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ASYMPTOTIC BEHAVIOR IN GRAIN GROWTH

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ABSTRACT

Hillert's model of grain growth consists of a drift term in size space that leads asymptotically to a distribution function and a growth exponent not often observed. Later theories introduce a diffusion term that is either assumed to dominate the drift term or a correction to it. This paper shows that the lower order drift term alone determines asymptotic grain growth behavior. A possible conclusion is that experimental results may need to be reinterpreted.

1. INTRODUCTION

Grain growth is the process by which the average size of grains in a polycrystalline material increases. Unlike computer models, which simulate the detailed behavior of individual grains, analytic theories for grain growth generally take a statistical approach based on the continuity equation

$$\frac{\partial f}{\partial t} = -\frac{\partial j}{\partial R}, \quad (1)$$

where f is the distribution function for grains of size R at time t and j is the current in size space. Grains are assumed to be equiaxed, so that R is the radius of a sphere having equal volume, and parameters such as the number of sides of a grain are ignored. A "model" for grain growth consists of writing down an expression for j .

Hillert [1] started with the assumption that the boundary between two grains will migrate with a velocity proportional to its curvature. Additional assumptions about the behavior of grains in a mean field led to the expression

$$j_{\text{Hillert}} = v f$$
$$v = M_0 \left(\frac{1}{R_*} - \frac{1}{R} \right), \quad (2)$$

with v the drift velocity in size space and R_* a time-dependent critical radius. Since the current has no other terms, this is known as a drift theory. Hillert was able to show asymptotically that the distribution function becomes self-similar when plotted in terms of the reduced variable R/R_* and that R_* grew as $t^{1/2}$. Unfortunately, experimental results do not generally support his predictions. Measured distributions tend to be broader with a gentler cutoff at the large grain sizes, and the fitted growth exponents show a spread between 1/4 and 1/2 [2].

Louat [3] has developed a theory in which curvature plays no role. He contends that grain growth occurs through the random motion of grain boundaries and introduces a diffusive current

$$j_{\text{Louat}} = -D_0 \frac{\partial f}{\partial R}. \quad (3)$$

Even though his model has been shown to violate volume conservation [4], Louat paved the way for modification of Hillert's theory. Hunderi and Ryum [5], for example, have suggested that grain growth contains elements of both deterministic drift and random walk. This paper considers the asymptotic behavior of Hillert's model with a diffusional correction:

$$j = j_{\text{Hillert}} + j_{\text{diffusion}}. \quad (4)$$

Since Louat's diffusion current is inadmissible, the question remains of what form the diffusive term should take.

2. DERIVATION OF THE DIFFUSION TERM

2.1 Grain growth as a discrete process

Analytic theories of grain growth usually classify grains in terms of the size R , but we are free to change this variable to any function of R . In the case of three-dimensional grain growth, for example, using the number of atoms k in a grain to replace R is just as valid if not more natural. There is, however, one essential difference between the two representations: R is a continuous variable, whereas k is discrete. We shall see shortly that treating grain growth as random walk in a discrete space actually determines the form of the diffusion current when continuum approximation of the rate equation is taken.

Given an assembly of grains, let us construct the distribution function H_k , the number of grains with k atoms. Since grains always shrink or grow by the exchange of atoms, we can model growth with transitions between bins (Fig. 1). In the general case, that of biased random walk, the forward and backward transition coefficients are not the same, the difference of which leads to a non-zero drift velocity [6]. Here we are concerned with unbiased random walk, for which the forward and backward coefficients are equal. Calling the transition rate $\mu_k H_k$, where μ_k is the transition coefficient, and taking into account the flux from neighboring bins, we obtain the rate equation for the population at bin k

$$\frac{dH_k}{dt} = \mu_{k-1}H_{k-1} - 2\mu_k H_k + \mu_{k+1}H_{k+1} \quad (5)$$

2.2 Continuum approximation

In order to obtain a partial differential equation, let us replace k by a continuous variable V ,

$$\begin{aligned} V &= \varepsilon k \\ \varepsilon &= \text{volume of one atom,} \end{aligned} \quad (6)$$

representing the volume of a grain, and introduce continuous distribution function h and diffusion coefficient D :

$$\begin{aligned} h(V, t) &= \frac{H_k(t)}{\varepsilon} \\ D(V) &= \varepsilon^2 \mu_k. \end{aligned} \quad (7)$$

Substituting these functions into the rate equation and performing a Taylor expansion for all terms, we obtain an infinite order partial differential equation [7], which, to leading order in ε , is just the diffusion equation

$$\frac{\partial h}{\partial t} = \frac{\partial^2}{\partial V^2}(Dh). \quad (8)$$

Since Hillert's flux is always written in terms of R , we should transform this equation to the same coordinate system. It can be shown [7] that the general result for grain growth in n dimensions is the diffusion equation

Fig. 1 The distribution function H_k is the number of grains having k atoms. The arrows represent the shrinking or growing of k -atom grains.

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial R} \left(\frac{1}{R^{n-1}} \frac{\partial}{\partial R} \left[\frac{D}{R^{n-1}} f \right] \right), \quad (9)$$

which implies that the correction to Hillert's current in equation (4) should take the form

$$j_{diffusion} = \frac{1}{R^{n-1}} \frac{\partial}{\partial R} \left(\frac{D}{R^{n-1}} f \right). \quad (10)$$

Mulheran and Harding [8] have given a physically motivated theory for the diffusion coefficient D . They argue that D must scale with the number of atoms on the surface of a grain

$$D = D_0 R^{n-1}. \quad (11)$$

We will use this diffusion coefficient in the following section.

3. ASYMPTOTIC ANALYSIS

We are now ready to consider the behavior of the full rate equation

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial R} \left(M_0 \left[\frac{1}{R} - \frac{1}{R_*} \right] f \right) + \frac{\partial}{\partial R} \left(\frac{1}{R^{n-1}} \frac{\partial}{\partial R} \left[\frac{D}{R^{n-1}} f \right] \right). \quad (12)$$

While the following dimensional analysis is not rigorous, a more detailed argument leads to the same result [7]: Taking Mulheran and Harding's choice for D , we see that the terms in equation (12) have dimensions

$$\frac{1}{t} \sim \frac{1}{R^2} + \frac{1}{R^{n+1}}. \quad (13)$$

Since the average size increases with time, the diffusion term will eventually become negligible relative to the drift term for $n = 2$ or 3 . This shows that asymptotically the solution of the enhanced equation is identical to Hillert's.

4. DISCUSSION

Given that Hillert's predictions do not agree with experimental results and that his asymptotic solution is unchanged by a diffusional correction, we can perhaps conclude that Hillert's theory requires major revision. Alternately, we could argue that the *interpretation* of experimental results needs further consideration. This viewpoint can be made defensible by looking at the variation of the average grain size with time.

Using simple dimensional analysis once again, we can assert that at some short time when the average size is sufficiently small, the diffusion term actually dominates the drift term. In this limit the average size must be growing like $t^{1/(n+1)}$, in contrast with the asymptotic limit when it varies as $t^{1/2}$. There must exist a transition zone during which the exponent increases smoothly between the values $1/(n+1)$ and $1/2$ (Fig. 2). Because the decay toward steady state is governed by a power law rather than by an exponential, the transient regime may be considerable. If an experiment is not carried out for a sufficiently long time, it is possible to mistake the transient for the steady state. This is of course only one explanation for the scatter of growth exponents observed experimentally.

Fig. 2. Schematic variation of the average grain size with time. The slope of the plot gives the growth exponent, which varies smoothly through the transition zone between the values $1/(n+1)$ and $1/2$.

5. CONCLUSION

We have shown that adding a diffusion term to Hillert's theory of grain growth has no effect on the asymptotic solution. However, the transient solution now contains a transition zone governed by slow power law decay. Unless an experiment is followed for a sufficiently long time, it is possible to mistake the transient regime for the steady state.

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