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Investigating the von Neumann–Mullins relation under triple junction dragging

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Abstract

The influence of triple junction mobility on the rate of size change is investigated by square-lattice Monte Carlo Potts model simulations. For normal, grain-boundary-controlled grain growth the classical von Neumann–Mullins relation ($\dot{A} \propto n - n_c$) is fulfilled for individual polyhedral grains as well as for polycrystalline grain microstructures. For triple-junction-controlled grain growth the number of neighboring grains is related self-similarly to the radius change rate ($\dot{R} \propto (n - n_c)/n$), which is also shown to be fulfilled for individual grains and polycrystalline microstructures.

Keywords: Grain growth; Nanocrystalline material; Triple junctions; Monte Carlo simulation; von Neumann–Mullins relation

1. Introduction

As long ago as 1952 von Neumann presented a fundamental relation for 2-D soap froth relating the rate of size change to the number of sides [1]. A couple of years later Mullins applied this idea to normal grain growth in two dimensions, yielding a rule of motion [2] that is known today as the von Neumann–Mullins law. This law states:

$$\dot{A} = -m_{gb}\gamma_{gb}\left(2\pi - \frac{\pi}{3}n\right) = m_{gb}\gamma_{gb}\frac{\pi}{3}(n-6). \quad (1)$$

Here m_{gb} is the grain boundary mobility, γ_{gb} is the grain boundary surface tension, A is the area of a grain and n is the number of sides or neighbors of that grain and the number of triple points, respectively, for any value of $n > 0$. In contrast, $n = 0$ corresponds to the case of zero triple points describing a grain embedded in a larger matrix grain with one grain boundary. Specifically, the rate of area change $\dot{A}$ is independent of the shape of the grain boundaries. As a result, all grains of an ensemble with $n > 6$ sides will grow and grains with $n < 6$ sides will shrink and finally disappear. Only those grains with six sides are stable, making $n = 6$ the critical number of neighboring grains n_c. In particular, the von Neumann–Mullins law is a self-similar time-independent function that holds whenever the average grain area increases linearly with time.

In this model grain boundaries are considered as plane curves and their migration is always directed toward the centre of curvature with a speed that is proportional to the curvature itself. It is assumed, in particular, that all grain boundaries of the polycrystalline microstructure are characterized by a unique value for the surface tension as well as by the same mobility. This is in agreement with the uniform boundary model [3] and neglects any dependence of the boundary properties m_{gb} and γ_{gb} on the misorientation or crystallographic orientations of the boundaries, where, in particular, the grain boundary mobility m_{gb} does not depend on the velocity of grain boundary migration.

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Finally, it is also assumed that only the grain boundaries contribute to their migration, and triple junctions are only geometrical properties. It follows from the surface tension equilibrium that the stable number of grains meeting in a vertex is always three and the associated triple junction angle is 120°.

Over the years, the von Neumann–Mullins law has been verified by experiments [4,5], theoretical considerations [6,7], and computer simulations [8,9]. However, especially in the last decade the influence of the triple junction drag on grain growth kinetics has become increasingly important. Triple junction drag is the principal explanation for the thermal stability of nanocrystalline materials (see overview in Ref. [10]). While there is intense activity in this field of research, and there are also many publications available regarding the production as well as the mechanical properties of nanocrystalline materials, statements regarding grain microstructural changes during coarsening are generally limited to information on the temporal evolution of the average grain size and on initial grain size distributions.

However, as long ago as 1998 Gottstein and Shvindlerman [11] considered the influence of triple junction dragging on the von Neumann–Mullins relation. Their work is based on the idea that in nanocrystalline materials the influence of the triple points of a 2-D grain network is non-negligible. In particular, the triple point mobility, which is considered to be different from that of the adjoining boundaries, influences the migration of the triple point and hence also the motion of the adjacent boundaries. To that aim, Gottstein and Shvindlerman [12] derived a relationship between triple junction mobility and the dihedral angles forming; they had to distinguish between grains with $n < 6$ neighbors and grains with $n > 6$ neighbors, and they derived two separate expressions for the rate of area change for grains with few sides ($n \leqslant 6$):

$$\dot{A} = -\frac{m_{gb}\gamma_{gb}}{1+\frac{2\cos\theta-1}{2\theta}}[2\pi - n(\pi-2\theta)]. \tag{2a}$$

And with many ($n > 6$) sides:

$$\dot{A} = \frac{m_{gb}\gamma_{gb}}{1-\frac{1-2\cos\theta}{\ln(\sin\theta)}}[n(\pi-2\theta)-2\pi]. \tag{2b}$$

Both equations are functions of θ, which is half the dihedral angle of the grain at the triple junction and depends strongly on the ratio of the mobilities of grain boundaries m_{gb} and triple junctions m_{tj} (cf. also Refs. [13,14]). It follows that grains with few ($n < 6$) sides will still shrink, but more slowly than in case of normal grain growth, and grains with many ($n > 6$) sides will grow, but also more slowly than for normal grain growth. In particular, for normal grain growth with an equilibrium angle at the triple points of 120°, i.e. $\theta = \pi/3$, Eqs. (2a) and (2b) include as a limiting case the classical von Neumann–Mullins-law, Eq. (1).

Moreover, while Eqs. (2a) and (2b) have been found to be in good agreement with network-model simulations [15], they also suffer from one particular drawback: they consist of two separate equations, instead of a holistic single solution for all numbers of sides. Hence, in the present paper we investigate the influence of triple junction mobility on the rate of size change by square-lattice Monte Carlo Potts model simulations. We show, in particular, that for triple-junction-controlled grain growth the number of neighboring grains n is related self-similarly to the radius change rate by the von Neumann–Mullins-type relation $\dot{R} \propto (n - n_c)/n$ as has been derived recently by Streitenberger and Zöllner [16], and find it to be fulfilled for individual grains as well as for polycrystalline grain microstructures.

2. A holistic growth laws for triple-junction-controlled grain growth

In a recent paper, Streitenberger and Zöllner [16] derived an expression for the rate of size change for grain growth under triple junction dragging based on the general form of the evolution equation of a single grain of linear grain size R:

$$R\dot{R} = m_{gb}\gamma_{gb}\alpha\left(n^{\frac{1}{D-1}} - n_c^{\frac{1}{D-1}}\right), \tag{3}$$

where the dimension is $D = 2$ for 2-D grain growth, n_c is the critical number of neighbors for which $\dot{R}(R = R_c) = 0$ is associated with the critical grain radius R_c, and α is a constant. Eq. (3) represents specifically for normal grain growth the von Neumann–Mullins law, Eq. (1), as the area change rate of a grain with the parameters $n_c = 6$ and $\alpha = 1/6$. However, for triple-junction-controlled grain growth α cannot be predicted theoretically, but from simulations we find that it takes—as we will see below—a much smaller value.

Then again, while it is assumed for normal grain growth (on the micrometer size scale) that only the grain boundaries and their properties control the migration kinetics, limited triple junction mobility is considered to be the main reason for the nanocrystalline growth kinetics. In particular, Gottstein and Shvindlerman [17] derived a principle expression giving the velocity of a boundary in terms of the intrinsic mobilities m_{gb}, m_{tj}, m_{qp} of grain boundaries, triple junctions and quadruple junctions:

$$v = \frac{m_{gb}\gamma_{gb}K}{1+\frac{m_{gb}}{am_{tj}}+\frac{m_{gb}}{a^2m_{qp}}}, \tag{4a}$$

where K is the curvature of the boundary and a is the boundary junction spacing. Considering grain growth in two dimensions and introducing the intrinsic size parameter $\lambda = m_{gb}/m_{tj}$, Eq. (4a) takes the simplified form $v = m_{eff}\gamma_{gb}K$ with an effective mobility:

$$m_{eff} = \frac{m_{gb}}{1+\lambda/a}, \tag{4b}$$

of a grain boundary reduced by the drag effect of the adjoining triple junctions. It follows that under the assumption that the average boundary junction spacing and the average curvature scale with the average grain size as $a \sim \langle R\rangle$ and $K \sim \langle \mathrm{R}\rangle^{-1}$, respectively, two different types of growth kinetics in polycrystals can be predicted [17]. Grain growth