A 3D PROBABILISTIC CELLULAR AUTOMATON FOR THE SIMULATION OF RECRYSTALLIZATION AND GRAIN GROWTH PHENOMENA

MAX-PLANCK PROJECT REPORT

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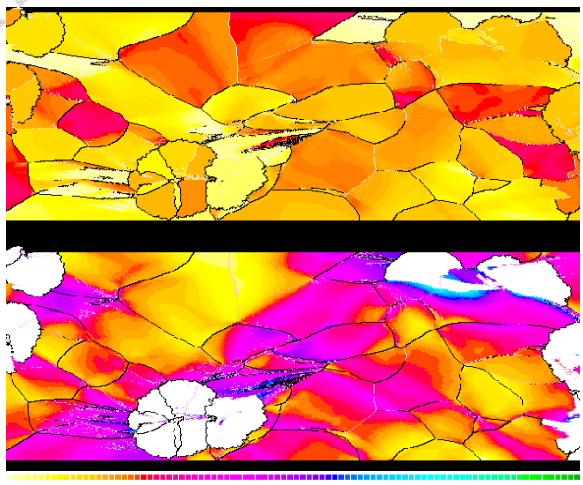

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Abstract of Progress Report

This MPG progress report presents applications of a 3D stochastic cellular automaton model for the spatial, kinetic, and crystallographic simulation of mesoscale transformation phenomena that involve non-conserved structural field variables and the motion of sharp interfaces, such as encountered in the fields of recrystallization and grain growth. The automaton is discrete in time, physical space, and orientation space. It is defined on a 3D cubic lattice considering the first, second, and third neighbor shell. The local transformation rule that acts on each lattice site consists of a probabilistic analog of the linearized symmetric Turnbull rate equation for grain boundary segment motion. All possible switches of cells are simultaneously considered using a weighted stochastic sampling integration scheme. The required input parameters are the mobility data for the grain boundaries, the local crystallographic texture, and a local stored energy measure as a function of space.

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Fundamentals of the Model

The material properties are regarded as continuum field quantities. For applying cellular automaton algorithms, physical space (sample) must be discretized into a regular array of equally shaped cells. Time t and space $\boldsymbol{x}=(x_1,x_2,x_3)$ are independent variables. The crystal grain orientation $\boldsymbol{g}=\boldsymbol{g}(\varphi_1,\phi,\varphi_2)$ and mechanical, interface, or electromagnetic contributions to the Gibbs free energy G_t are dependent variables. The local transformation rule of the automaton consists of the probabilistic analog of a linear symmetric rate equation for thermally activated grain boundary segment motion under the influence of free energy gradients as introduced by Turnbull [1]. The automaton is defined on a spatially discrete 3D cubic lattice considering the first, second, and third neighbor shell. Each discrete lattice cell is characterized by an orientation and a value for the stored free energy (e.g. deformation energy in recrystallization simulations). The physical size of each lattice cell can be scaled by microstructure, e.g. by the local dislocation cell size. The possible switches of all cells in the automaton are in each time step simultaneously considered. The actual switch of cells adjacent to cells with different energy and/or orientation is made in accord with their switching probability, which is calculated by using the segment rate equation with local energy and mobility data, by using a weighted stochastic sampling integration scheme. The boundary mobility m is a function of the crystal misorientation $\Delta\boldsymbol{g}$ and the boundary plane inclination $\boldsymbol{n}$. Both quantities are derived dependent variables. The method requires the incorporation of experimental or theoretical data for grain boundary mobilities and energies as a function of their crystallographic misorientation. The transformation rate equation is scaled by the physical size of the lattice cells λ, the maximum admissible statistical integration variance σ, and the boundary mobility m.

The new approach allows one the fast discrete 3D simulation of the evolution of grain microstructures in physical and crystallographic orientation space at a realistic time and space scale. It considers the initial microstructure including crystallographic textures, grain boundary characteristics (energy, mobility), and driving forces. The following paragraphs provide a brief derivation of the governing rate equation, the probabilistic equivalent of which serves as local transformation rule, explain the switching scheme, and present some examples.

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Rate Equation of Boundary Motion and Probabilistic Analogue as Transformation Rule

According to Turnbull [1] a phenomenological symmetric rate equation, which describes grain boundary motion in terms of isotropic single-atom diffusion processes perpendicular through a homogeneous planar grain boundary segment under the influence of free energy gradients, can be written,

$$\dot{\boldsymbol{x}} = \boldsymbol{n}\,\upsilon_{\mathrm{D}}\,\lambda_{\mathrm{gb}}\,c\left\{\exp\left(-\frac{\Delta G-\Delta G_{\mathrm{t}}/2}{k_{\mathrm{B}}T}\right)-\exp\left(-\frac{\Delta G+\Delta G_{\mathrm{t}}/2}{k_{\mathrm{B}}T}\right)\right\} \tag{1}$$

where $\dot{\boldsymbol{x}}$ is the interface velocity, υ_{D} the Debye frequency, λ_{gb} the jump width through the interface, c the intrinsic concentration of in-plane self diffusion carrier defects (e.g. grain boundary vacancies or shuffle sources), $\boldsymbol{n}$ the normal of the grain boundary segment, ΔG the Gibbs enthalpy of motion through in the interface, ΔG_{t} the Gibbs enthalpy associated with the transformation, k_{B} the Boltzmann constant, and T the absolute temperature. Bold symbols indicate vector quantities. The Debye frequency is of the order of 10^{13}–10^{14} /s and the jump width of the order of the magnitude of the Burgers vector. After insertion of the enthalpy, entropy, and driving force, eq. (1) becomes

$$\dot{\boldsymbol{x}} = \boldsymbol{n}\,\upsilon_{\mathrm{D}}\,\lambda_{\mathrm{gb}}\exp\left(-\frac{\Delta H^{\mathrm{f}}-\Delta S^{\mathrm{f}}T}{k_{\mathrm{B}}T}\right)\left\{\exp\left(-\frac{\Delta H^{\mathrm{m}}-T\Delta S^{\mathrm{m}}-\frac{p\Omega}{2}}{k_{\mathrm{B}}T}\right)-\exp\left(-\frac{\Delta H^{\mathrm{m}}-T\Delta S^{\mathrm{m}}+\frac{p\Omega}{2}}{k_{\mathrm{B}}T}\right)\right\} \tag{2}$$

where p is the gradient in Gibbs enthalpy across the interface (driving force), Ω the atomic volume, ΔS^{f} the entropy of formation, ΔH^{f} the enthalpy of formation, ΔS^{m} the entropy of motion, and ΔH^{m} the enthalpy of motion. The atomic volume is of the order of b^3, where b is the magnitude of the

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Burgers vector. While ΔS^{f} mainly quantifies the vibrational entropy, ΔS^{m} contains configurational and vibrational portions. Summarizing these terms leads to

$$\dot{\boldsymbol{x}} = \boldsymbol{n}\upsilon_{\mathrm{D}}\,\mathrm{b}\exp\left(-\frac{\Delta S^{\mathrm{f}}+\Delta S^{\mathrm{m}}}{k_{\mathrm{B}}}\right)\sinh\left(\frac{p\,\Omega}{k_{\mathrm{B}}T}\right)\exp\left(-\frac{\Delta H^{\mathrm{f}}+\Delta H^{\mathrm{m}}}{k_{\mathrm{B}}T}\right)$$
$$\approx \boldsymbol{n}\upsilon_{\mathrm{D}}\,\mathrm{b}\exp\left(-\frac{\Delta S^{\mathrm{f}}+\Delta S^{\mathrm{m}}}{k_{\mathrm{B}}}\right)\left(\frac{p\,\Omega}{k_{\mathrm{B}}T}\right)\exp\left(-\frac{\Delta H^{\mathrm{f}}+\Delta H^{\mathrm{m}}}{k_{\mathrm{B}}T}\right) \qquad (3)$$

This approximation reproduces the well known phenomenological Turnbull expression

$$\dot{\boldsymbol{x}} = \boldsymbol{n}\,m\,p = \boldsymbol{n}\,m_0\exp\left(-\frac{Q_{\mathrm{gb}}}{k_{\mathrm{B}}T}\right)p \qquad (4)$$

where m is the mobility and Q_{gb} the activation energy of boundary motion. Eq. (3) gives

$$m_0 = \frac{\upsilon_{\mathrm{D}}\,\mathrm{b}\,\Omega}{k_{\mathrm{B}}T}\exp\left(-\frac{\Delta S^{\mathrm{f}}+\Delta S^{\mathrm{m}}}{k_{\mathrm{B}}}\right) \quad \text{and} \quad Q_{\mathrm{gb}} = \Delta H^{\mathrm{f}}+\Delta H^{\mathrm{m}} \qquad (5)$$

Eqs. (1)–(5) provide a phenomenological kinetic picture of grain boundary motion, where the atomistic processes associated with a particular grain boundary segment are statistically described in terms of $m_0 = m_0(\Delta\boldsymbol{g}, \boldsymbol{n})$ and $Q_{\mathrm{gb}} = Q_{\mathrm{gb}}(\Delta\boldsymbol{g}, \boldsymbol{n})$. Since it is difficult to quantify some of the physical parameters in eq. (5), particularly with respect to their dependence on the misorientation, it is pertinent to use experimental rather than theoretical mobility data wherever possible [2,3].

The major task of the here suggested simulation approach now consists in the calculation of the switching *probabilities* of all cells which have neighboring cells with different energy and/or orientation under consideration of the crystallographic character of the boundary segments between them. The actual switching *decision* is for each cell then made by using a conventional weighted stochastic sampling integration method (Monte Carlo scheme). After this step the states (energy, orientation) of all cells are updated in synchrony. As will be shown below, the use of

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experimentally determined mobility data automatically introduces the correct time and space scale into the prediction.

The approach described requires the replacement of the deterministic rate equation of boundary segment motion, eqs. (3),(4), by a probabilistic analog which can be solved by weighted stochastic sampling. For this purpose eq. (4) is first separated into a deterministic part, $\dot{\boldsymbol{x}}_0$, which depends weakly on temperature, and a probabilistic part, *w*, which depends strongly on temperature:

$$\dot{\boldsymbol{x}} = \dot{\boldsymbol{x}}_0 w = \boldsymbol{n}\frac{k_B T m_0}{\Omega}\frac{p\Omega}{k_B T}\exp\left(-\frac{Q_{gb}}{k_B T}\right) \text{ where } \dot{\boldsymbol{x}}_0 = \boldsymbol{n}\frac{k_B T m_0}{\Omega} \text{ and } w = \boldsymbol{n}\frac{p\Omega}{k_B T}\exp\left(-\frac{Q_{gb}}{k_B T}\right) \tag{6}$$

This equation could in principle serve as a probabilistic analog of the Turnbull rate equation. However, unlike boundary and vertex dynamics models [e.g. 3,4], the present simulations are carried out on a given spatial grid with an arbitrary cell size λ_m. The value of λ_m will usually be much larger than the atomic spacing b. If a moving boundary segment sweeps a cell, the grain thus grows (or shrinks) by λ_m^3 rather than b^3. This scaling length turns eq. (6) into

$$\dot{\boldsymbol{x}} = \dot{\boldsymbol{x}}_0 w = \boldsymbol{n}\left(\lambda_m \nu\right) w \qquad \text{where} \qquad \nu = \frac{k_B T\, m_0^{max}}{\Omega\, \lambda_m} \tag{7}$$

ν can be regarded as the eigen-frequency of the chosen grid. m_0^{max} is the maximum occurring pre-exponential factor of the mobility. Since the switching probability of the cells is obtained by stochastic sampling, the above eigen-frequency is too small and its use as the basic attack frequency would entail a substantial statistical error. It is thus necessary to normalize the above equation by an attack frequency ν_0, so that

$$\dot{\boldsymbol{x}} = \dot{\boldsymbol{x}}_0 w = \boldsymbol{n}\lambda_m\, \nu_0\left(\frac{\nu}{\nu_0}\right) w = \hat{\dot{\boldsymbol{x}}}_0\left(\frac{\nu}{\nu_0}\right) w = \hat{\dot{\boldsymbol{x}}}_0 \hat{w} \tag{8}$$

where

$$\hat{w} = \left(\frac{\nu}{\nu_0}\right)\frac{p\,\Omega}{k_B T}\exp\left(-\frac{Q_{gb}}{k_B T}\right) = \frac{m_0^{max} p}{\lambda_m\, \nu_0}\exp\left(-\frac{Q_{gb}}{k_B T}\right) \tag{9}$$

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While $\hat{\dot{x}}$ is determined by the grid size and the frequency, $\hat{w}$ is determined by the temperature and experimental data. An appropriate value for the normalization or grid attack frequency ν_0 can be identified by some straightforward statistical considerations. It is physically plausible that the maximum occurring probability in one integration step can never be larger than one, i.e.

$$\hat{w}^{\max} \leq \frac{m_0^{\max} p^{\max}}{\lambda_m \nu_0^{\min}} \exp\left(-\frac{Q_{\mathrm{gb}}^{\min}}{k_{\mathrm{B}} T}\right) \tag{10}$$

where $p^{\max}$ is the maximum occurring driving force, $\nu_0^{\min}$ the minimum allowed attack frequency, and $Q_{\mathrm{gb}}^{\min}$ the minimum occurring activation energy. The statistical variance σ associated with stochastic sampling is proportional to $1/\sqrt{N}$, where N is the number of trials. The physical constraints for the normalization frequency imposed by eq. (10) are thus increased by the statistical condition that the maximum possible switching probability $\hat{w}^{\max}$ should not only be smaller than one but even be smaller than some maximum allowed statistical variance σ, i.e. $\hat{w}^{\max} \leq \sigma$. The appropriate attack frequency for a set of given parameters can thus be calculated according to

$$\nu_0^{\min} \geq \frac{m_0^{\max} p^{\max}}{\lambda_m \sigma} \exp\left(-\frac{Q_{\mathrm{gb}}^{\min}}{k_{\mathrm{B}} T}\right) \tag{11}$$

The simulation proceeds by switching all cells according to their proper statistical weight, determined by the local mobility and driving pressure. The probability of the fastest occurring boundary segment to realize a local transformation amounts to σ. The characteristic time constant of the simulation is $1/\nu_0^{\min}$. All transformations (switch of cell state) are updated synchronously once per time interval. Except for the probabilistic evaluation of the single transformation steps, the approach is entirely deterministic and should not be confused with conventional kinetic Monte Carlo methods. Further details of the method are given in [5].

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Example 1: 3D Recrystallization of an Aluminium Single Crystal

Figure 1 shows an example of a 3D recrystallization simulation of a heavily deformed aluminum single crystal. The deformed crystal had a uniform near-cube orientation and an initial dislocation density of 10^{15} m^{-2}. The driving force was due to the stored elastic energy. Crystal recovery and the back driving force arising from boundary curvature were not considered. The simulation used site saturated nucleation conditions with a pseudo-activation energy of 0.45 eV. The nuclei were statistically distributed in physical and orientation space. Euler space was discretized into a set of 936 possible discrete orientations. The density of nuclei amounted to $7.47 \cdot 10^{23}$ m^{-3}. The grid size was $80 \cdot 80 \cdot 80$ $(\mu m)^3$. The activation energy of the grain boundary mobility amounted to 1.46 eV (all boundaries had the same mobility). The temperature was 800 K. The elementary time constant of the simulation was 1.53 s. Figure 1a shows the sample with 10.05 vol.%, Figure 1b with 21.74 vol.%, and Figure 1c with 38.42 vol.% recrystallized grains. According to the random distribution of nuclei and the absence of special boundaries the final recrystallization texture was random.

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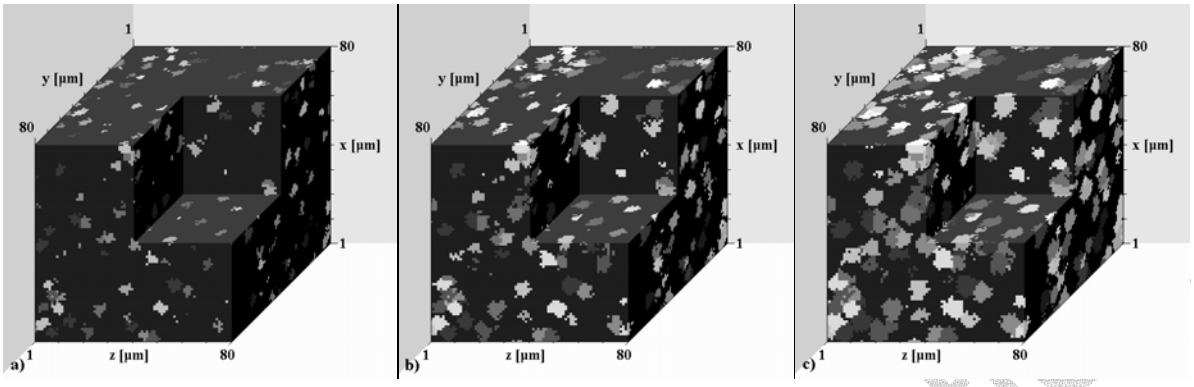

Figure 1: 3D recrystallization simulation. Metal: Al, initial dislocation density: 10^{15} m^{-2}, recovery and boundary curvature were not considered, site saturated nucleation conditions, 936 discrete orientations, grid size: 80·80·80 $(\mu m)^3$, cell size: 0.1 µm, activation energy of grain boundary mobility: 1.46 eV, $\ln(m_0/\gamma)$= 16.0 $\mu m^2/s$, γ= 0.7 J/m^2, temperature: 800 K, time constant: 1.53 s, periodic boundary conditions. (a) 4.59 s, 10.05 vol.% recrystallized, (b) 6.12 s, 21.74 vol.% recrystallized, (c) 7.65 s, 38.42 vol.% recrystallized.

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Example 2: 3D Grain Growth in an Aluminium Polycrystal

Figure 2 shows subsequent stages of a 3D grain growth simulation in aluminium. The driving force was calculated from the local boundary curvature. The simulation used periodic boundary conditions, a grid size of 32·32·0.5 $(\mu m)^3$, and 936 discrete texture components. All boundaries had identical mobilities, using Q=1.6 eV, $\ln(m_0/\gamma)$= 16.0 $\mu m^2/s$, and γ= 0.7 J/m^2.

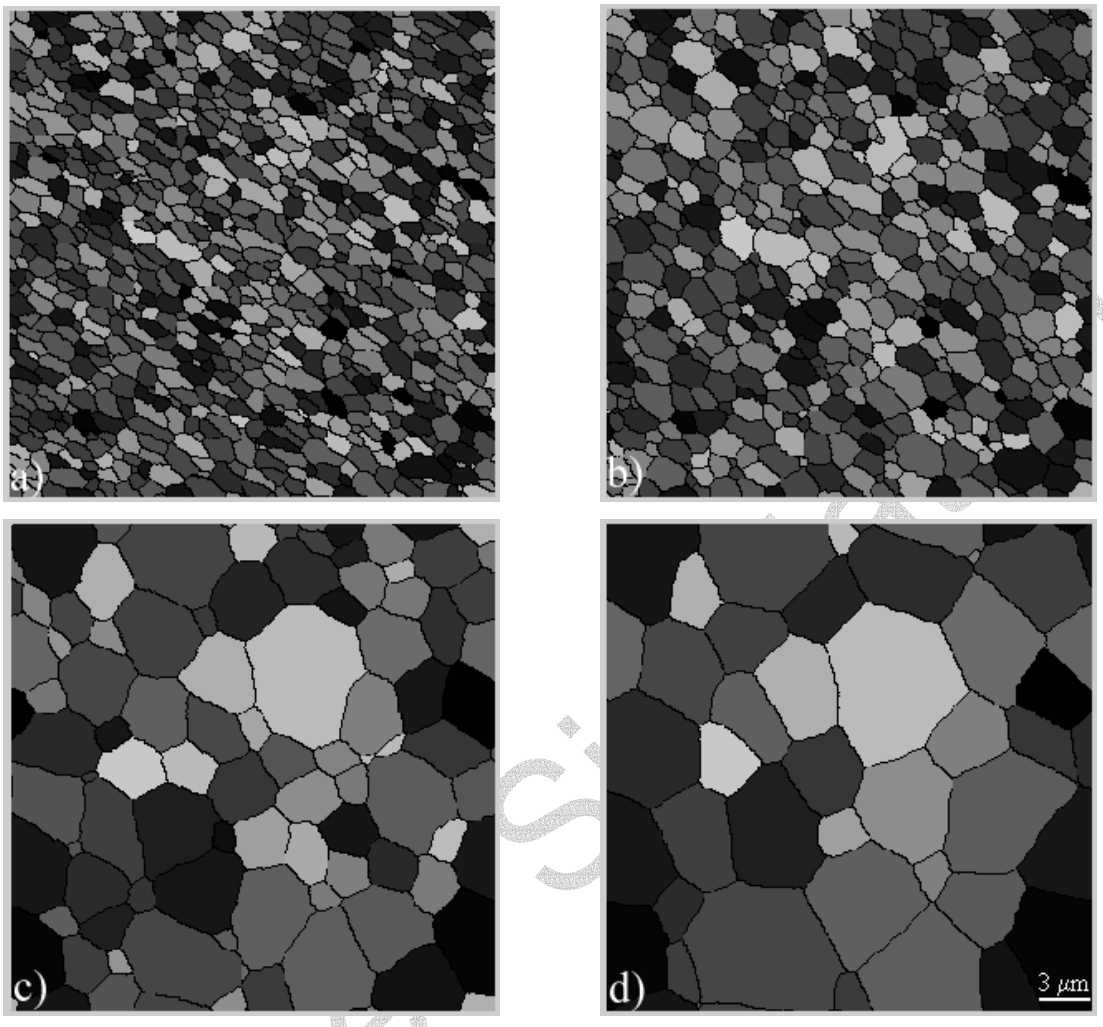

Figure 2: Subsequent sections from 3D grain growth simulation, Al, periodic boundary conditions, grid size: 32·32·0.5 $(\mu m)^3$, cell size: 0.1 µm, 936 texture components, Q=1.6 eV, $\ln(m_0/\gamma)$= 16.0 $\mu m^2/s$, γ= 0.7 J/m^2, 800 K, (a) 15.1 s, (b) 75.5 s, (c) 755 s, (d) 1510 s.

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