Available online at www.sciencedirect.com
ScienceDirect
Acta Materialia 59 (2011) 955–961
Acta MATERIALIA
www.elsevier.com/locate/actamat

On the analytical solution for self-similar grain size distributions in two dimensions

C.S. Pande, K.P. Cooper *

Naval Research Laboratory, Washington, DC 20375, USA

Received 22 April 2010; received in revised form 17 September 2010; accepted 10 October 2010
Available online 11 November 2010

Abstract

In a recent publication an analytical solution of the Fokker–Planck continuity equation for the grain size distribution for two-dimensional grain growth in the long time limit (self-similar state) was provided. It used von Neumann–Mullins law and the results of Rios and Glicksman, but was based on a stochastic formulation first proposed by Pande. In this paper this analytical solution is compared with experimental and computer simulation distributions. It is found that grain size distribution, as obtained by simulations of two-dimensional grain growth, although in agreement with our analytical results, may in fact differ from experimentally obtained grain size distributions in thin films. It is also shown mathematically that in the two limiting cases the general solution is reduced to the Hillert or Rayleigh distributions.
Published by Elsevier Ltd. on behalf of Acta Materialia Inc.

Keywords: Grain size distribution; Grain growth; Stochastic model

1. Introduction

Grain growth is a well-known phenomenon in the evolution of crystalline microstructures, resulting in an increase in average grain size with time. This happens by the motion of grain boundaries and the gradual disappearance of the smallest grains during annealing treatment. Grain growth under the usual circumstances is known to approach a quasi-stationary (self-similar) distribution of grain sizes after a transient period. For a review of this see Atkinson [1]. In a recent publication [2] a size-based continuum stochastic formulation was presented based on topological considerations. As expected, that analysis led to a Fokker–Planck equation for the size distribution, which can yield a unique self-similar asymptotic state that could be reached from any arbitrary initial state. The Fokker–Planck equation was obtained using a stochastic formulation first proposed by Pande [3] and employing von Neumann–Mullins law and the results of Rios and Glicksman [4]. We also showed that the boundary conditions are sufficient to determine the "strength" of the diffusion term D in terms of the parameters already determined by Rios and Glicksman [4]. The approximate analytical solution of the Fokker–Planck equation presented in Pande and Cooper [2] was limited to two dimensions and was based on the assumption of quasi-stationary distributions reached in the long time limit. This is so-called normal grain growth, when only the scale varies with some power of time, the grain size distribution remaining self-similar. The mathematical expression for grain size distribution thus obtained has, in principle, no adjustable parameters.

In this paper the analytical solution is compared with experimental and simulated distributions. The grain size distributions obtained by computer simulation agree well with our analytically obtained distribution. However, in some cases there appears to be a discrepancy between our approximate analytical results and the experimental results. The reasons for this discrepancy are discussed. In addition, the approximate analytical solution is further considered to show mathematically that in the two limiting cases for one

* Corresponding author. Tel.: +1 202 767 0181.
E-mail address: khershed.cooper@nrl.navy.mil (K.P. Cooper).

1359-6454/$36.00 Published by Elsevier Ltd. on behalf of Acta Materialia Inc.
doi:10.1016/j.actamat.2010.10.019

of the constants the general solution is reduced to a Hillert or a Rayleigh distribution [1,2] (see Appendix A).

2. Analytical formulation

For the sake of completeness a brief summary of the analytical formulation is given below. For full details see Pande and Cooper [2].

von Neumann [5] and Mullins [6] showed that the growth rate of an individual grain, dC/dt, growing under the influence of its curvature-driven motion, is given by the expression

$$\frac{dC}{dt} = M(n-6), \tag{1}$$

where C is the area of an n-sided grain and M is a constant. A relation between n and C is needed in order to obtain a grain size distribution from this relation.

The first attempt to relate grain radius R or grain area C and n was made by Hillert [7], who gave a comprehensive and consistent theoretical treatment of grain growth in both two and three dimensions. Using heuristics, he argued that

$$n \cong k\frac{R}{\overline{R}}, \tag{2}$$

where k is a constant and $\overline{R}$ is the mean of the grain size distribution.

Eq. (2) leads to an equation for $F(R, t)$ in the mean field model:

$$\frac{\partial F(R,t)}{\partial t} = \frac{\partial}{\partial R}\left[\left(\frac{A}{R} - \frac{B}{\overline{R}}\right)F(R,t)\right], \tag{3}$$

where A and B are constants. Surprisingly, predictions from this equation are in serious disagreement with the experimental results. In Pande and Cooper [2] we showed why models based on a mean field approach cannot explain many properties of grain growth observed experimentally, no matter what form of growth rate is assumed. Hence, there is a need for a new approach, namely a stochastic treatment [3,8–11].

Mathematically, a stochastic process in its simplest form is described by a function of two variables, one of which is time, and involves both a deterministic term and a random term. Specifically, in this treatment relation (2) is retained, except that it is noted that it is a statistical relation and not an exact one.

The stochastic continuity or Fokker–Planck equation in this case is given by:

$$\frac{\partial F(R,t)}{\partial t} = \frac{\partial}{\partial R}\left[\left(\frac{A}{R} - \frac{B}{\overline{R}}\right)F(R,t)\right] + D\frac{\partial F^2(R,t)}{\partial R^2}, \tag{4}$$

where A, B and D are arbitrary constants yet to be determined. On comparison with the mean field continuity Eq. (3) it is seen that it has an additional term, called the diffusion term. The magnitude of the diffusion term could, however, be small. As a first approximation we took D to be constant, independent of time and grain size.

The constant A is a material parameter that can be determined as shown in Rios and Glicksman [4]. The other two constants, B and D, can be determined exactly from boundary conditions, as shown in Sections 3 and 4. So, in principle, there are no adjustable constants in our model.

The continuity equation (Eq. (4)) can be recast as an ordinary differential equation by imposing the experimental observation of self-similarity of the grain size distribution. We assume that all grain sizes are accessible and that the total area (mass) of the polycrystalline system is conserved and finite. Appropriate boundary conditions for the size distribution $F(R, t)$ may thus be written as:

$$F(0,t) = F(\infty,t) = 0. \tag{5}$$

The area (mass) conservation requirement can be expressed in integral form as:

$$\int_0^\infty R^2 F(R,t)dR = \text{constant}. \tag{6}$$

From the self-similarity condition of the grain size distribution, the spatial and temporal components of $F(R, t)$ can be separated [20] so that it can be expressed as:

$$F(R,t) = t^{-3/2} f(x), \tag{7}$$

where $x \equiv R/\bar{R}(t)$ and $f(x)$ is the grain size distribution for the scaled variable x. Here $\bar{R}$ is defined as the mean (first moment) of the distribution, and it can be shown to vary with time as [1]:

$$\overline{R} = 2\lambda t^{1/2} \tag{8}$$

where λ is a constant. The shape of the renormalized grain size distribution is time invariant, but the scale factor $\bar{R}$ increases as the square root of annealing time.

Using Eqs. (7) and (8), Eq. (4) can be rewritten as:

$$D\frac{d^2 f(x)}{\partial x^2} + \left[\frac{A}{x} - B + 2x\right]\frac{df(x)}{dx} + \left[6 - \frac{A}{x^2}\right]f(x) = 0. \tag{9}$$

Let

$$\varepsilon = D/\lambda^2, \tag{10}$$

and

$$\alpha = B/\lambda^2, \tag{11}$$

and A/λ^2 can be shown to be equal to $\alpha + \varepsilon$ [2].

Eq. (9) is then rescaled as:

$$\varepsilon\frac{d^2 f(x)}{dx^2} + \left[\frac{\alpha+\varepsilon}{x} - \alpha + 2x\right]\frac{df(x)}{dx} + \left[6 - \frac{\alpha+\varepsilon}{x^2}\right]f(x) = 0 \tag{12}$$

The solution to Eq. (12) must also satisfy the constraint condition given by Eqs. (5) and (6). An approximate analytical solution of this equation was given in Pande and Cooper [2]. Eq. (12) can be solved exactly for two limiting cases where the driving force is either due only to diffusion (Rayleigh) or to the drift velocity (Hillert).

In the first limiting case [11] the Rayleigh grain size distribution occurs when $\alpha = 0$ and $\varepsilon \neq 0$. This means that all