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ScienceDirect

Acta Materialia 67 (2014) 134–144

Acta MATERIALIA

www.elsevier.com/locate/actamat

A phase-field model for grain growth with trijunction drag

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Received 19 September 2013; received in revised form 5 December 2013; accepted 7 December 2013

Abstract

A phase-field model has been developed to study the effect of triple junction (TJ) mobility on 2-D grain growth kinetics. The method captures the results of past work such as a linear increase in the average grain size with time, but can also follow the transition from TJ-limited to grain boundary energy-limited growth. The distribution of grain boundary curvature is examined. In the low TJ mobility simulations the distribution has a peak at zero curvature and approaches the grain boundary mobility-limited steady-state distribution at larger sizes. Even for extremely low TJ mobility, a small fraction of the grain boundary length has non-zero curvature and thus a lack of self-similarity is observed for all TJ-limited simulations, even when the average size is increasing linearly in time. We find that the topology of the grain structure is independent of the degree of TJ drag, within the range of parameters employed in the simulation. The effects of TJ mobility increase as the grain size decreases, suggesting that TJ mobility can play a significant role in nanocrystalline grain growth kinetics.

Keywords: Grain growth; Triple junction drag; Computer simulation

1. Introduction

Grain growth and coarsening occur in many polycrystalline materials in order to reduce the interfacial free energy of the system. Especially during high-temperature processing and operation, the grain growth rate can be significant and can greatly affect properties such as yield strength.

Triple junctions (TJs), the line formed by the intersection of three grains, play an important role in grain growth kinetics due to their energy [1], mobility [2], impurity affinity [3] and larger volume fraction for small-grained materials [4]. TJs can thus also significantly affect properties, e.g. creep via enhanced diffusivity [5–7] or electrochemical corrosivity via enhanced electron mobility along triple lines [8]. In small-grained materials, there may be many competing mechanisms and driving forces that affect grain growth. However, it has been shown theoretically that TJs are more effective at "dragging" the growth rate of nanocrystalline grains, relative to vacancies, particles and impurities [9].

TJs are often assumed to have large mobility relative to the grain boundaries and thus move with the grain boundaries in order to maintain the TJ equilibrium angles [10]. However, as grain size decreases and approaches the nanoscale, the influence of TJs relative to grain boundaries increases [11–14]. In particular, TJs can have low mobility in small grains or at low temperatures and can significantly affect grain boundary curvatures, TJ angles and the overall kinetics [15,2,16–23].

As the TJ mobility approaches zero, the grain boundary curvatures approach zero and the driving force for grain growth becomes the deviation of the TJ angles from their equilibrium values. Tricrystal experiments have shown that the TJ angles deviate from equilibrium as the temperature decreases, suggesting that kinetics are grain boundary mobility limited at high temperatures and TJ mobility limited at low temperatures [2,16,20]. This temperature

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1359-6454/$36.00
http://dx.doi.org/10.1016/j.actamat.2013.12.012

dependence of Zn tricrystals and bicrystals was shown to exhibit Arrhenius behavior, with TJs having a larger activation energy [16]. Furthermore, it has been proposed that low TJ mobility results in linear growth kinetics, i.e. $\langle D\rangle \sim t$ where $\langle D\rangle$ is the average grain size [15,2,16]. Such kinetics have been observed in nanocrystalline Fe [24,25] and molecular dynamics simulations of nanocrystalline Ni [26].

Importantly, TJ mobility has a larger effect for smaller grains, suggesting that nanocrystalline grain growth kinetics is largely determined by TJ mobility. Thus it is essential to understand TJ mobility in order to understand nanocrystalline grain growth kinetics as well as to design and build robust nanocrystalline materials. In particular, accurately modeling TJ mobility is important for predicting the effect of TJs on grain growth and grain stabilization in nanocrystalline materials [27,2]. Molecular dynamics [28,19], network [22], virtual vertex [29,23] and Potts [30] models have been used to model TJ drag, demonstrating results mostly consistent with theory and experiment. The vertex models and Potts models have observed linear kinetics, as well as a widening of the grain size distribution and a lack of self-similarity during TJ mobility-limited grain growth.

The phase-field model, however, has the advantage of smooth interfaces, no need to explicitly track trijunctions, and the ability to incorporate any number of conserved and non-conserved parameters such as impurity concentration [31,32]. Because impurities have been seen to preferentially segregate to triple lines, it is important to study TJs using a model that can incorporate long-range diffusion. Thus, this model is the first step to combining the effects of diffusion- and TJ-limited grain growth.

2. Theory

2.1. Triple junction mobility

An analytical theory for the simplest TJ geometry – seen in – was developed by Gottstein and Shvindlerman to calculate the TJ velocity, mobility and angle [2,18,15]. The shape of the grain boundary $y(x)$ for the $n < 6$ geometry is given by:

$$y(x) = \xi \arccos\left[e^{-\frac{x}{\xi}+c_1}\right] + c_2 \tag{1}$$

where $\xi = \frac{a}{2\theta_a}$, $c_1 = \ln(\sin\theta_a)$, $c_2 = -\xi\left(\frac{\pi}{2} - \theta_a\right)$, and n is the number sides of the grain. There are only two degrees of freedom: if the grain size, a, and the dihedral angle, $2\theta_a$, are known, then the grain boundary (GB) shape can be uniquely determined.

For grains with fewer than six sides, the TJ angles inside the grain are less than their equilibrium values and the grain shrinks (middle grain in Fig. 1(a)). In this system with isotropic grain boundary energies, the TJ velocity is:

$$V_{TJ} = m_{TJ}\sigma(2\cos\theta_a - 1) \tag{2}$$

where V_{TJ} is the TJ velocity, m_{TJ} is the TJ mobility, and σ is the grain boundary energy.

By requiring that the TJ velocity be equal to the grain boundary velocity in the x-direction, the mobility parameter, Λ, can be defined:

$$\Lambda = \frac{m_{TJ}a}{m_{GB}} = \frac{2\theta_a}{2\cos\theta_a - 1} \tag{3}$$

where m_{TJ} and m_{GB} are the TJ and GB mobilities. Λ is dimensionless and for a given system describes the relative importance of TJ and grain boundary mobilities. For large m_{TJ} (grain boundary-limited kinetics), Λ is large and the denominator on the right side of Eq. (3) approaches zero and thus θ_a approaches the equilibrium isotropic value of 60°. For small m_{TJ} (TJ-limited kinetics), Λ approaches zero and θ_a approaches zero, and the TJ velocity is dictated by Eq. (2). Decreasing the grain size, a, decreases Λ as well as the TJ angle, and so TJs play a larger role for small grains. Furthermore, by simply measuring the angle and grain size in such a system, the relative TJ and grain boundary mobilities can be determined. A similar analysis can be done for $n > 6$; see Refs. [2,15,18].

For polycrystalline systems, Λ', described by Eq. (4), is used to measure the overall effect of TJs [33,34]:

$$\Lambda' = \frac{m_{TJ}\langle D\rangle}{2m_{GB}} \tag{4}$$

where $\langle D\rangle$ is the average grain size, or effective grain diameter. In polycrystals, the grain growth kinetics is typically described by:

$$\langle D\rangle \sim kt^n \tag{5}$$

where k is a rate constant, and n is the grain growth exponent. Theoretically, growth limited by grain boundary curvature has a growth exponent of 1/2. In two dimensions, Gottstein and Shvindlerman proposed that grain growth can be described by Eq. (6), which consists of a grain boundary term and a TJ term [35,13].

$$\frac{1}{m_{GB}\sigma}\left(\langle D\rangle^2 - \langle D_o\rangle^2\right) + \frac{1}{m_{TJ}\sigma}\left(\langle D\rangle - \langle D_o\rangle\right) = t \tag{6}$$

For small grains, the linear TJ term dominates and $\langle D\rangle \sim t$; the growth exponent is 1. For large grains, the parabolic grain boundary term dominates and $\langle D\rangle \sim \sqrt{t}$; the growth exponent is 1/2. Thus, for small grains the growth is driven by TJ angles, and for large grains it is driven by GB curvature.

Gottstein and Shvindlermann developed equations for the rate of area change of individual grains, comparable to the Von Neumann–Mullins equation, but with TJ mobility taken into account:

$$\frac{dA}{dt}(n) = \frac{m_{GB}\sigma\pi}{3(1+1/\Lambda)}\left(n\frac{6+\sqrt{3}\Lambda}{2+\sqrt{3}\Lambda} - 6\right), \quad n < 6 \tag{7a}$$

$$\frac{dA}{dt}(n) = \frac{m_{GB}\sigma\pi}{3(1+1/\Lambda)}\left(n\left(1 - \frac{6}{\pi\Lambda B}\right) - 6\right), \quad n > 6 \tag{7b}$$