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Scripta Materialia 54 (2006) 993–997
Scripta MATERIALIA
www.actamat-journals.com

Grain boundary engineering with particles

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Received 17 May 2005; received in revised form 29 July 2005; accepted 21 November 2005
Available online 22 December 2005

Abstract

This paper analyses a number of good candidate mechanisms for grain boundary engineering using particles, such as particle coherency, anisotropic boundary energy and boundary mobility mechanisms. The paper speculates on why these grain boundary engineering mechanisms are rarely observed in experiment and assesses the potential for computer modelling to elucidate the phenomenon further.

Keywords: Zener pinning; Grain growth; Abnormal grain growth; Grain boundary energy

1. Introduction

Second phase particles are employed to control many aspects of microstructure. They are used to control nucleation rate and texture evolution during recrystallisation of metal alloys; to influence grain growth and grain boundary sliding in metal alloys and ceramics; and to determine texture via abnormal grain growth in nickel, iron-silicon and many other alloys. However, there has been very little focus on the use of second phase particles to control the character of grain boundaries; in other words, the use of particles for grain boundary engineering. Whether this is due to lack of mechanism or to a lack of experimentation is the focus of this paper.

The character of a grain boundary enters the physics of the particle–boundaries interactions in the form of the boundary energies. Consider a boundary interacting with a single particle as shown in Fig. 1 which depicts a migrating grain boundary with a radius of curvature, ρ, interacting with a spherical particle of radius, r. It is evident that there are three surface tensions to consider, the boundary surface tension, γ, and the two particle/boundary surface tensions, γ_{AP} and γ_{BP}. These surface tensions dictate the equilibrium shape of the boundary near the particle, which is a catenoid of revolution often called a dimple. This shape determines the pinning force which is given by the expression:

$$F = 2\pi r\gamma \sin\theta \cos(\pi/2 - \alpha + \theta) \tag{1}$$

where θ is the bypass angle and $\gamma_{AP} - \gamma_{BP} = \gamma\cos\alpha$. When the particle is incoherent $\gamma_{AP} = \gamma_{AP}$ the force can be calculated as a simple function of the dimple shape:

$$F(y_0) = 2\pi r\gamma \sin\theta \cos\theta \tag{2}$$

where y_0 is the size of the dimple (see Fig. 1). When a grain boundary interacts with a large number of particles the pinning stress on the boundary is a sum of the forces exerted by each particle and so depends on the position of each particle relative to the boundary. A method to sum the contributions of these relative positions for a boundary migrating through a random array of particles was developed by Hellman and Hillert [1]. A boundary moving through an array of particles is considered to be a multi-dimpled entity, see Fig. 2(a). All particles trailing the mean position of the boundary (reference sphere) exert a pinning force on the boundary. If there are N_v particles per unit volume, they will exert a pinning stress:

$$\sigma_z = N_v \int_0^{y_{\max}} F(y_0)\,\mathrm{d}y_0 \tag{3}$$

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1359-6462/$ - see front matter
doi:10.1016/j.scriptamat.2005.11.040

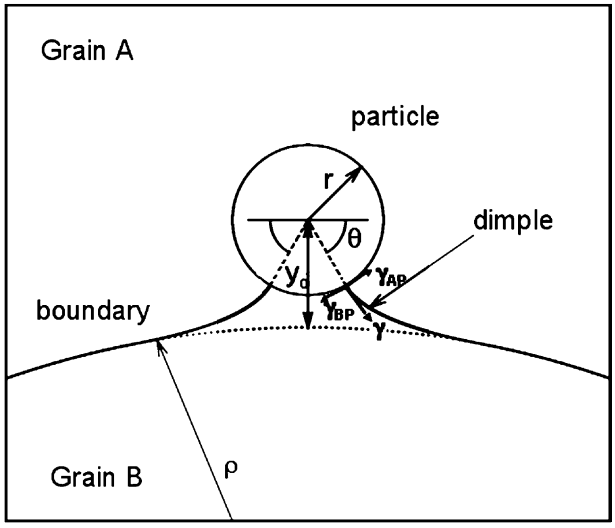

Fig. 1. A schematic of the formation of a dimple during grain boundary bypass of a particle. r is radius of the particle, ρ is the radius of boundary curvature, θ is the boundary bypass angle, the boundary surface tension is γ, the two particle/boundary surface tensions are γ_{AP} and γ_{BP}, and y_0 is the distance of the boundary from the particle center.

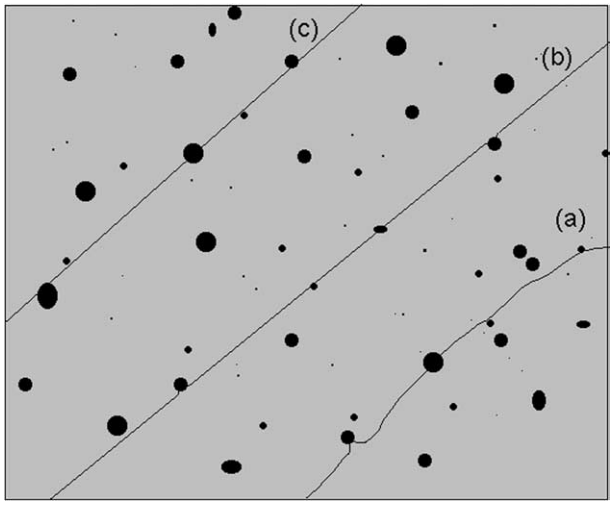

Fig. 2. Boundaries migrating in a particle array: (a) a curved isotropic boundary which assumes a multi-dimpled shape; (b) a faceted boundary in which dimple formation is repressed due to the anisotropic nature of the surface tension; (c) an idealised flat boundary which does not form dimples.

where y_{max} is the maximum size of a dimple. However, this represents an overestimate of the pinning stress since it takes no account of the fact that particles in front of the boundary, whose centers lie within r of the mean position of the boundary tend to pull the boundary forward. The value of σ_z can be corrected by adjusting the integral limits in Eq. (3), by assuming that the effects of the particles in front and behind the boundary, whose centers lie within r of the boundary exactly cancel out. The net pinning stress is therefore due to particles whose centers lie further than r from the boundary. Louat [2] reevaluated Eq. (3) with r as the lower limit of the integral yielding a value for the pinning stress:

$$\sigma_z = \frac{3\beta f \gamma}{4r} \tag{4}$$

where f is the volume fraction of particles, $\beta = 1$ is a function of ρ/r [3]. By equating this pinning stress with the driving stress for grain growth, $F_d = \gamma/R$, we can derive the Zener–Smith expression for the grain size of a pinned microstructure [4,5]:

$$R_z = \frac{4r}{3\beta f} \tag{5}$$

What this shows, from a grain boundary engineering perspective, is that the pinned grain size is independent of the character of the pinned boundary. Although the surface tension of the boundary, γ, appears in the functional form of both the driving stress and pinning stress, γ cancels. However, we have only dealt with the incoherent, isotropic case, we will consider coherent and anisotropic cases next.

2. Particle coherency effects

When a particle is coherent with a matrix phase then α will not equal $\pi/2$ in Eq. (1) and so the pinning force will be increased to a maximum of $2F(y_0)$ when $\theta = 0$ and $\alpha = 0$. The origin of this increased pinning force is the increased boundary energy that is required to replace a coherent boundary with a incoherent one. This coherency effect has been shown to have a direct result on the orientation of particles, which rotate in response to the torque of this pinning force [6]. From a grain boundary engineering perspective there is a possibility that boundaries of certain types can be frozen into the microstructure by a thermomechanical treatment that would cause particles decorating target boundaries to rotate into coherency with one of the matrix grains.

The driving force for rotation of a particle within a matrix grain, F_{rot}, can be estimated using a Gibbs–Thompson expression:

$$F_{rot} \approx \frac{\Delta\gamma \cdot \Omega}{r^2} \tag{6}$$

where $\Delta\gamma$ is the change in boundary energy, r is the particle radius and Ω is the atomic volume. Using $v = mF$:

$$v \approx \frac{D}{kT}\frac{\Delta\gamma \cdot \Omega}{r^2} \tag{7}$$

where v is the average velocity and $m = D/kT$ is the rotation mobility. Assuming $v = r/t$:

$$t_{rot} \approx \frac{kTr^3}{D\Delta\gamma\Omega} \tag{8}$$

This derivation shows the strong r^3 dependence on the kinetics of rotation.

Harris et al. [7] have observed a similar phenomenon, grain rotation in polycrystals. They analysed the mecha-