_{krit}$=700 (Simulation I, Fig. 3a-c) results in a large number of nucleation sites. Accordingly this simulation shows moderate grain growth with no preferred orientations and a rather fine grained microstructure at the end. The simulation with $\rho_{krit}$=800 (Simulation II, Fig. 4a-c) also shows a relatively large amount of nuclei, but the grains start to mutually obstruct each others growth. However it is observed that there are also orientations, which disappear during simulation. Besides there are orientations, which do not change at all. With a critical dislocation density of $\rho_{krit}$=900 (Simulation III, Fig. 5a-c) there are only a few grains growing enormously at the cost of their neighbors. At the end of the recrystallization almost the whole simulated microstructure consists of only one large grain (Fig. 5c). Only the obviously very stable orientation in the center of the mapping could resist the growth of the preferentially oriented grains. However this stable orientation was not able to grow itself.

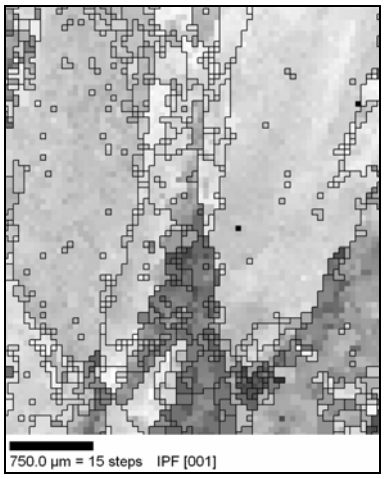



Fig. 3a) Simulation I, beginning state

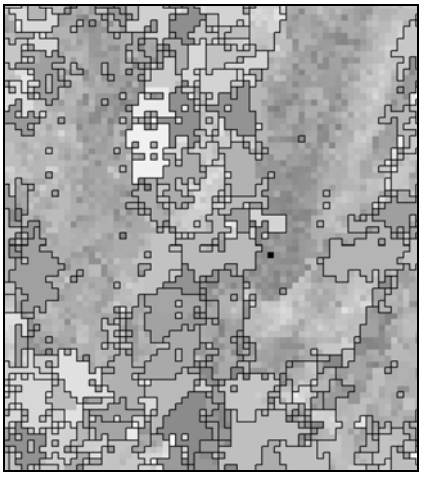


Fig. 3b) Simulation I , intermediate state

Fig. 3c) Simulation I , final state

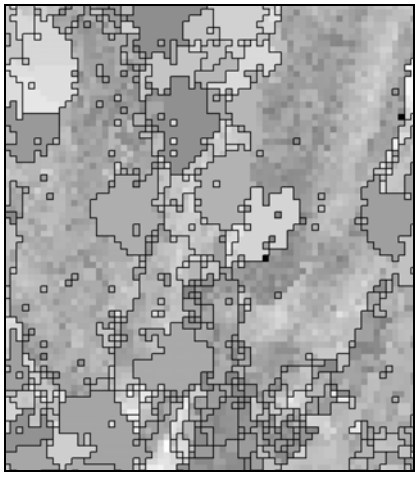


Fig. 4a) Simulation II, beginning state

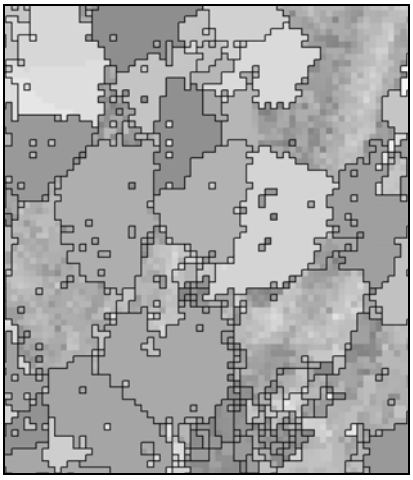


Fig.4b) Simulation II , intermediate state

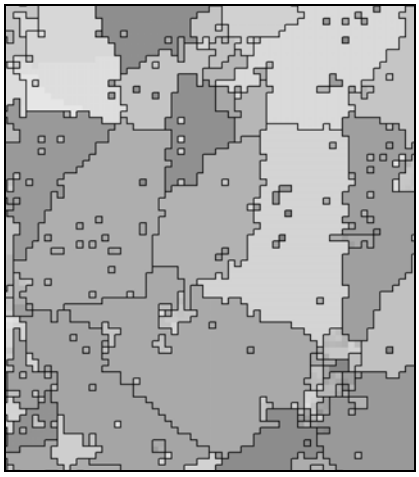


Fig.4c) Simulation II , final state

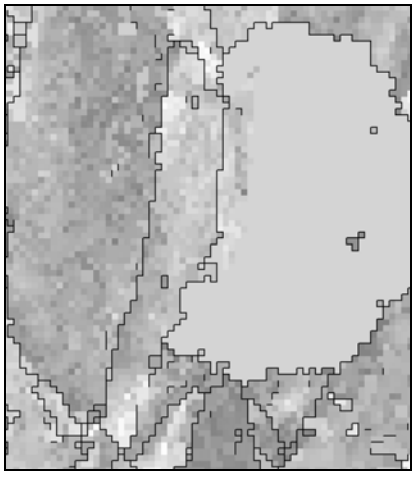


Fig. 5a) Simulation III, beginning state

Fig. 5b) Simulation III , intermediate state

Fig. 5c) Simulation III , final state

From the recrystallization kinetics (Fig. 6) one can see very clearly that the recrystallization becomes slower with increasing $\rho_{krit}$. It is remarkable that the simulation with a critical dislocation density of 900 takes extremely long compared to the other simulations. In the Cahn-Hagel plots (Fig. 7a-c) this fact is seen even more clearly. For simulations with a critical dislocation density of 700 and 800 first the cellsize increases briefly, then, however, it decreases clearly. During the simulation with $\rho_{krit}$=900 the cell size generally increases, except for sudden small decreases (Fig. 7c, i.e. at 40% and 60%) that are followed by continuing increasing cell size. These small decreases can be correlated to be complete disappearance of grains with weaker orientations.

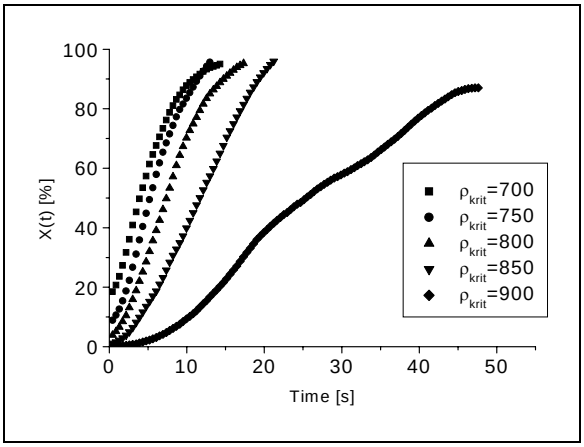



Fig. 6) Recrystallization kinetics

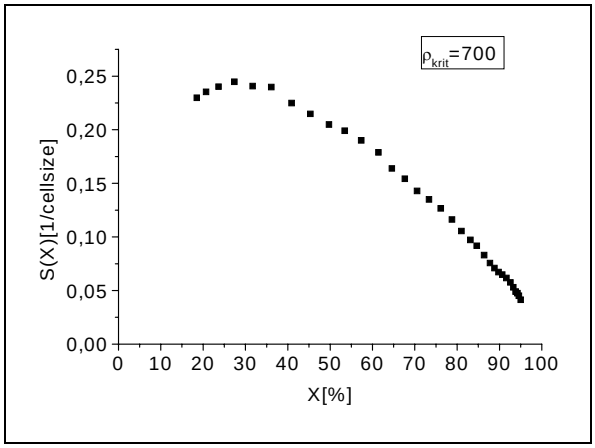



Fig. 7a) Cahn-Hagel plot, simulation I

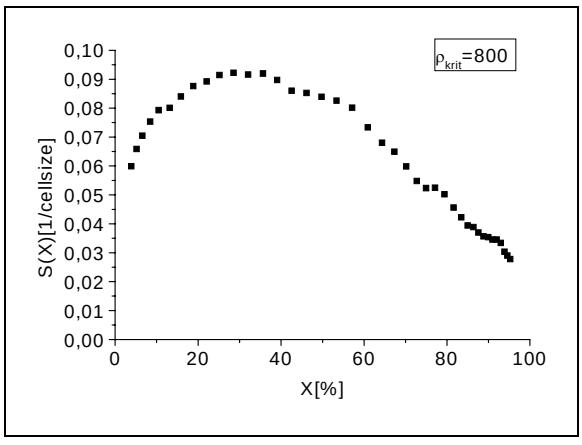



Fig. 7b) Cahn-Hagel plot, simulation II

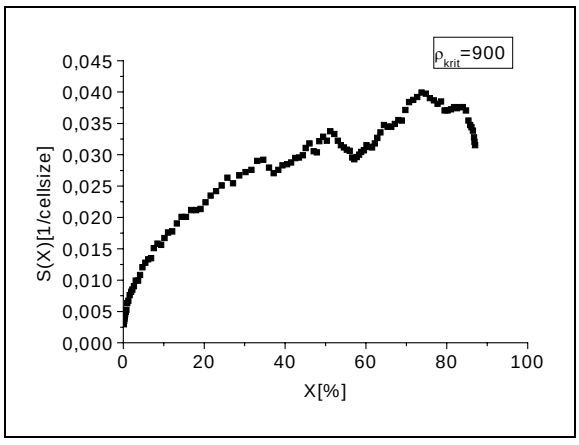



Fig. 7c) Cahn-Hagel plot, simulation III

# DISCUSSION

**Comparison of Simulation and Experiment.** Compared to the experiment, the simulations show a size effect stamming from the mesh, particularly in the case of $\rho_{krit}$=700 (Fig. 3b-c). That difference in the grid effect is due particularly to the very rigid separation between preferred and non-preferred orientations. Since $\rho_{krit}$ is very sharply defined and doesn't have a gradual transition (as it is the case in reality), the simulation develops clusters in the microstructure. The comparison of the final states in simulation after complete recrystallisation (Fig. 3c,4c,5c) with the final state in the experiment (Fig. 1c) shows that the simulation with $\rho_{krit}$=800 matches closely to reality. Simulation II (Fig. 4c) corresponds with the experiment regarding the final grain size of most of the grains. However, it is noticeable, that the difference in growth behavior between the individual grains in the simulation is smaller than in the experiment. This discrepancy means, the final microstructure of the simulation has a more homogenous grain size than the experiment. However, these results show that in the experiment and in the simulation the same grains grow preferentially, and other orientations, which disappear in the experiment, turnout to be instable during simulation too.

**Outlook.** In future simulations the separation between preferred and non preferred orientations will be described in a less discrete way. So-called special boundary conditions for the simulation will be tested. Furthermore the comparison between simulation and experiment will be put on a statistically larger basis.

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