

Influence of subgrain boundaries on coarsening of grain structures

D. Zöllner, W. Skrotzki

Institut für Strukturphysik, Technische Universität Dresden, Haeckelstraße 3, D-01069 Dresden, Germany

dana.zoellner@ovgu.de

Abstract. In the present work, the influence of subgrain boundaries on the coarsening kinetics of individual grains embedded in an average environment as well as within a grain structure is investigated. It is found that a specific introduction of subgrain boundaries not only influences the speed with which grains shrink or grow, but in contrast to the von Neumann-Mullins-law, a distinct manipulation of the location of the subgrain boundaries allows even grains with few edges to grow, while grains with many edges shrink. During these circumstances one fact stays the same: the area of the individual grains is a linear function of annealing time as long as the environment does not change.

1. Introduction

In the classical treatment of normal grain growth the von Neumann-Mullins-law [1-3]

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

describes the temporal evolution of individual grains, according to which the area, A , of a two-dimensional grain increases or decreases linearly with time solely depending on the number of neighboring grains or edges, n . The rate of area change $\dot{A}(n)$ is independent of the shape of the grain. The materials parameters taken into account are the specific boundary mobility, m , and the boundary surface tension, γ . It follows directly from Eq. (1) that all grains of an ensemble with more than six edges will grow and all those with less than six edges will shrink making six the critical number of neighboring grains. However, this relation holds only under the assumption of ideal grain coarsening, where all boundaries are of high angle type. In such a case three grains always meet at a vertex forming 120° dihedral angles.

In contrast, processes like severe plastic deformation (SPD) introduce a large number of subgrain boundaries within the framework of grain refinement by a multi-step process [4,5]. Initially the dislocations are distributed more or less homogeneously throughout the grain structure. During deformation they start to rearrange themselves forming cells. With ongoing deformation more dislocations enter the cell walls changing them to subgrain boundaries. The misorientation along these boundaries is rather small such that they are clearly of low angle type. As deformation continues, continuous dynamic recrystallization leads to a fine steady state grain structure [6].

However, quite often during the grain refinement process the steady state grain structure is not reached such that within the grain structure a majority of the grain boundaries may very well be of low angle type, for which the classical treatment of grain coarsening as described by Eq. (1) does no longer hold. In order to understand resulting microstructural changes and therewith also property changes due to thermal treatments, the migration of low angle grain boundaries has been of great scientific interest



for decades (e.g., [7-9]). For example a combined experimental and computational study [7] has shown that the simulated shrinkage of cylindrical grains with low angle $\langle 1\ 0\ 0 \rangle$ boundaries results in a strongly decreasing boundary mobility with decreasing misorientation angles smaller than 10° . The shape evolution of the analyzed grains can be related directly to energy computations.

In the present work, the influence of subgrain boundaries on the coarsening kinetics of individual grains is systematically investigated under two conditions: In the first case, the grains are each embedded in an average environment neglecting structural changes around the grains focusing purely on the interplay of a grain with its associated subgrain boundaries. In the second step, it is shown how individual grains connected to subgrain boundaries behave within a polycrystalline grain ensemble.

2. Simulation method

The Monte Carlo Potts model has been in use for simulation of grain coarsening phenomena for more than 30 years. It is a lattice based method that is in its basics rather simple, but allows in its specifics complex modeling. Among others the grain boundaries of a microstructure can be manipulated individually giving them a well-defined form as well as distinct values for mobility and energy. Following the standard procedure, the grain structures are mapped in the current investigations onto a quadratic 2D lattice, where each lattice point is a Monte Carlo Unit. The time unit of the simulation is one Monte Carlo Step comprising N reorientation attempts, where N is the total number of MCUs of the lattice. In each reorientation attempt the local energy of a selected lattice point is minimized (for details refer to, e.g., [10-12]).

Particularly for the present investigations certain grain boundaries are introduced as subgrain boundaries with lower values of boundary energy, γ_{SB} , and mobility, m_{SB} , therewith treating them as low angle grain boundaries compared to the common high angle grain boundaries with γ_{GB} and m_{GB} . The influence of energy, mobility, location and number of these subgrain boundaries is examined carefully.

3. Simulation results

3.1. Subgrain boundaries in individual grains

According to Eq. (1) we know that the area change rate of an n -edged grain is proportional to the boundary energy, where a lower energy means a smaller rate of growth for $n > 6$ or rate of shrinkage for $n < 6$. For example an ideal grain with five edges embedded in an average environment should have a rate of shrinkage of $\dot{A}(n=5) = -m\gamma\pi/3$. This is, of course, true for a grain with high angle boundaries only (compare [3]). If a number of subgrain boundaries is introduced and put solely inside the five-edged grain, they will strongly interact with the high angle boundaries and therewith influence the motion of the five edges and also influence the growth kinetics of the grain in total as it is shown in figure 1.

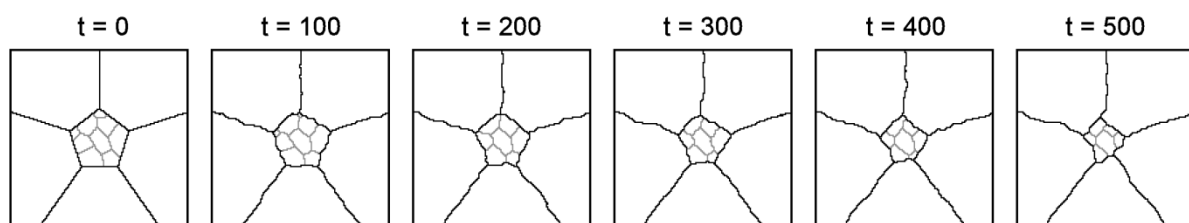


Figure 1. Temporal development of a five-edged grain with internal subgrain boundaries (in grey).

Apparently, the morphology of the grain changes because the subgrain boundaries exert a drag on the adjoining high angle boundaries. The strength of the drag strongly depends on the subgrain boundary energy as presented in figure 2a. The linear relation between grain area (which is the area enclosed by the high angle boundaries) and annealing time only holds as long as the morphology of

the grain does not change. A reduction in the number of grain boundaries (high angle as well as low angle type) changes the relation $A(t)$, e.g., lower left hand in figure 2a. The limiting case for $\gamma_{SB} = \gamma_{GB}$ yields normal-like coarsening behavior with only high angle boundaries and has the highest rate of shrinkage, which equals to the fastest shrinkage. The smaller the energy of the subgrain boundaries, the slower is the grain shrinking tending to zero for $\gamma_{SB} \ll \gamma_{GB}$. A systematic parameter variation shows that the rate of area change, $\dot{A} = \frac{dA}{dt}$, is a linear function of $\ln(\gamma_{SB}:\gamma_{GB}) = \ln(\bar{\gamma})$ connecting the two limiting cases and introducing the relative energy $\bar{\gamma} = \gamma_{SB}:\gamma_{GB}$ (figure 2b). A similar behavior can be observed when the subgrain boundary mobilities are changed as presented in figure 2c.

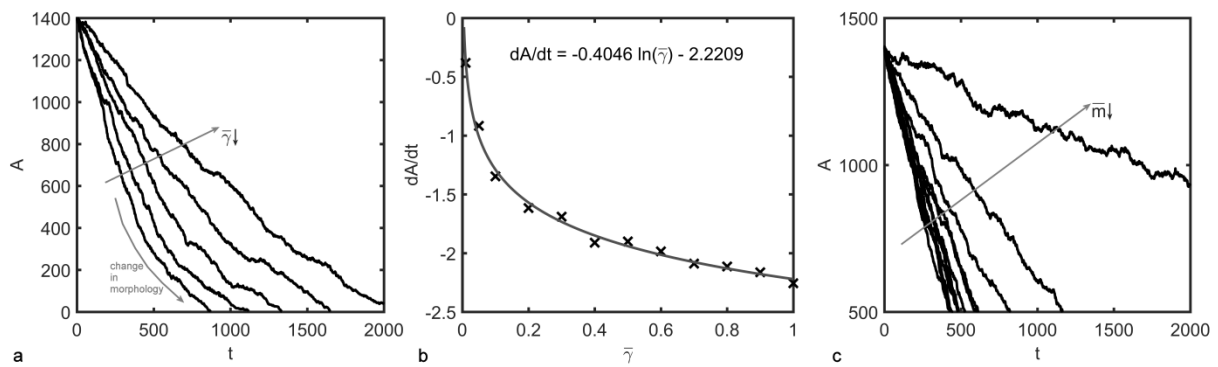


Figure 2. a – Temporal development of the area of a five-edged grain with internal subgrain boundaries (as in figure 1) changing with the relative energy; b – Resulting initial rate of area change depending on relative energy; c – Temporal development of the area of a five-edged grain with internal subgrain boundaries changing with the relative boundary mobility.

In addition, an immense influence on the growth kinetics is the number of subgrain boundaries present as shown in figures 3a and b. An increase in the number of internal subgrains, n' , all with the same energy and mobility increases the rate of shrinkage of a five-edged grain such that $\dot{A} \propto n'$ for a broad range of n' . Hence, apart from the relations $\gamma_{SB}:\gamma_{GB}$ and $m_{SB}:m_{GB}$, also the number of internal subgrain boundaries influences the shrinkage of grains with fewer than six edges.

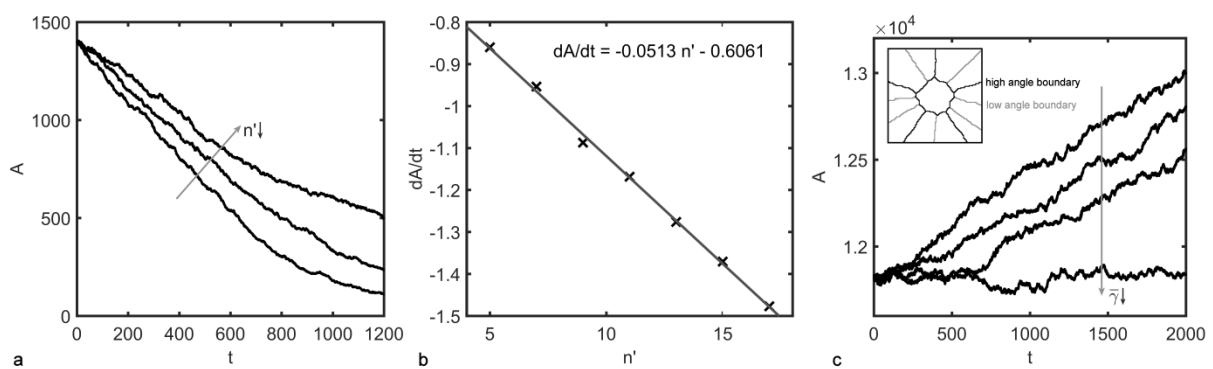


Figure 3. a – Temporal development of the area of a five-edged grain with different numbers of internal subgrains; b – Resulting initial rate of area change depending on the number of subgrains n' ; c – Temporal development of the area of a five-edged grain with external subgrain boundaries.

On the other hand, a selective placement of subgrain boundaries on the outside of the central grain yields an external drag effect. The fastest growth is naturally reached for the limiting case of $\gamma_{SB} = \gamma_{GB}$, whereas a reduction of the energy of the subgrain boundaries slows the temporal development down and tends to zero for $\gamma_{SB} \ll \gamma_{GB}$ (figure 3c). A similar behavior of nearly constant size can also be achieved by introduction of internal and external subgrain boundaries of higher energy.

In contrast, grains with more than six edges should grow according to Eq. (1). However, as shown in figure 4, the internal subgrain boundaries of a nine-edged grain with $\gamma_{SB} < \gamma_{GB}$ force the grain to shrink. Initially A is a linear function of t up to a point, where the number of internal boundaries is reduced therewith also reducing the rate of shrinkage (dotted line) in agreement with figures 3a and b.

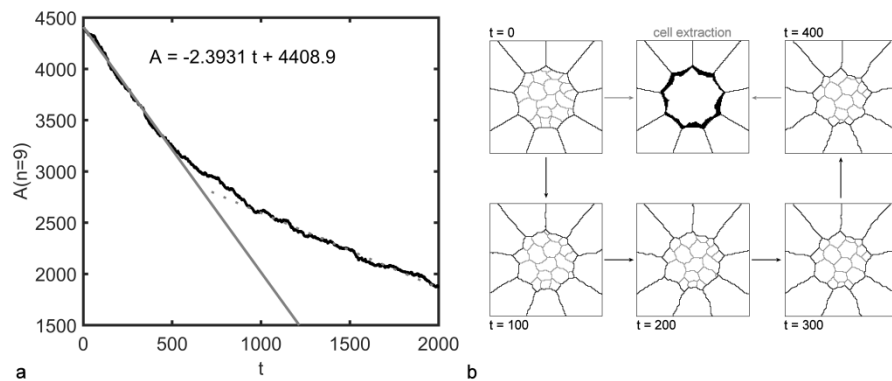


Figure 4. Temporal development of a nine-edged grain with internal subgrain boundaries that shrinks due to the drag of the subgrains in contrast to the prediction according to Eq. (1). High angle boundaries are plotted in black and low angle boundaries in grey.

3.2. Subgrain boundaries in polycrystalline aggregates

As discussed above, during SPD microstructures can be achieved that contain many subgrain boundaries. This is shown exemplarily in figure 5a for a grain structure produced by accumulative roll bonding (ARB) of thin aluminum sheets using commercially pure aluminum (99.5 wt.% Al). The high angle grain boundaries are marked in red and the low angle boundaries in blue [13].

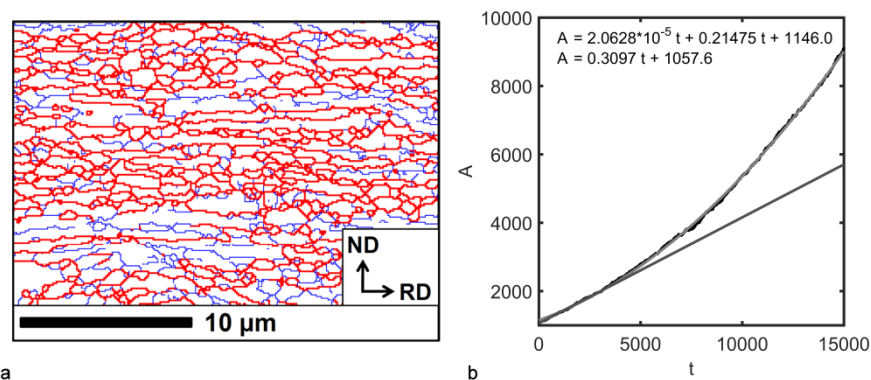


Figure 5. a – Grain boundary structure in commercially pure aluminium after 6 ARB cycles. Low angle grain boundaries (between 3° and 15°) and high angle grain boundaries ($> 15^\circ$) are coloured blue and red, respectively [13]; b – Temporal development of the size of a nine-edged grain with many subgrain boundaries in neighboring grains.

How does such a neighborhood influence the growth kinetics? To model this, the considerations above are extended by embedding in a first step a nine-edged grain in a polycrystalline aggregate, where all nine neighboring grains are relatively large and contain many subgrain boundaries. The mobility and energy of the low angle subgrain boundaries is assumed to be 10% of that of the high angle boundaries. As a result it is seen in figure 5b that the speed of growth is initially constant (linear least-squares fit), but then starts to increase with increasing annealing time (quadratic least-squares fit for long annealing times). This is due to the fact that the growing grain gets into contact with more and

more subgrain boundaries. Consequently, as demonstrated in figures 3a and b, a higher number of subgrains n' increases the rate of shrinkage and also in this particular case growth.

Extending this consideration to polycrystalline aggregates by inserting subgrain boundaries into 1/3 or 2/3 of the grains, where the mobility and energy of the low angle subgrain boundaries is 15% of that of the high angle boundaries, it is demonstrated in figure 6 how the average and individual growth kinetics are influenced. Particularly, in figure 6a the temporal development of the areas of individual grains is shown for the microstructure with 1/3 of the grains containing subgrains. The grains that contain no subgrains (black curves) evolve normally: large ones grow, small ones shrink, and average grains stagnate (compare [14]), while all those grains that contain subgrains (grey curves) are mostly shrinking very fast even if they are rather large. This is in agreement with figures 2 and 4, where internal subgrain boundaries force the grains to shrink even if they have more than six edges and are larger than average, since most of the grains have basically no external subgrain boundaries in case of figure 6a. As a result, after approximately 500 annealing time steps most of the grains containing subgrains are about to vanish. This in turn changes the average growth law as shown in figure 6b, where the loss of many grains between $t = 500$ and $t = 1000$ speeds up the average growth kinetics. In contrast, the microstructure, where 2/3 of the grains contain subgrain boundaries shows a slightly different behavior regarding the individual growth kinetics (figure 6c). Subgrain-free grains grow even when they are originally smaller than average, while grains that contain subgrains display a much more complex behavior. In this second case many such grains are surrounded by grains that also contain subgrain boundaries themselves, which can be shown to result in stagnation, growth, or shrinkage depending on the location and density of the subgrain boundaries.

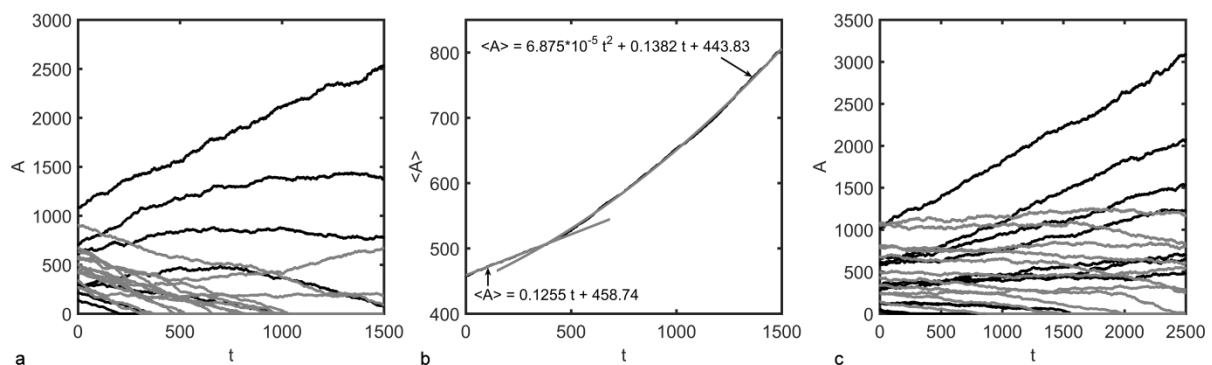


Figure 6. Temporal development of: a – area of individual grains for microstructure with 1/3 of the grains containing subgrain boundaries; b – associated average growth law; c – average growth law for microstructure with 2/3 of the grains containing subgrain boundaries. In images a and c grains that contain no subgrains are plotted in black, whereas grains that enclose subgrains are plotted in grey.

Taking a closer look at figure 6a, the area change rate as a function of the number of neighboring grains can be derived for different annealing times. Initially (see figure 7a) the grains not containing subgrains (black crosses) almost fulfill the von Neumann-Mullins-law, Eq. (1) (associated linear least-squares fit), whereas all those grains that contain subgrain boundaries (grey diamonds) form a separate cluster of data showing high shrinking rates independent of the number of edges (these data points have not been taken into account for the least-squares fit). As coarsening progresses, figures 7b and c show that the grains containing subgrain boundaries usually have a characteristically high rate of shrinkage, while for all other grains \dot{A} is a linear function of n with a critical number of edges slightly deviating from 6. Particularly in the last figure it can be seen that the microstructure balances the high shrinking rates (lower right hand side) with high growth rates of neighboring grains (upper right hand side). This can easily be understood from the fact that grain boundaries form a network. If a boundary moves rather fast to the center of a certain grain, it also moves just as fast away from the center of the adjunct grain.

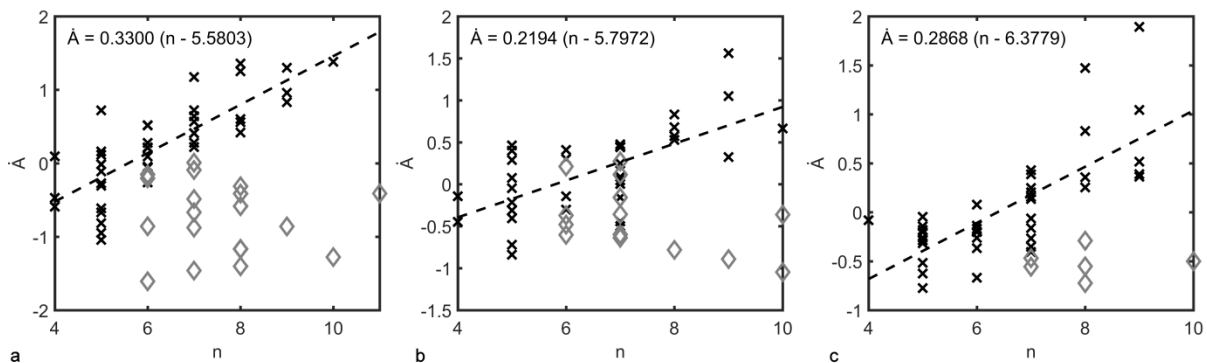


Figure 7. Area change rate of individual grains as a function of the number of neighboring grains for a microstructure with 1/3 of the grains containing subgrains. Black crosses mark all grains without internal subgrains and grey diamonds marks all those with internal subgrain boundaries: a – $t = 0$; b – $t = 500$; c – $t = 800$.

4. Summary

The present work shows the influence of subgrain boundaries on the coarsening kinetics of individual grains embedded in an average environment as well as within a polycrystalline grain ensemble. A specific introduction of subgrain boundaries not only influences the speed with which grains shrink or grow depending on their number of neighboring grains or edges, but in contrast to the von Neumann-Mullins-law a distinct manipulation of the location of the subgrain boundaries allows even grains with few edges to grow, while grains with many edges shrink. During these circumstances one fact stays the same: the area of the individual grains is always a linear function of annealing time as long as the environment does not change. However, once the number of internal or external subgrain boundaries changes clear deviations from the linear relation become visible. For polycrystalline grain aggregates produced by SPD this relation is even more complicated due to the complex interaction of area change rate, grain size respectively number of edges, and the existence or non-existence of subgrains within a grain and in its neighboring grains. Nevertheless, growth and shrinkage rates far larger and smaller, respectively, than under normal grain growth conditions have been observed.

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