8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

Monte Carlo simulation of nanocrystalline grain growth

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Key Words: *Monte Carlo simulation, grain growth, nanocrystalline materials.*

ABSTRACT

Grain growth in polycrystalline materials is known to be a non-equilibrium dissipative process. It is driven by a reduction of the Gibbs free energy that is associated with an entropy production. The temporal development towards a thermodynamic equilibrium proceeds under the constraints of metrical, topological and mechanical equilibrium properties in the space filling grain network.

In the present work nanocrystalline grain growth in polycrystals is modelled under the assumption that the mobility of grain boundaries is limited at small grain sizes. In particular, following the works of Gottstein, Shvindlerman, Novikov and others (cf. e.g. [1]), it is assumed that the grain boundary mobility depends, for two-dimensional grain growth, on the triple junction distance.

Therefore, a new intrinsic length scale λ has been introduced, reducing the mobility m_0 of the grain boundary to

$$m = \frac{m_0}{1+\frac{\lambda}{a}},$$

where a is the triple junction distance.

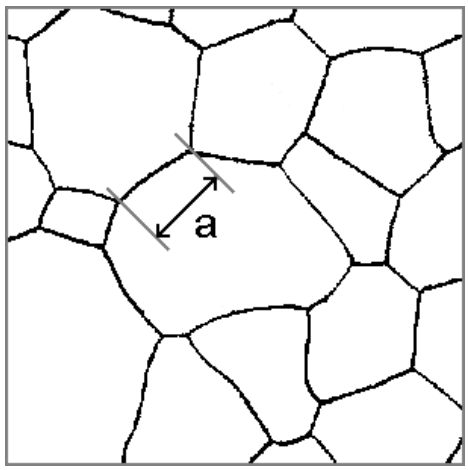

Figure 1. Grain structure with triple junction distance a.

Based on this assumption the Monte Carlo Potts model algorithm (compare [2] and the literature within) has been modified. The implemented algorithm allows now the simulation of grain growth controlled by size effects.

For initially very small grains a linear grain growth kinetics is observed (cf. Fig. 2a), which is in agreement with the experimental results of [3]. Furthermore, an approximately quasi-stationary self-similar coarsening regime is reached, where the

grain size distributions are shifted to smaller relative grain sizes. The coincidence of the distributions implies a universal size distribution as can be seen in Figure 2b.

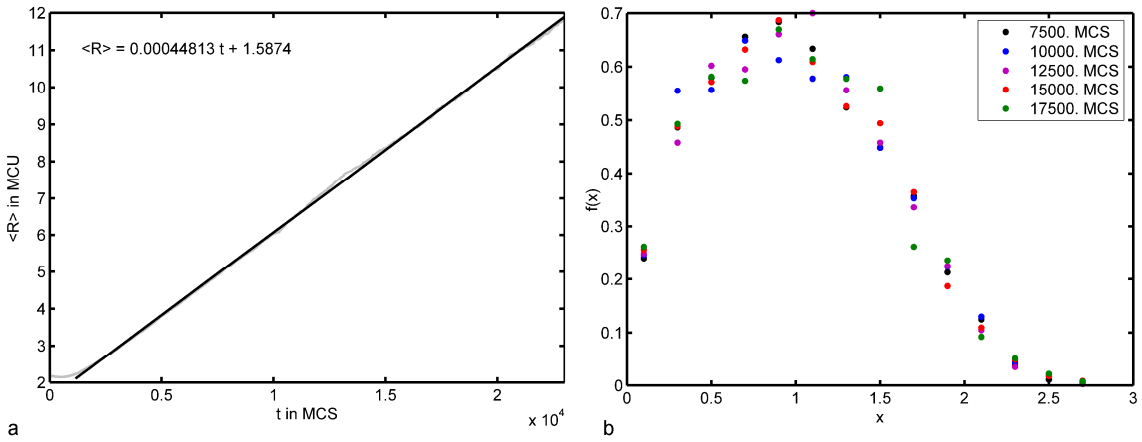

Figure 2: a – Mean grain size vs. time showing a linear growth kinetics; b – Universal grain size distribution shifted to smaller relative grain sizes $x = R/\langle R\rangle$.

This linear growth regime can adequately be described by a statistical mean-field approach based on the generalized Lifshitz-Slyozov-Wagner theory (cf. [4] and the literature within) yielding an analytical grain size distribution function

$$f(x) = \frac{D x_0^D \mathrm{e}^D (x + x_c)}{(x_0 - x)^{2+D}} \cdot \mathrm{e}^{\frac{-D\left(x_0^2 + x_c x\right)}{x_0 (x_0 - x)}}$$

that is in good agreement with the simulation results (compare Fig. 3).

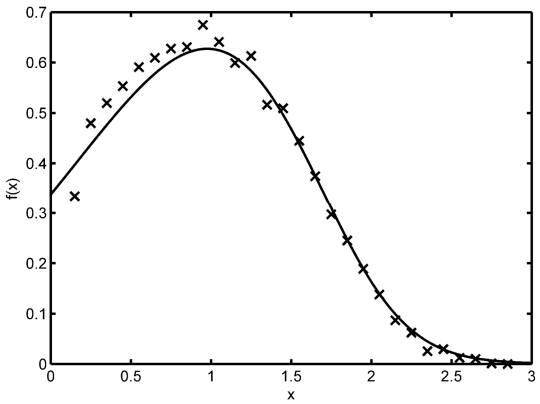

Figure 3: Self-similar grain size distribution together with analytic fit.

REFERENCES

[1] V. Y. Novikov, "On the influence of triple junctions on grain growth kinetics and microstructure evolution in 2D polycrystals", *Scripta Mater.*, **52**, 857–861 (2005).

[2] D. Zöllner, *Monte Carlo Potts Model Simulation and Statistical Mean-Field Theory of Normal Grain Growth*, Shaker Verlag, 2006.

[3] C. E. Krill III, L. Helfen, D. Michels, H. Natter, A. Fitch, O. Masson, and R. Birringer, "Size-Dependent Grain Growth Kinetics Observed in Nanocrystalline Fe", *Phys. Rev. Letters*, **86**, 842–845 (2001).

[4] P. Streitenberger and D. Zöllner, "Effective growth law from three-dimensional grain growth simulations and new analytical grain size distribution", *Scripta Mater.*, **55**, 461–464 (2006).