Acta Materialia 96 (2015) 390–398

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Abnormal grain growth in the Potts model incorporating grain boundary complexion transitions that increase the mobility of individual boundaries

William E. Frazier *, Gregory S. Rohrer, Anthony D. Rollett

Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA 15213-3890, USA

ARTICLE INFO

Article history:
Received 16 April 2015
Revised 3 June 2015
Accepted 15 June 2015

Keywords:
Abnormal grain growth
Potts model
Complexions
Grain boundaries

ABSTRACT

The Potts model of grain growth was adapted for the purpose of simulating abnormal grain growth (AGG) resulting from grain boundary complexion transitions. The transition in grain boundary structure between specific complexion types results in changes in properties. Where the transitions decrease energy and increase the mobility of boundaries, AGG occurs provided that such transitions predominantly occur via propagation to adjacent boundaries. Thus the model increases the mobility of selected boundaries on the basis of their adjacency to zero, one, or a multiplicity of boundaries that have already transitioned. The effect of transitions to a high mobility complexion was investigated separately from the effect of changes in energy. The influence of the frequency of complexion transitions with different adjacencies on the occurrence of AGG was explored. The simulations show how propagating complexion transitions can explain the AGG observed in certain ceramic systems.

1. Introduction

Abnormal grain growth occurs in a wide variety of different materials systems, including alumina [1], yttria [2], barium titanate [3], boron carbide [4], tungsten carbides [5], nickel alloys [6], molybdenum alloys [7], and steels [8]. A variety of mechanisms have been proposed to explain AGG, but in the absence of inert particles or pores that pin most boundaries, it is generally agreed upon that the boundaries surrounding an abnormally large grain must have a sustained mobility and/or energy advantage. For example, Rollett et al. [9] used two dimensional Potts model simulations to show that a relatively large grain decreases in size relative to the average grain size unless the grain has a mobility advantage (a greater grain boundary velocity per applied driving force) and energy advantage (a lower grain boundary energy). Similar results were obtained in three dimensions [10]. Rollett and Mullins [11] analyzed relative growth rates of grains assigned a mobility and/or energy advantage and established a simple quadratic relationship between the maximum relative size and the two ratios; Humphreys [12] published a similar theory at the same time. A reasonable expectation from these analyses is that the tendency for a grain to grow abnormally should be related both to the mobility (and energy) advantage and to the fraction of the grain surface area that has that advantage. In order, however, for a given grain to grow to a large enough size relative to the average in order to be observable as abnormal, the property advantage must be sustained over a large number of changes in the boundaries on its perimeter. This in turn motivated the investigation of what effect propagating transitions in grain boundary structure and properties might have on abnormal grain growth.

In experimental studies of doped aluminas, Dillon and Harmer [13] associated abnormal grain growth with the presence of certain grain boundaries that not only had higher mobilities, but also had microscopically distinguishable structures and compositions [14]. These distinguishable grain boundary states have been called "complexions" [15]. More recently, it has been found that these higher mobility boundaries can also have lower grain boundary energies [16,17]. The coexistence of the high mobility, low energy grain boundary complexion with the lower mobility, higher energy complexion suggests that one of them is metastable with respect to the other and that there is a nucleation energy barrier associated with the transition from the metastable to equilibrium state. In fact, under the assumption that the number of abnormal grains is proportional to the number of transitioned grain boundaries, the temperature dependence of the transitioned boundaries is consistent with a thermally activated process. In the Ca doped alumina system, the nucleation barrier for a complexion transition was estimated to be 275 kJ · mol^{-1} [16].

* Corresponding author.

http://dx.doi.org/10.1016/j.actamat.2015.06.033
1359-6454/

It has also been observed that the abnormally large grains that occur are relatively rare. For example, if a grain is 10 times the average diameter, and makes up 10% of the total volume, then there are approximately 10,000 average grains for each abnormal grain. One open question is, what fraction of the grain boundaries must be transitioned to the high mobility, low energy complexion to lead to an abnormally large grain? While it seems clear that one high mobility boundary is unlikely to result in an abnormally large grain, it is also likely that it is not necessary to transition every single boundary surrounding a grain. The combined observations that abnormal grains are rare and that the abnormal grains must have multiple transitioned boundaries in close proximity suggest that the nucleation of new transitioned boundaries is not a random process. This suggests the hypothesis that grain boundaries in contact with transitioned boundaries are more likely to transition, which in turn leads to AGG.

There is some experimental evidence for this. Recent measurements of grain boundary energies around abnormally large grains in Ca doped yttria showed that the energies of boundaries around the largest grains were systematically lower than those around small grains separated from the large grains by at least five grain diameters [18]. This was taken as evidence that the boundaries around the largest grains have transformed to a lower energy, higher mobility complexion. However, the boundaries around small grains in contact with the larger grain had energies that were indistinguishable from the large grains. This suggests that these boundaries had transformed after contact with the fast growing grains.

The purpose of this paper is to show, through grain growth simulations, that abnormal grain growth can be stimulated if transitions of a fraction of grain boundaries to a high mobility, low energy complexion are accelerated by the presence of a neighboring, already transitioned boundary. Conversely, if the transformation to a high mobility, low energy complexion occurs randomly and without regard to the state of the adjacent boundaries, then abnormally large grains will not be observed.

2. Methods

The Potts model in this work is similar to that used by Rollett et al. [9] (and many others) to study abnormal grain growth in the mid and late 1980s, which in turn was based on the pioneering work of Anderson et al. [19]. The Potts model is itself a generalization of the Ising model for magnetism. A grid of "spins", or grain identity (ID) numbers, is assembled, and randomly selected spins can change spin to that of a neighbor with a probability dependent on the energy change associated with the change of spin and the "mobility" of the boundary between the neighbors. The local energy for site i in the grid is defined by the equation:

$$E = -\frac{J}{2} * \sum_{j}^{NN} (\delta_{S_i S_j} - 1)$$

Here, J is the grain boundary energy between i and j, S_i and S_j denote spin, δ is the Kronecker delta function [20], and NN is the number of nearest neighbor cells. In the basic (isotropic) Potts model, J is constant. Self evidently, the energy of the system is the sum (over i) of all the individual site energies. Thus, the probability of ID reorientation can be expressed by the piecewise defined function:

$$p = \begin{cases} M * J, & \Delta E < 0 \\ M * J * e^{\frac{-\Delta E}{T * kT}}, & \Delta E \geqslant 0 \end{cases}$$

Here, M is the grain boundary mobility, ΔE is the energy associated with the grain ID reorientation, T is temperature and k is the Boltzmann constant. It is important to understand that temperature in this context is not a physical temperature governing boundary migration rates, for example, but instead controls the disorder associated with the boundaries e.g. their roughness. To prevent artificial pinning effects associated with the cubic lattice of the Potts model simulation [21,22], we use a constant temperature value, $kT = 1.0$, in all of the described simulations.

The model incorporates the mobility and energy changes associated with transitions on grain boundaries by creating respective functions $M(i,j)$ and $J(i,j)$, which are defined as follows:

$$M(i,j) = \begin{cases} 1, & Tr(i,j) = 1 \\ M_{Min}, & Tr(i,j) = 0 \end{cases}$$

$$J(i,j) = \begin{cases} J_{Min}, & Tr(i,j) = 1 \\ 1, & Tr(i,j) = 0 \end{cases}$$

where the function $Tr(i,j)$ is an indicator that returns one when the grain boundary is transitioned and zero when the grain boundary is not transitioned, or nonexistent. Now, the fraction of transitioned grain boundaries, f_T, is the number of transitioned boundaries divided by the total number of grain boundaries:

$$f_T = \frac{\sum_i^{N_{IDs}} \sum_j^{N_{IDs}} Tr(i,j) * B(i,j)}{\sum_i^{N_{IDs}} \sum_j^{N_{IDs}} B(i,j)}$$

Here N_{IDs} is the number of grain IDs in the microstructure and $B(i,j)$ is an indicator that returns one when the grain boundary exists and zero when it does not. Although not a requirement in the Potts model, the grains are numbered uniquely.

We define three different rules for allowing boundaries to transition to the high mobility complexion. First and most obviously, the "N_0", or "Independent" rule specifies that some fraction of grain boundaries transition to the high mobility, low energy complexion regardless of the state of their neighboring boundaries. This condition ensures that at least some of the grain boundaries are transitioned in the simulation.

The second rule, the "N_1", or "Adjacency" rule, allows grain boundaries that border at least one already transitioned grain boundary to transition. Any boundary connected to an already transitioned grain boundary through a triple line can transition by this rule when selected. The adjacency transition is not a simple "enveloping" step, since the transition can occur for any grain boundary bordering the transitioned boundary by a triple line. This means that any three transitioned boundaries produced by this mechanism do not necessarily have to share one grain. The third and final rule, the "N_2", or "Double Adjacency" rule, allows grain boundaries to transition if they border two transitioned grain boundaries which are themselves adjacent. Schematic representations of these three rules can be seen in Fig. 1, and the requirements set by these rules are expressed mathematically in Table 1.

We stress that each transition made is characterized only by the mechanism that was initially used to transition the boundary. For example, a grain boundary may meet the criteria to perform an adjacency transition, but make an independent transition instead. Thus sometimes, by chance, some grain boundaries that made independent transitions will appear to have made adjacency transitions. In the same way, some grain boundaries that made adjacency transitions will become disconnected from their neighboring transitioned boundaries over time, and appear to have made independent transitions (see Table 2).

The numbers of grain boundaries that can undergo each type of transition to the high mobility grain boundary complexion by a given mechanism, $\{N_I, N_{Adj}, N_{DAdj}\}$, can be calculated in the following manner. Grain boundaries are "sites" for independent transitions when (a) the grain boundary in question exists and (b) the grain boundary has not already transitioned i.e. $Tr(i,j) = 0$ and

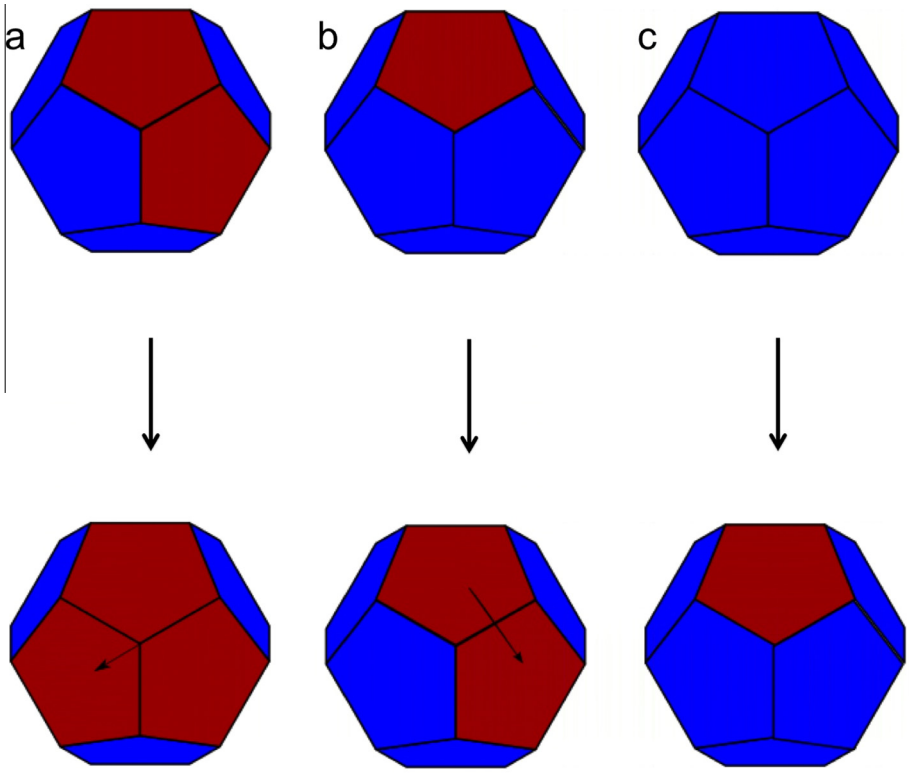

Fig. 1. (a) The "Independent" grain boundary transition, (b) the "Adjacency" grain boundary transition, and (c) the "Double Adjacency" grain boundary transition. Here the blue surfaces represent not transitioned grain boundaries and the red surfaces represent the transitioned grain boundaries. Note that in the case of the adjacency transition, mechanism is not a simple "enveloping" step, as the transition can occur for any grain boundary bordering the transitioned boundary by a triple line. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1
The different grain boundary transitioning mechanisms and their conditions.

Type of transition	Explanation	Transitioning condition
The "N_I" or "Independent" transition	Grain boundary transitions without preferential site	$Tr(i,j) = 0,\ B(i,j) = 1$
The "N_{Adj}" or "Adjacency" transition	Preferential site for grain boundary transition provided by one previously transitioned grain boundary	$Tr(i,j) = 0,\ B(i,j) = 1$ $\sum_k^{NN_j} Tr(i,k) + \sum_l^{NN_i} Tr(j,l) > 0$
The "N_{DAdj}" or "Double Adjacency" transition	Preferential site for grain boundary transition provided by two adjacent, previously existing transitioned grain boundaries	$T(i,j) = 0,\ B(i,j) = 1$ $\sum_k^{NN_j}\sum_l^{NN_j} Tr(i,k) * Tr(i,l) * B(l,k) + \sum_m^{NN_i}\sum_n^{NN_i} Tr(j,m) * Tr(j,n) * B(m,n) > 0$

Table 2
A table showing the expected grain boundary transitioning behavior that will come from different variations in the independent, random branching and percolated transition limits.

Scenario	Expected behavior
$N_0 > N_2 = N_1 = 0$	Only independent transitions appear
$N_1 > N_0 > N_2 = 0$	Independent transitions and adjacency transitions appear
$N_2 > N_1 > N_0 > 0$	Independent transitions, adjacency transitions, and double adjacency transitions appear
$N_2 > N_0 > N_1 = 0$	Independent transitions appear, and double adjacency transitions may appear

$B(i,j) = 1$. Therefore, the number of grain boundaries that can undergo an independent transition, N_I, is:

$$N_I = \sum_I^{N_{IDs}}\sum_j^{N_{IDs}} \frac{(1 - Tr(i,j)) * B(i,j)}{2}$$

We divide the summation by two to prevent grain boundaries from being double counted. Similarly, grain boundaries that are sites for adjacency transitions meet these previous two conditions, but also (c) at least one of the neighboring boundaries is transitioned. This means that the grain boundary shares a triple line with some neighbor of the first grain that has a transitioned boundary with the second grain, or some neighbor of the second grain that has a transitioned boundary with the first grain. These two conditions, of course, are not mutually exclusive. This condition can therefore be expressed mathematically as:

$$\sum_k^{NN_j} Tr(i,k) + \sum_l^{NN_i} Tr(j,l) > 0$$

Applying a summation over all possible grain boundaries and once again dividing by two to prevent double counting, we have N_{Adj}, the number of grain boundaries in our simulation that are sites for adjacency transitions:

$$N_{Adj} = \sum_i^{N_{IDs}}\sum_j^{N_{IDs}} \left(\left[\begin{cases} 1/2, & \sum_k^{NN_j} Tr(i,k) + \sum_l^{NN_i} T(j,l) > 0 \\ 0, & \text{else} \end{cases} \right] * (1 - Tr(i,j)) * B(i,j) \right)$$

Finally, grain boundaries that are sites for double adjacency transitions meet the first two conditions stated, but also (d) two adjacent grain boundaries that are themselves adjacent to each other are both transitioned. These two conditions as well are not mutually exclusive. We can express this statement mathematically as:

$$\sum_{k}^{NN_j}\sum_{l}^{NN_j} Tr(i,k) * Tr(i,l) * B(l,k) + \sum_{m}^{NN_i}\sum_{n}^{NN_i} Tr(j,m) * Tr(j,n) * B(m,n) > 0$$

Once again, we apply a summation and divide by a factor of two to prevent double counting, yielding our expression for N_{DAdj}, the number of grain boundaries in our simulation that are sites for double adjacency transitions.

$$N_{DAdj} = \sum_{i}^{N_{IDs}}\sum_{j}^{N_{IDs}} \left(\begin{bmatrix} 1/2, & \sum_{k}^{NN_j}\sum_{l}^{NN_j} Tr(i,k) * Tr(i,l) * B(l,k) + \sum_{m}^{NN_i}\sum_{ln}^{NN_i} Tr(j,m) * Tr(j,n) * B(m,n) > 0 \\ 0, & \text{else} \end{bmatrix} * (1 - Tr(i,j)) * B(i,j) \right)$$

The number of sites that can be transitioned by each rule on a given step, N_T, is simply the minimum between the preset limit, R, which defines the number of complexion transitions allowed per step, and the number of sites available. Each respective mechanism of transition only occurs when the fraction of transitioned boundaries is below that mechanism's preset limit. These preset limits are put in place to reflect the assumption that most grain boundaries are not transitioned.

$$N_{T,I} = \begin{cases} \min(N_I, R_I), & f_T < N_0 \\ 0, & f_T \geqslant N_0 \end{cases}$$

$$N_{T,Adj} = \begin{cases} \min(N_{Adj}, R_{Adj}), & f_T < N_1 \\ 0, & f_T \geqslant N_1 \end{cases}$$

$$N_{T,DAdj} = \begin{cases} \min(N_{DAdj}, R_{DAdj}), & f_T < N_2 \\ 0, & f_T \geqslant N_2 \end{cases}$$

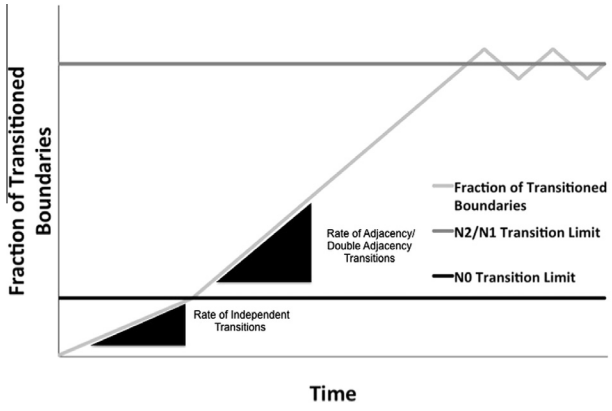

Fig. 2. A plot of the fraction of transitioned boundaries as a function of time during simulations. The model transitions boundaries at a constant rate until the fraction of boundaries transitioned reaches a preset threshold, at which point the model stops transitioning boundaries and some grain boundaries are eliminated. The oscillations at long times indicates that, in the event that the fraction of transitioned boundaries falls below the preset limit, transitions are added at the same rate until the fraction of transitioned boundaries has once again exceeded the threshold.

In each round of transitions, the model first makes independent transitions, then adjacency transitions, and finally double adjacency transitions. An illustration of how the fraction of transitioned boundaries should change with time can therefore be seen in Fig. 2:

Amended with these rules, the Potts model was used with a 100 by 100 by 100 grid with ~2500 grains for 10^7 time steps, transitioning grain boundaries at a rate of $R_I = R_{Adj} = R_{DAdj} = 50$ every 5000 time steps. Although much larger domains are feasible on current computers, this domain size allowed large numbers of configurations to be tested, such that several hundred simulations were performed using different set values of N_0, N_1, and N_2. Among the different variations of the three parameters that can exist, certain combinations were singled out for scrutiny.

The condition $N_0 > N_2 = N_1 = 0$ ensures that only the independent transitions are allowed. In such simulations, no propagation of transitions will occur.

The condition $N_1 > N_0 > N_2 = 0$ ensures that the grain boundaries will only make independent or adjacent transitions. This scenario increases the probability of a given grain boundary transitioning if it borders an already transitioned grain boundary; double adjacency, however, has no effect. The propagation of transitioned boundaries through the microstructure is completely random with adjacency transitions, but transitioned boundaries will be more likely to share a common grain.

The condition $N_2 > N_1 > N_0 > 0$ allows for independent, adjacency, and double adjacency grain boundary transitions. Preferred sites created by the independent and adjacent transitions should provide many sites for double adjacency transitions and grains transitioned in this way will always share a grain with at least two other transitioned boundaries.

Finally, the condition of $N_2 > N_0 > N_1 = 0$ allows for independent and double adjacency transitions, but *disallows* adjacency transitions. In other words, the probability of a grain boundary transitioning increases upon adjacency to two transitioned boundaries that are themselves adjacent, but not upon adjacency to one single transitioned boundary. This means that sites for double adjacency transitions will only appear once two neighboring grain boundaries undergo independent transitions.

For this work, special attention was given to the region of the parameter space in which the total number of independent, adjacency, and double adjacency boundaries consisted of less than 1% of the boundaries because preliminary simulations suggested that this region contained a frontier that, when crossed, AGG goes from being highly unlikely to highly likely. In an effort to determine how the likelihood of AGG changed with the changing parameters and gain insight into what features of a grain may promote AGG besides the formation of grain boundary complexions, an additional three sets of simulations were run: one with a pair of inserted independent transitions allowing for varying fractions of adjacency transitions, one with an independent transition bordering an adjacency transition allowing for varying fractions of double adjacency transitions, and finally one with a varying fraction of independent transitions allowing for a high number of double adjacency transitions.

Each simulation was checked for the presence of abnormal grains at $t = 10^7$, with an abnormal grain being defined as having a volume ten times that of the average grain. Although normal grain size distributions extend out to this multiple of the average size, the criterion was found to correspond well to visual inspection of microstructures. Visual representations of the simulations were collected as each simulation progressed. Visual inspection of a subset of the evolving microstructures confirmed the numerical indications of AGG.

3. Results

Fig. 3 shows the occurrence of AGG in the region in which between 0 and 100 adjacency transitions were allowed (limited to 0.6% of all boundaries in the microstructure) and independent transitions, with a ratio of N_1:N_0 of at most 60. Note that the curves apparent in the figure are a consequence of the controls on transition rates in the code and have no significance per se.

It is obvious from this plot that the occurrence of AGG becomes more likely as more adjacency transitions are allowed in the simulation, and becomes close to certain after around 0.3% of all boundaries (roughly 60 boundaries in the simulation) are allowed to make the adjacency transition. Fig. 4 shows a microstructure from one of these simulations.

Here, an abnormal grain with multiple transitioned boundaries has clearly appeared, which demonstrates that AGG can occur with a simple "random branching" propagation of complexion transition propagation over triple lines, as some grains gain enough transitioned boundaries to grow abnormally simply by chance. Further, AGG can also occur when transitions are only allowed to propagate by the double adjacency rule, as shown in Fig. 5. With enough independent transitions allowed in the simulation, occasionally some of them come into contact, allowing the transitions to propagate by the double adjacency rule. Thus, as with when only adjacency and independent boundary transitions were allowed, some grains gained enough transitioned boundaries to grow abnormally. However, when only independent grain boundary transitions are allowed, abnormal growth does not occur, as Fig. 6 demonstrates.

Results from models propagating transitions from a single independent transition, an independent adjacency junction or randomly touching independent transitions show a clear region where AGG is possible. When only adjacency transitions were allowed to propagate from the independent transition, AGG became close to certain after roughly 0.3% of boundaries (roughly 60 boundaries) were allowed to make adjacency transitions, which can be inferred from Fig. 8 as the cumulative probability of AGG in the set of such simulations becomes roughly linear at this point.

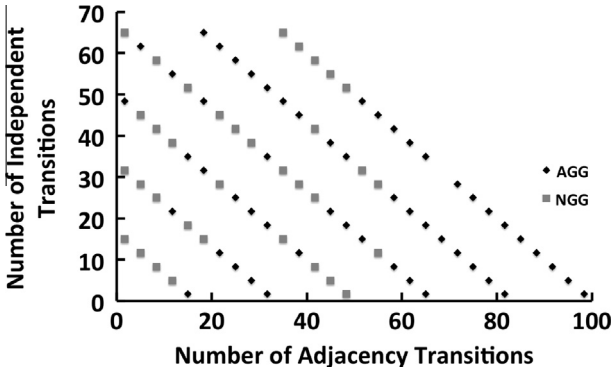

Fig. 3. A plot of the occurrence of AGG with varying numbers of independent transitions and adjacency transitions in a microstructure initially containing 19,629 boundaries.

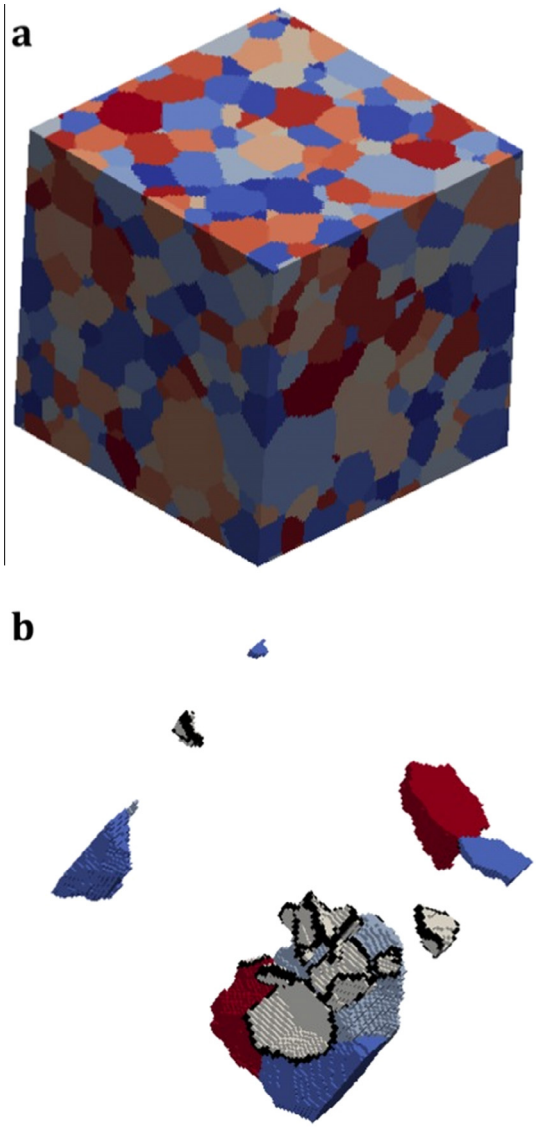

Fig. 4. (a) The microstructure and (b) the transitioned boundaries (filtered for $M > 0.5$) colored white and outlined in black, with abnormal grains in blue, light blue, and red formed from adjacency and independent transitions in the modified Potts model after 10^7 MCS, with $N_0 = 0.0001$ (~3 boundaries), $N_1 = 0.005$ (~85 boundaries), and $N_2 = 0$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 8 shows that, when only double adjacency transitions were allowed to propagate from the independent adjacency junction, the occurrence of AGG became close to certain after a much smaller fraction of boundaries was transitioned – the cumulative probability plot becomes linear with only 0.05% of grain boundaries allowed to transition (~10 boundaries). Further, Fig. 7 shows that when double adjacency transitions were essentially free to occur, but constrained by the presence of randomly touching independent transitions, the cumulative probability of AGG becomes linear after the fraction of transitioned boundaries allowed to occur by independent transitions is roughly 0.1%.

In addition, Fig. 9 shows the fraction of transitioned boundaries on abnormal grains at $t = 10^7$ in three different scenarios. In the first scenario, independent and adjacency transitions occurred, in the second, independent and double adjacency transitions occurred, and in the third all three types of transitions were allowed to occur. Grain boundaries that make double adjacency transitions are guaranteed to share a grain with at least two other

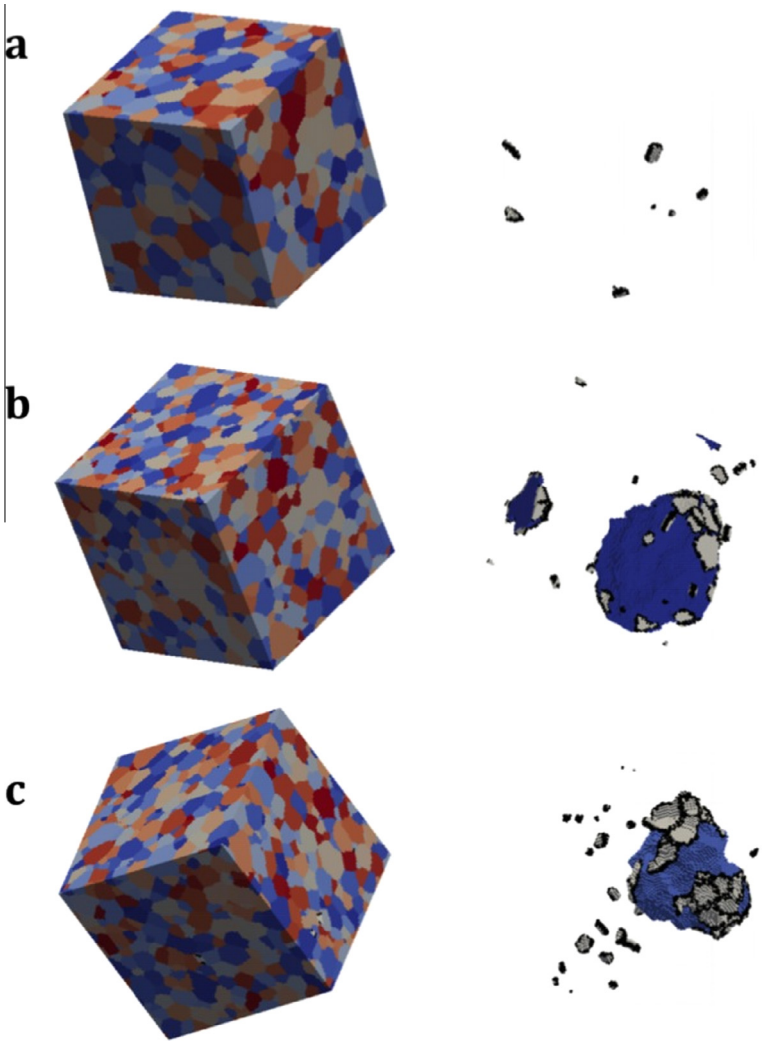

Fig. 5. Grain growth over 10^7 steps for $N_2 = 0.9\%$ and $N_0 = 0.114\%$ after 10^7 steps: (a), $N_2 = 0.9\%$ and $N_0 = 0.276\%$ after $3 * 10^6$ steps; (b) $N_2 = 0.9\%$ and $N_0 = 0.816\%$ after $3 * 10^6$ steps. Resulting microstructures are shown on the left and transitioned grain boundaries in the microstructures are shown on the right (filtered for $M > 0.5$) in white and outlined in black, as well as the present abnormal grains, which are blue. AGG is clear in (b) and (c), with connectivity between transitioned grain boundaries obviously high. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

transitioned grain boundaries, so microstructures experiencing AGG in the first scenario should on average have a smaller fraction of their transitioned boundaries on the abnormal grains themselves than in the third scenario.

The number of abnormal grains was also tracked in these simulations, as well as whether or not abnormal grains appeared to cluster or impinge. "Clustering" of abnormal grains in this case was regarded as a situation in which one abnormal grain forms while in contact with an abnormal neighbor, while simple "impingement" was regarded as two abnormal grains growing into each other. In each of the three scenarios abnormal grains appeared with only one percent of all boundaries transitioned, but scenario three resulted in an over twofold increase in the number of abnormal grains per volume.

4. Discussion

There is a relatively simple probabilistic explanation for why AGG occurs in the simulations where the transitioned boundaries with high mobility are added in clusters and why AGG does not occur when the grain boundary transitions are independent, i.e. spatially correlated. If we assume that the probability of any grain boundary transitioning over a period of time is one percent and that a typical fourteen sided grain needs half of its boundaries to transition to become abnormal, this suggests that the probability of a particular grain growing abnormally is $p = (0.01)^7 = 10^{-14}$. At most only one in a trillion grains could possibly be abnormal and this would never be observed.

However, assuming that a boundary neighboring a transitioned boundary is more likely to transition by a factor of fifty, then the chances of *a grain* accumulating enough transitioned boundaries to grow abnormally is roughly $p = (0.01)(0.5)^6 = 0.000156$. Dillon and Harmer [23] estimate similar abnormal grain number fractions in their observations of AGG in Ca doped alumina, and speculate that the fraction of abnormal grains in a "typical" microstructure is on the order of 1 in 10,000 to 1 in 1,000,000.

We can make simple probabilistic estimates that two transitioned boundaries will share a triple line, the requirement in our simulations for a double adjacency transition, in an analogous fashion to estimating the probability that two individuals in a room share a common birthday. If we assume that grains have on average fourteen grain boundaries [24], then the total number of boundaries in the system is about seven times the number of grains, Q. Each grain boundary (or facet) on average is enclosed by five triple lines, so transitioning one grain boundary in the

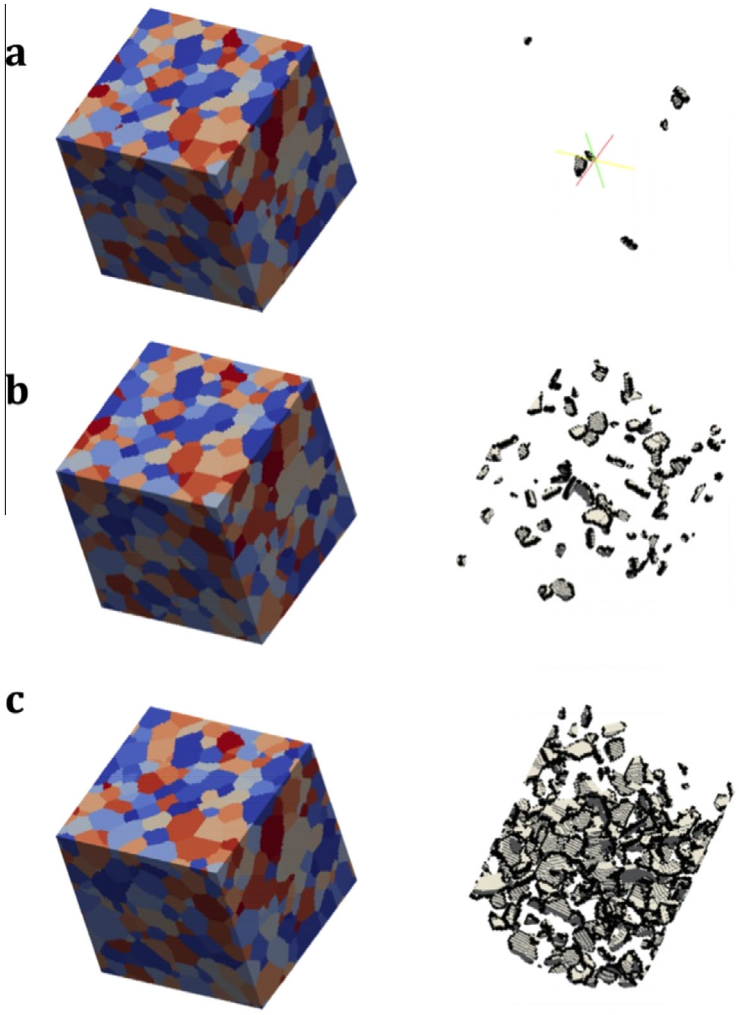

Fig. 6. Grain growth over 10^7 steps for N_0 thresholds of 0.1% (a), 1% (b), and 10% (c) of all grain boundaries, with no N_1 or N_2 transitions allowed. Resulting microstructures are shown on the left and transitioned grain boundaries in the microstructures are shown on the right (filtered for $M > 0.5$) in white, outlined in black. No AGG is present and no isolated clusters of transitioned boundaries are present.

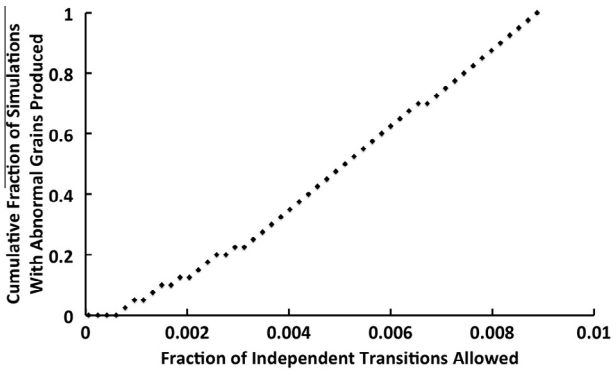

Fig. 7. The cumulative probability of AGG in the set of simulations upon allowing for a set fraction of independent transitions and a set fraction of double adjacency transitions.

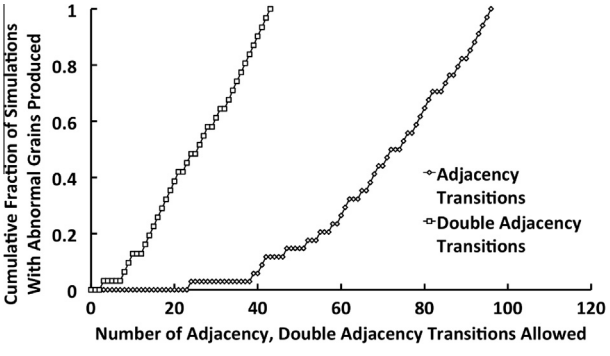

Fig. 8. The cumulative fraction of all simulations performed in which AGG occurred when a set number of adjacency transitions and a set number of double adjacency transitions were allowed to occur. Note that double adjacency transitions result in AGG at substantially smaller fractions.

microstructure means that on average eleven grain boundaries (five neighboring boundaries from each grain, plus the transitioned grain boundary itself) cannot transition in order to avoid forming a double adjacency site. Therefore, the total number of "people" in the room is N_T, the number of transitioned boundaries, the total number of possible "birthdays" is $7Q$, and every additional "person" eliminates eleven birthdays. We can then estimate the probability that at least two transitioned grain boundaries in the system will come into contact as:

$$P_{Site} \approx 1 - \prod_{i=1}^{N_T} \left(1 - \frac{11i}{7Q}\right)$$

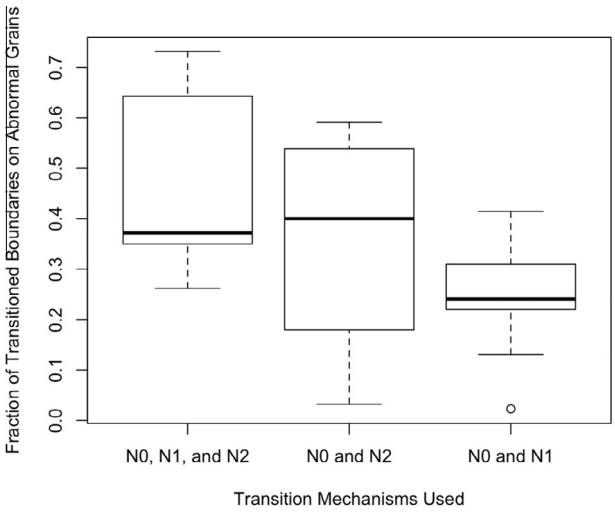

Fig. 9. Box and whisker plots of the fraction of transitioned boundaries on abnormal grains after 10^7 MCS in simulations allowing for either the independent and double adjacency propagation mechanisms, the independent and adjacency propagation mechanisms, or the independent, adjacency, and double adjacency propagation mechanisms. Ten simulations were performed for each combination of transition types.

When $Q = 3000$ (~21,000 grain boundaries) and $N_T = 100$ (~0.5% of all boundaries transitioned), the probability of at least two of these boundaries being in contact, thus creating a double adjacency site is approximately 93%. With less than one in one hundred boundaries in the system transitioned, we can expect at least a few grain boundaries in the system to meet the criteria for making a double adjacency transition, if this type can occur.

Many attempts to model different forms of AGG make some grains "special" either due to an advantageous orientation, high stored energy (in a case of recrystallization), or giving a single particular grain low energy subgrains. For example, Park et al. [20] have demonstrated that a single grain with several low angle subgrains can grow abnormally in the Potts model when a fraction of its grain boundaries are allowed to have low energies, as long as the growth occurs in the presence of particles. Simulations performed by Rollett et al. [9] picked a single grain and gave its boundaries high mobility and low energy, also resulting in AGG. This latter case begs the question of how a given grain can sustain a perimeter with special properties. This only has a simple answer in the case of a subgrain structure with low mosaic spread but an occasional subgrain is sufficiently misoriented with respect to the average that its perimeter is consistently a high angle and therefore high mobility boundary [25–27].

However, there are a number of simulations that do not need to seed the microstructure for AGG to appear. As just mentioned, coarsening of subgrain structures has been modeled by making the grain boundary energy and mobility dependent on grain boundary misorientation and including a cutoff misorientation above which grain boundary mobility and energy both increase [25–27]. The AGG that emerges in this model has been shown to be representative of the apparent nucleation of new grains in primary recrystallization. Kim and Park [28] has shown that AGG can occur in a phase field simulation that includes solute drag via breakaway of boundaries from their pinning atmospheres. No variations in grain boundary mobility or energy anisotropy, variation in texture, particle pinning, or seeded sites of any kind were needed or included. The mechanisms of complexion transition formation and propagation employed in this work are hypothetical, but demonstrate an analogous, seedless mechanism by which AGG can occur.

The results of this work suggest that abnormal grains form because transitioned grain boundaries form clusters within the microstructure, germinating from a small number of transitioned grain boundaries. If this is indeed true, then preventing the most vulnerable grain boundaries from appearing could possibly control AGG. Alternatively, if abnormal grains form because certain high energy grain boundaries changing complexion occasionally come into contact and allow others to transition, keeping these boundaries separated could control AGG.

5. Conclusions

A mesoscale model of grain growth incorporating the selected transition of some grain boundaries to a high mobility complexion has been developed. This model shows that complexion transitions on a subset of grain boundaries to a higher mobility state can lead to abnormal grain growth provided that adjacency is allowed to influence the transition rate. If, however, such transitioned boundaries are randomly dispersed in the microstructure, they are unlikely to initiate abnormal grain growth. The key to obtaining abnormal growth is when the nucleation of transitioned boundaries is stimulated by the presence of an adjacent, already transitioned boundary, so that clusters of transitioned boundaries are formed, resulting in a few abnormally large grains. The results suggest that the nucleation of complexion transitions occurs heterogeneously such that a transition on any given grain boundary increases the probability of a complexion transition on an adjacent boundary so that clusters of transitioned boundaries are created.

Acknowledgment

This work at Carnegie Mellon University was supported by the Office of Naval Research under grant N00014-11-1-0678.

References

[1] S.I. Bae, S. Baik, Sintering and grain growth of ultrapure alumina, J. Mater. Sci. 28 (1997) 4197–4204.
[2] S. Lartigue-Korinek, C. Carry, L. Priester, Multiscale aspects of the influence of yttrium on microstructure, sintering and creep of alumina, J. Eur. Ceram. Soc. 22 (2002) 1525–1541.
[3] J.G. Fisher, S.-Y. Choi, S.-J.L. Kang, Abnormal grain growth in barium titanate doped with alumina, J. Am. Ceram. Soc. 89 (2006) 2206–2212.
[4] M.P. Harmer, S.J. Dillon, Optimizing grain boundary complexions to produce dense pressure-less sintered boron carbide (B_4C), Internal Report to Air Force Office of Scientific Research, 2008.
[5] T. Li, Q. Li, J.Y.H. Fuh, P.C. Yuh, L. Luh, C.C. Wu, Effects of AGG on fracture toughness of tungsten carbide, Mater. Sci. Eng., A 587 (2007) 445–446.
[6] L. Cheng, G.D. Hibbard, Abnormal grain growth via the migration of planar growth interfaces, Mater. Sci. Eng., A 492 (2008) 128–133.
[7] D.L. Worthington, N.A. Pedrazas, P.J. Noell, E.M. Taleff, Dynamic abnormal grain growth in molybdenum, Metall. Mater. Trans. A 44 (2013) 5025–5038.
[8] J. Mizera, J.W. Wyrzykowski, K.J. Kurzydlowski, Description of the kinetics of normal and abnormal grain growth in austenitic stainless steel, Mater. Sci. Eng., A 104 (1988) 157–162.
[9] A.D. Rollett, D.J. Srolovitz, M.P. Anderson, Simulation and theory of abnormal grain growth – Anisotropic grain boundary energies and mobilities, Acta Metall. 37 (1989) 1227–1240.
[10] G.S. Grest, D.J. Srolovitz, M.P. Anderson, A.D. Rollett, Abnormal grain growth in three dimensions, Scr. Metall. Mater. 24 (1990) 661–665.
[11] A.D. Rollett, W.W. Mullins, On the growth of abnormal grains, Scripta Mater. 36 (1997) 975–980.
[12] F.J. Humphreys, Unified theory of recovery, recrystallization and grain growth, based on the stability and growth of cellular microstructures – II. The effect of second phase particles, Acta Mater. 45 (1997) 5031–5039.
[13] S.J. Dillon, M.P. Harmer, Relating grain-boundary complexion to grain-boundary kinetics I: Calcia-doped alumina, J. Am. Ceram. Soc. 91 (2008) 2304–2313.
[14] S.J. Dillon, M. Tang, W.C. Carter, M.P. Harmer, Complexion: a new concept for kinetic engineering in materials science, Acta Mater. 55 (2007) 6208–6218.
[15] P.R. Cantwell, M. Tang, S.J. Dillon, J. Luo, G.S. Rohrer, M.P. Harmer, Grain boundary complexions, Acta Mater. 62 (2014) 1–48.
[16] S.J. Dillon, M.P. Harmer, G.S. Rohrer, The relative energies of normally and abnormally growing grain boundaries in alumina displaying different complexions, J. Am. Ceram. Soc. 93 (2010) 1796–1802.

[17] S.A. Bojarski, J. Knighting, S. Ma, W. Lenthe, M.P. Harmer, G.S. Rohrer, The relationship between grain boundary energy, grain boundary complexion transitions, and grain size in Ca-doped yttria, Mater. Sci. Forum 753 (2013) 87–92.
[18] S.A. Bojarski, S. Ma, W. Lenthe, M.P. Harmer, G.S. Rohrer, Changes in the grain boundary character and energy distributions resulting from a complexion transition in Ca-doped yttria, Metall. Mater. Trans. A 43 (2012) 3532–3538.
[19] P.S. Sahni, G.S. Grest, M.P. Anderson, D.J. Srolovitz, Kinetics of the Q-state Potts model in two dimensions, Phys. Rev. Lett. 50 (1983) 263–266.
[20] C.S. Park, T.W. Na, H.K. Park, B.J. Lee, C.H. Han, N.M. Hwang, Three-dimensional Monte Carlo simulation for the effect of precipitates and sub-boundaries on abnormal grain growth, Scripta Mater. 66 (2013) 398–401.
[21] D. Zöllner, A new point of view to determine the simulation temperature for the Potts model simulation of grain growth, Comput. Mater. Sci. 86 (2014) 99–107.
[22] M.A. Miodownik, K.G.F. Janssens, D. Raabe, E. Kozeschnik, B. Nestler, Computational Materials Engineering, Elsevier Academic Press, 2007.
[23] S.J. Dillon, M.P. Harmer, Demystifying the role of sintering additives with "Complexion", J. Eur. Ceram. Soc. 28 (2008) 1485–1493.
[24] S. Hilgenfeldt, A.M. Kraynik, S.A. Koehler, H.A. Stone, An accurate von Neumann's Law for three-dimensional foams, Phys. Rev. Lett. 86 (2001) 2685–2688.
[25] E.A. Holm, M.A. Miodownik, A.D. Rollett, On abnormal grain growth and the origin of recrystallization nuclei, Acta Mater. 51 (2003) 2701–2716.
[26] E.A. Holm, M.A. Miodownik, K.J. Healy, A subgrain growth model for strain-free grain nucleation during recrystallization, Mater. Sci. Forum 467–470 (2004) 611–616.
[27] S.Y. Wang, E.A. Holm, J. Suni, M.H. Alvi, P.N. Kalu, A.D. Rollett, Modeling the recrystallized grain size in single phase materials, Acta Mater. 59 (2011) 3872–3882.
[28] S.G. Kim, Y.B. Park, Grain boundary segregation, solute drag and abnormal grain growth, Acta Mater. 56 (2008) 3739–3753.