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Mobility driven abnormal grain growth in the presence of particles

E. Fjeldberg[1], E. Holm[2], A.D. Rollett[3] and K.Marthinsen[1]

[1]Norwegian University of of Science and Technology (NTNU), N-7491 Trondheim, Norway.

[2]Sandia National Laboratories, Albuequerque, NM, USA,

[3]Carnegie Mellon University, Pittsburgh, PA, USA.

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Abstract. Simulation of mobility-driven abnormal grain growth in the presence of particles in a 3D Potts Monte Carlo model has been investigated, and even though the driving force in this case is identical to normal grain growth, Zener pinning does not occur. Instead the particles seem merely to have a small inhibiting effect on the number of abnormal grains, and this effect only has a noticeable influence for volume fractions of particles above 5vol%.

Introduction

The preferential or discontinuous evolution of a few grains in a recrystallised polycrystal is termed abnormal grain growth (AGG). Abnormal grain growth is observed in a wide variety of polycrystalline metals and ceramics, and it may or may not be desirable. For example, the abnormal growth of {110} < 001 > Goss-oriented grains in transformer steel improves magnetic permeability and loss properties [1]. In contrast, abnormal growth in copper films used in electronic interconnects causes a bimodal grain size distribution that is detrimental to reliability [2]. The avoidance of abnormal grain growth at high temperature is generally an important aspect of grain size control in steels and nonferrous alloys, e.g. aluminium. Dunn and Walter [3] have reviewed its occurrence in a wide variety of materials.

According to Humphreys [4, 5, 6] abnormal grain growth cannot occur in an "ideal grain assembly" (i.e. a simple single-phase uniform grain structure with constant and isotropic properties). Most assumptions concerning the origin of abnormal grain growth assume some kind of advantage, as a condition for the occurrence of abnormal grain growth. This advantage is most commonly related to size, but can also be related to texture where certain special boundaries experience a higher mobility, or, in the case of thin films, surface effects, (see e.g. [7] and references therein).

It is also well known that second-phase particles can be used to control grain size during normal grain growth [8]. The use of particles to refine grain size is important in e.g. steel making and in the welding of certain metal alloys, including aluminium [9]. However, it is also common knowledge that abnormal grain growth can develop in a matrix pinned by particles when the pinning force somehow is lowered [10, 11].

In spite of a lot of work and many efforts, the general conditions and behaviour of abnormal grain growth is poorly understood. In a recent work Holm et al. [12] used a 2D Potts Monte Carlo model to test whether abnormal subgrain growth (mobility driven) could be a possible nucleation mechanism for recrystallisation. This work was later transferred to 3D simulations [13].

The present work is an extension of these previous papers and is particularly focused on the influence of particles on mobility-driven abnormal grain growth, an aspect which not has previously been investigated. The question we will be discussing here, with no particular reference to nucleation of recrystallisation, is if mobility-driven abnormal (sub-)grain growth can be reduced or inhibited by adding second-phase particles to the microstructure. If this is possible, materials which are weakened due to abnormal grain growth, can get considerably improved by addition of second-phase particles.

Monte Carlo Simulation method

To simulate (sub-)grain evolution a Potts Monte Carlo model, which successfully has been applied to grain growth [14, 15], abnormal grain growth [13, 16] and particle effect problems (Zener pinning) [17], has been used. First a microstructure is mapped onto a 3D discrete lattice by assigning each volume element in the lattice a crystallographic orientation O_i so that all lattice sites within a (sub-)grain have the same orientation. Inert particles are incorporated by assigning clusters of sites a unique, non-changeable index without any crystallographic orientation.

The grain boundaries are represented only implicitly as surfaces separating neighbour elements of unlike orientation, where the misorientation rotation matrix for the subgrain boundary, separating subgrains i and j, are given by $M = O_i O_j^{-1}$. For a cubic material, M corresponds to 24 geometrically equivalent rotation angle/axis pairs. We define the misorientation angle θ_{ij} to be the smallest of these rotation angles, regardless of axis (often called the disorientation angle).

In this model, we wish to limit subgrain orientations to those that appear in the initial subgrain structure, and the microstructure evolves by motion of the subgrain boundaries alone. This subgrain boundary motion is simulated by selecting a random lattice element and choosing a candidate orientation at random from among its neighbour orientations. The change in system energy, ΔE, for reorienting the site to the new orientation is given by

$$E = \frac{\gamma_0}{2} \sum_{i=1}^{N} \sum_{j=1}^{nn} \left(1 - \delta_{S_i S_j}\right) \tag{1}$$

where γ_0 is the grain boundary energy, the first sum is taken over all lattice sites, N, the second sum is taken over the nn nearest neighbours (equal to 26 in a simple cubic three dimensional lattice) of site i and δ_{SiSj} is the Kronecker delta. The reorientation is performed with probability P(_E) given by

$$p(\Delta E) = \begin{cases} p_0 & if\ \Delta E \le 0 \\ p_0 \exp\left(-\dfrac{\Delta E}{k_B T}\right) & if\ \Delta E > 0 \end{cases} \tag{2}$$

where

$$p_0 = \frac{M(\theta_{ij})\gamma_0}{M_m} \tag{3}$$

Here $M(\theta_{ij})$ is the intrinsic mobility of the boundary between subgrains Si and Sj , which has a misorientation angle θ_{ij} between them and Mm is the maximum reduced mobility in the system, thus a reorientation is accepted with a probability proportional to the normalised boundary mobility [18]. The mobility function used is:

$$M(\theta_{ij}) = \begin{cases} 1.0 & \theta_{ij} \ge \theta_m \\ 0.001 & \theta_{ij} < \theta_m \end{cases} \tag{4}$$

where θ_m is a critical misorientation angle defining the mobility for each boundary. The current simulations were performed on a fully periodic, 3D, cubic lattice. The thermal energy term $k_B T$ was set low enough to prevent boundaries from disordering but high enough to minimise lattice pinning, and it is normalised so that all boundaries have the same roughness independent of boundary energy. After each reorientation attempt, the time clock is incremented by 1/N Monte Carlo steps

(MCS). The initial microstructures were constructed by distributing (3x3x3) cubic particles at random until the specific particle volume fraction was reached. To approximate a continuum crystallographic texture, Q = 1000 different, discrete orientations were allowed. A specialised algorithm [19] was used to increase the time efficiency of the simulations. The microstructures were allowed to evolve until a certain maximum number of abnormal grains had been reached, typically 1000 MCS, and numerical data points represent the average of 10 independent simulation runs.

Results and discussion

The simulations were run with a sharp texture most easily described by the misorientation distribution function (MDF) seen in Fig. 1.

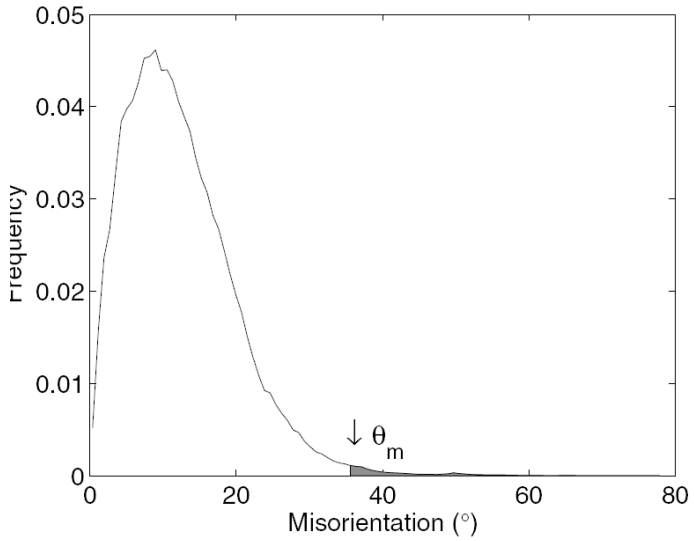


Figure 1 Initial misorientation distribution for the subgrain structures analysed in the text. The plot shows schematically the role of θ_m in determining which boundaries have a high mobility.

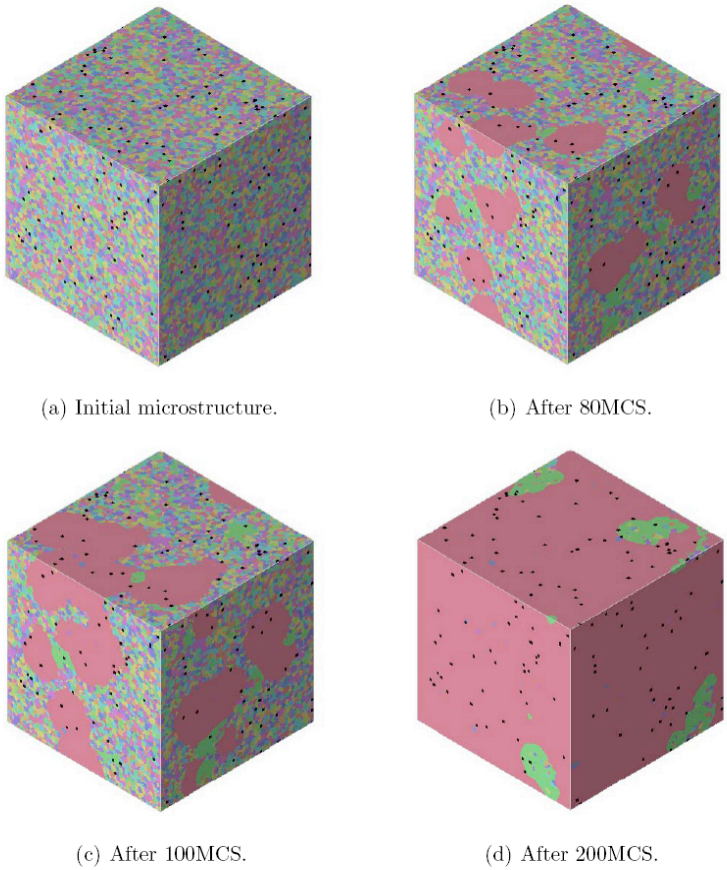
The time evolution of the microstructure for a vol% of particles of 1 and 10 are illustrated in Figs. 2 and 3, respectively. It is clearly seen that we get abnormal grain growth even in the presence of particles, and the abnormal grains grow to a size far larger than the Zener limit, see e.g. [4]. It is also seen that the abnormally growing grains in Fig. 2 (1vol% of particles) develops faster than the abnormally growing grains in Fig. 3 (10 vol% of particles), i.e. an increasing particle fraction clearly leads to a slower development of abnormally growing grains.

The following assumption, based on only running the simulations over shorter times (valid up to 1000MCS), was made to define an abnormal grain: When a grain gets at least 15 times larger than the average initial grain size, it is definned as abnormal.

The simulations were performed on a fully periodic 200x200x200 lattice in the case of $k_BT = 0.5$ and $k_BT = 1.0$, while, because of instabilities, a 100x100x100 lattice was used for $k_BT = 1.5$. The effect of volume fraction of particles f = 0.0; 0.01; 0.02; 0.05 and 0.1 on the time for when the maximum fraction of abnormal grains was reached, was analysed for all simulation temperatures, and compared in Fig. 4. This shows that there is only a small increase in latency time to reach the maximum number of abnormal grains as the particle fraction increases. Actually, for particle fraction of 5vol%, it can be argued that the latency time is constant. At the same time this also clearly shows that $k_BT = 1.0$ is a sufficiently low value for the simulation temperature while it still minimises the lattice pinning.

The frequency of abnormal grains as a function of particle fraction was investigated, and the results are seen in Fig. 5. The figure shows only a small decrease (< 20% decrease) in the frequency of AGG as the particle fraction increases from 0 to 10vol%. Especially the difference between a volume fraction of particles between 0 and 5vol% seem to be extremely small, and an assumption

of no decrease in the AGG frequency within these particle fractions falls well within the standard deviation. However, due to poor statistics and thus large standard deviations for the data in the low particle vol% regime, these data may also be interpreted alternatively. As indicated by the dotted line in Fig. 4, a linear decrease, although weak, may also be assumed between the number fraction of abnormal grains and all vol% of particles.



(a) Initial microstructure. (b) After 80MCS.

(c) After 100MCS. (d) After 200MCS.

Figure 2 The microstructure after different times for the case of 1 vol% of particles.

Summary

Simulation of mobility-driven abnormal grain growth in the presence of particles has been investigated, and even though the driving force in this case is identical to normal grain growth, Zener pinning does not occur. Instead the particles seem to merely have a small inhibiting effect on the number of abnormal grains, and this effect only has a noticeable inuence for volume fractions of particles above 5vol%. This means Zener pinning is not operative since the static particles do not inhibit the abnormal grain growth in these initially unpinned microstructures.

Also, since this effect is so small, the material will still contain a considerable amount of abnormal grains, i.e. adding particles will not inhibit abnormal grain growth only reduce the number of abnormal grains and delay their growth.

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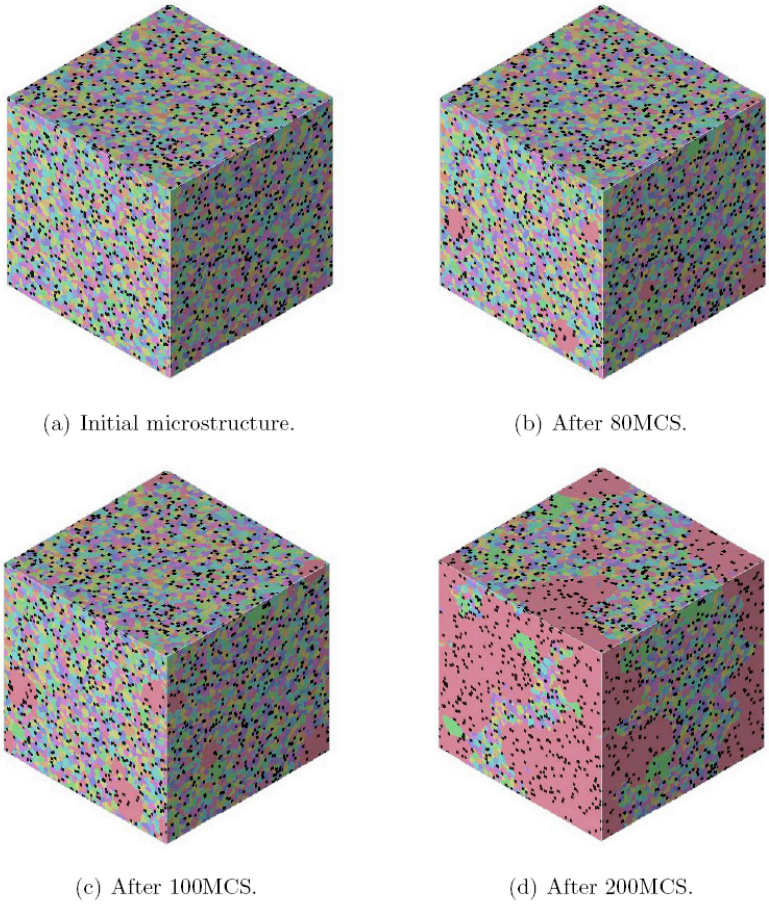

(a) Initial microstructure. (b) After 80MCS.

(c) After 100MCS. (d) After 200MCS.

Figure 3 The microstructure after different times for the case of 10 vol% of particles.

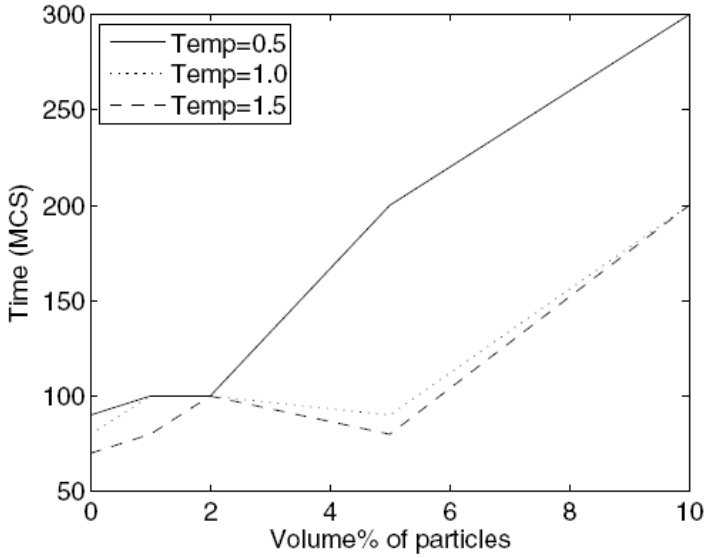

Figure 4 The time when the maximum number fraction of abnormal grains is reached as a function of the vol% of particles.

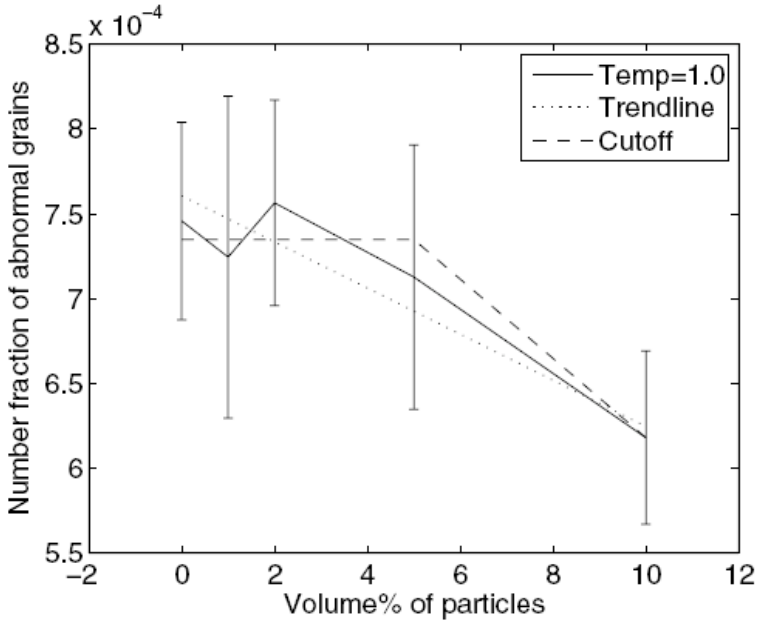

Figure 5 Number fraction of abnormal grains versus the vol% of particles together with the standard deviation. Two interpretations of the data at low vol% of particles are indicated. Dotted line: Linear trend; dashed line: Cutoff in number fraction below 5vol%.

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