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Influence of the local topology on the von Neumann-Mullins-relation

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ABSTRACT

The von Neumann-Mullins-relation is one of the most fundamental laws of microstructural coarsening enabling a prediction of the kinetics of individual cells in many cellular structures ranging from foams to polycrystalline metals and alloys. The derivation of this relation is based on the assumption of ideal coarsening, regular cells, and a constant environment. However, in reality this is rarely the case. Hence, in the present work it is shown how the local topology and local topological changes influence the growth kinetics of individual grains.

1. Introduction

Our understanding of cellular structures—like soap foams or polycrystalline grain structures—is of fundamental importance in order to improve materials properties in production and application. This is particularly significant for microstructural coarsening, since microstructures and materials properties are closely related. To this end, Smith [1] developed one of the first physically motivated grain growth theories. Already in 1952, he pointed out the importance of the angles at triple junctions, i.e. those places where three cells meet. They control the morphology of individual cells and therewith also the topology of the whole structure as well as the kinetics during coarsening. Under the assumption of an isotropic energy of the cell boundaries and a balance of surface tension, the dihedral angles in three adjacent cells are always 120°.

In the same year, von Neumann presented in a written discussion a relation for two-dimensional soap froth relating the rate of size change to the number of sides [2]. And while this has been von Neumann's only contribution to materials science, it has become one of the most essential equations in the theory of two-dimensional coarsening processes. A couple of years later, Mullins applied this idea to normal grain growth in two dimensions yielding a rule of motion [3] that is well-known today as the von Neumann-Mullins-law stating

$$\dot{A}(n) = -m\gamma\left(2\pi - \frac{\pi}{3}n\right) = m\gamma\frac{\pi}{3}(n-6), \tag{1}$$

where the only two materials parameters under consideration are m as the specific boundary mobility and γ as the boundary surface tension. The parameter n describes the number of edges or neighbors of the considered cell respectively grain and therewith also the number of triple points. In addition, the area is given by A, and the rate of area change $\dot{A}(n)$ is independent of the shape of the grain boundaries depending rather only on the number of edges. As a basic result of $\dot{A} \propto n - 6$ the growth behavior of all cells is fixed such that all the cells of an ensemble with more than six edges will grow and all those with less than six edges will shrink, whereas those cells with exactly six are stable marking a critical number of neighboring cells for $n = 6$. It follows that the von Neumann-Mullins-law is a self-similar and time-independent function.

Obviously, a constant area growth rate implies that the area of the cell or grain changes linearly with time. However, this is true only under those idealized circumstances described by von Neumann and Mullins [2,3]. In a real foam or polycrystalline grain structure the topology of the structures changes constantly, e.g., by vanishing cells or neighbor switching events [4]. As a result, there will always be deviations from Eq. (1) for individual cells in real materials.

Over the years, the von Neumann-Mullins-law has been proven to be true again and again by experiments, theoretical considerations as well as computer simulations; to name just a few:

- Palmer et al. [5] have shown that for example succinonitrile is a good system for investigating coarsening in thin films. They were able to examine the behavior of individual grains in such films and found that the vast majority of the grains fulfills the

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von Neumann-Mullins-relation. Only a small fraction of grains show a deviating behavior either because they have low angle boundaries or due to the finite thickness.

- Hunderi and Ryum [6] have re-analyzed the von Neumann-Mullins-law and proven that Eq. (1) is exactly correct under the classical assumptions made by von Neumann and Mullins. Hence, they confuted an argument that the relation might be only approximately correct. In particular, they solved the equation even numerically for some centro-symmetrical grains.
- Zöllner et al. [7] as well as Streitenberger and Zöllner [8] extended that classical von Neumann-Mullins relation applying it to junction limited grain growth as it may occur in nanocrystalline materials. They showed by analytic theories and Potts model simulations that for coarsening under triple junction control not the area change rate $\dot{A}$ but the radius change rate $\dot{R}$ is a self-similar function of the number of sides n.
- Moldovan et al. [9] used a mesoscopic simulation approach to study the coupling and competition between grain-boundary-curvature driven and grain-rotation-coalescence induced grain growth in a ⟨0 0 1⟩ textured columnar microstructure. Particularly they extended the von Neumann–Mullins-relation successfully based on averaged grain boundary properties to include also the effect of grain rotations.
- Also Kim [10] analyzed the von Neumann–Mullins-law by 2D Potts model simulations on a hexagonal grid. Though, these considerations suffer from a simple drawback, namely the use of zero temperature Potts model simulations. Such zero temperature grain growth simulations include the effect that the boundaries cling to the underlying grid resulting in unphysical behavior (see [11]).

In the present paper it will be shown that the von Neumann-Mullins-law is indeed fulfilled for individual cells resp. grains evolving in a constant environment as expected. However, as a main focus it will be shown how the local topology and associated topological changes influence the growth kinetics of individual grains yielding clear deviations from the classical von Neumann-Mullins-equation.

2. Simulation method

2.1. Standard Potts model

The modern Monte Carlo Potts model is based on the classical works of Anderson, Srolovitz, Grest, and Sahni, who applied the Potts model more than 30 years ago for the first time to the problem of grain growth [12,13] opening up the possibility to predict some of the main features of polycrystalline grain microstructures during thermal annealing. In the succeeding years many different areas of application have been established, for example

- anisotropic and abnormal grain growth,
- texture-controlled grain growth,
- influence of second phase particles,
- pore migration,
- grain growth under thermal gradients,
- static and dynamic recrystallization,
- sintering, and
- junction limited grain growth as may occur in nanocrystalline materials.

But also the coarsening of foams has been investigated thoroughly. The ongoing success of the Potts model for such investigations of coarsening is based on different reasons. In particular, it is a mesoscopic simulation model that allows the observation of large cellular ensembles over long time spans making statistical analyses possible, which is quite different compared to molecular dynamics simulations that are usually limited to a small number of cells. But most of all, such simulation techniques enjoy control over kinetic and thermodynamic materials parameters affecting coarsening far greater and more precise than can be realized experimentally.

Before starting a simulation some technical grid parameters have to be selected. In the current investigations, a two dimensional polygonal network is mapped onto a simple quadratic lattice with eight nearest neighbors (first and second nearest), which are in the present case not weighted. Each grid point is called Monte Carlo Unit and contains a certain area of a cell.

Following the standard procedure the specific boundary energy γ and the specific boundary mobility m are the only materials parameters under consideration. Hence, it has been reasonably assumed that, e.g., segregation or precipitations at boundaries express themselves phenomenologically in changed parameters of the Potts model [14]. Basically, the algorithm minimizes the total lattice energy by a series of local orientation changes, where the final orientation of a grid point under consideration is calculated by

$$p = \begin{cases} \frac{m}{m_{\max}} \frac{\gamma}{\gamma_{\max}}, & \Delta E \leqslant 0 \\ \frac{m}{m_{\max}} \frac{\gamma}{\gamma_{\max}} \cdot \exp\left(\frac{-\Delta E}{T_S}\right), & \Delta E > 0 \cdot \end{cases} \tag{2}$$

Here T_S is the simulation temperature also called effective lattice temperature, and the constants $m_{\max}$ and $\gamma_{\max}$ denote the maximum values of mobility and energy. As a result, setting $m = m_{\max}$ and $\gamma = \gamma_{\max}$ yields a simulation of normal grain growth respectively ideal coarsening. Hence, the areas of the grains are given in Monte Carlo Units, whereas the time unit is a Monte Carlo Step. For more details compare, e.g., [11,14].

2.2. Controversial use of the simulation temperature

Historically, Potts model simulations were carried out as zero temperature simulations ($T_S = 0$). This simplifies the algorithm, especially Eq. (2), such that the new orientation is only accepted in case that the energy of the grid is reduced by the change in orientation. As a result, no thermal fluctuations occur and the runtime of the algorithm is reduced, which has been a computational advantage particularly in the 1980s and 1990s. For this reason, there are many zero temperature Potts model simulation studies available in literature (compare review [11] and the literature within). Nevertheless, using such an approach is extremely problematic as the algorithm then aligns the cell boundaries with the underlying lattice. As a result, the boundaries are often straight and cling to the lattice, which is highly unphysical.

However, this effect can easily be eliminated by introduction of a non-zero simulation temperature T_S just as presented in Eq. (2), where an increase in T_S activates thermal fluctuations that result in a roughening of the grain boundaries. As it has been shown in Ref. [11], the actual choice of the simulation temperature needs to be done very carefully since Potts model simulations exhibit a so-called order-disorder transition, and one has to keep in mind that T_S is, of course, not a real temperature. While the real temperature controls the mobilities of the boundary interfaces, the simulation temperature has an effect only on the roughness of said boundaries. Nevertheless, an algorithm has been proposed in [11] to find for a given set of lattice parameters one adequate simulation temperature that yields curvature driven grain growth kinetics exactly as predicted theoretically.

Within the present work, it will also be shown how the simulation temperature influences the von Neumann-Mullins-law, and