Acta Materialia 115 (2016) 442–447

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

A new treatment of transient grain growth

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ARTICLE INFO

Article history:
Received 27 January 2016
Received in revised form
10 May 2016
Accepted 10 May 2016
Available online 18 June 2016

Keywords:
Grain size distribution
Grain growth
Growth kinetics
Thermodynamic modelling
Numerical solution of integro-differential equations

ABSTRACT

The grain radius R distribution function $f(R,t)$ with $R_c(t)$ as critical grain radius is formulated, inspired by the Hillert self-similar solution concept, as product of $1/R_c^4$ and of a shape function $g(\rho,t)$ as function of the dimension-free radius $\rho = R/R_c$ and time t, contrarily to the Hillert self-similar solution concept with time-independent $g(\rho)$. The evolution equations for $R_c(t)$ as well as for $g(\rho,t)$ are derived, guaranteeing that the total volume of grains remains constant. The solution of the resulting integro-differential equations for $R_c(t)$ and $g(\rho,t)$ is performed by standard numerical tools. Remarkable advantages of this semi-analytical concept are: (i) the concept is a deterministic one, (ii) its computational treatment is very efficient and (iii) the shape function $g(\rho,t)$ remains localized in a fixed interval of ρ. The shape function $g(\rho,t)$ evolves towards the well-known Hillert self-similar distribution, which is demonstrated for two initial shape functions (one of them is triangular). Also a study on "nearly" self-similar distribution functions proposed as useful approximations of experimental data is presented.

1. Introduction

Spontaneous processes as grain growth, and recently also grain refinement, are still a topic of research, especially with respect to the methods treating these phenomena. Two basic thermodynamic concepts exist to describe the evolution of ensemble of grains,

(i) the distinct grain concept working with individual grains approximated by circles or polygons in 2D and by spheres or polyhedrons in 3D;
(ii) the grain size or radius distribution concept working with size or radii distribution functions for grains approximated as in (i).

As tools applied to the treatment of the distinct grain concepts the cellular automaton approach [1] and its combination with Monte Carlo [2] and Monte Carlo Potts [3] simulations, the level-set method [4], the phase field method [5,6] and the Thermodynamic Extremal Principle (TEP) [7] can be mentioned. An immediate advantage of the TEP is that it is applicable to both a/m concepts, for the TEP see the overview [8]. This has become possible by formulating Onsager's and Ziegler's extremal principles in terms of discrete parameters characterizing the state of the system, the so-called "characteristic parameters", see [9,10].

This paper is now devoted to show a new approach within the grain radius distribution concept. The first key assumption is the formulation of the distribution function in the dimension-free variable $\rho = R/R_c$ with R being the effective radius of a grain and R_c the so-called critical radius, for details see the next section. The second key assumption is the mathematical structure of the distribution function $f(R,t)$ (with t being the time) as

$$f(R,t) = \frac{1}{R_c^4(t)} g(\rho,t), \quad (1)$$

where $g(\rho,t)$ is a dimension-free shape function. In a previous distribution concept [11] it was assumed that the dependence on time t is only implicit due to the time dependence of the set of parameters $\mathbf{p}(t)$ characterizing the shape function $g(\rho,\mathbf{p}(t))$. Going back to the seminal works by Hillert five decades ago, see [12] and the later overview [13], Hillert introduced $g(\rho)$ as time-independent version of $g(\rho,t)$. The shape function $g(\rho)$ results from the self-similar solution of the Hillert evolution equations for individual grains derived from mean field approach (note that ρ is equivalent to u and $g(\rho)$ to $P(u)$ in the Hillert notation). For sake of completeness it should be mentioned that as dimension-free

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http://dx.doi.org/10.1016/j.actamat.2016.05.020
1359-6454/

variable also R/a instead of R/R_c with a being a parameter different to R_c, has been applied, see [14,15].

Let us now consider that the function g depends explicitly on time t as a second variable, i.e. $g = g(\rho, t)$. The goal of this paper is formulating and solving the evolution equations for $R_c(t)$ and $g(\rho, t)$ for transient grain growth taking into account that the volume of the grain ensemble is kept constant.

2. A short overview on the distribution concept for grain growth

Let us shortly repeat the features of a distribution function $f(R, t)$. We introduce two material properties, the specific grain boundary energy γ and the grain boundary mobility M, see Sun and Deng [16] for quantification of M. The time derivative is denoted by a dot. One understands with $\mathrm{d}N = f(R, t)\mathrm{d}R$ the number of grains with their radius R from the interval $\langle R, R + \mathrm{d}R\rangle$. The total number of grains N follows then as

$$N(t) = \int_0^\infty f\left(\tilde{R}, t\right)\, \mathrm{d}\tilde{R} \tag{2}$$

and its rate $\dot{N}$ as

$$\dot{N}(t) = \int_0^\infty \frac{\partial f}{\partial t}\mathrm{d}\tilde{R}. \tag{3}$$

The evolution equation for the grain radius R reads as

$$\dot{R} = \alpha\left(\frac{1}{R_c} - \frac{1}{R}\right),\ \alpha = 2\gamma M. \tag{4}$$

This equation has also been derived rigorously by the TEP in [7]. Obviously small (subscritical) grains ($R < R_c$) shrink and large (supercritical) grains ($R > R_c$) grow. The critical radius R_c can be calculated by using the condition that the volume V of all the grains must remain as a constant quantity, i.e., $\dot{V} = 0$. Since $\mathrm{d}N = f(R, t)\mathrm{d}R$ grains, see above, cover the volume $\mathrm{d}V = 4\pi/3\cdot R^3\mathrm{d}N$, their volume changes as $\mathrm{d}\dot{V} = 4\pi R^2\dot{R}\mathrm{d}N$. Note also that the total number of grains N changes only by disappearance of grains with $R \to 0$, which, however, does not contribute to the rate of the total volume $\dot{V}$, as the volume of disappearing grains is zero. Inserting of Eq. (4) in $\mathrm{d}\dot{V}$ and performing the integration $\int \mathrm{d}\dot{V} = \dot{V} = 0$ yield

$$R_c(t) = \int_0^\infty \tilde{R}^2 f\left(\tilde{R}, t\right)\mathrm{d}\tilde{R} \Bigg/ \int_0^\infty \tilde{R} f\left(\tilde{R}, t\right)\mathrm{d}\tilde{R}. \tag{5}$$

Furthermore, we introduce $\overline{R}$ as the radius corresponding to a grain with the average grain volume

$$\overline{R}(t) = \left(\int_0^\infty \tilde{R}^3 f\left(\tilde{R}, t\right)\mathrm{d}\tilde{R}\Big/N\right)^{1/3}. \tag{6}$$

The distribution function $f(R, t)$ is subjected in the R, t-space to the so-called continuity equation, for details see, e.g. [11,14,15], reading as

$$\frac{\partial f}{\partial t} + \frac{\partial\left(f\dot{R}\right)}{\partial R} = 0. \tag{7}$$

Keep in mind that R is considered in Eq. (7) as the R-coordinate in the R, t-space and that the rate $\dot{R}$ represents the rate of the grain radius given e.g. by Eq. (4). The integration of Eq. (7) with respect to R in the interval $\langle A, B\rangle$ yields

$$\int_A^B \frac{\partial f}{\partial t}\, \mathrm{d}\tilde{R} = \left(f\dot{R}\right)\Big|_{R=A} - \left(f\dot{R}\right)\Big|_{R=B}. \tag{8}$$

For $A = 0$ and $B \to \infty$ with $f|_{R\to\infty} = 0$ for $\dot{R}\big|_{R\to\infty}$ as a finite quantity, the rate $\dot{N}$, Eq. (3), can be calculated with Eq. (8) as

$$\dot{N} = \int_0^\infty \frac{\partial f}{\partial t}\mathrm{d}\tilde{R} = \left(f\dot{R}\right)\Big|_{R=0}. \tag{9}$$

For $R \to 0$ Eq. (4) provides the rate of the grain radius as $\dot{R} = -\alpha/R$ and its insertion into Eq. (9) leads to $\dot{N} = -\alpha f/R$. Since $\dot{N}$ is supposed to be a finite quantity, f/R must assume an indeterminate form with $f = 0$ for $R = 0$. L'Hopital's rule yields $\dot{N} = -\alpha\partial f/\partial R$ for $R \to 0$.

A question may arise, what about a distribution function with $f \neq 0$ for $R \to 0$. In this case $\dot{N} = -\alpha f/R$ tends to infinity, which means that small grains with $R \to 0$ suddenly disappear and f obtains immediately the value zero. Thus, it makes not much sense to assume nonzero values of f for $R \to 0$.

For $A = 0$ and $B = R$ the combination of Eqs. (8) and (9) provides

$$\int_0^R \frac{\partial f}{\partial t}\mathrm{d}\tilde{R} = -\left(f\dot{R}\right)\Big|_R + \dot{N}. \tag{10}$$

Inserting Eq. (4) into Eq. (7) (or in differentiated form of Eq. (10)) provides the evolution equation for f as

$$\frac{\partial f}{\partial t} = -\frac{\partial\left(f\dot{R}\right)}{\partial R} = -\alpha\frac{\partial\left(f\left(\frac{1}{R_c} - \frac{1}{R}\right)\right)}{\partial R}. \tag{11}$$

Note that Eq. (11) does not include $\dot{N}$, since $\dot{N}$ is independent of R and, see Eq. (3), disappears in differentiated form of Eq. (10). Finally, Eq. (11), completed with Eq. (5), can be solved numerically by accounting for the boundary conditions $f = 0$ at $R = 0$ and $R \to \infty$. As solution concept a finite difference scheme in R and the Euler integration scheme for t can be used. For grain growth the value of $\dot{N}$ is given from the solution of Eq. (11) by $\dot{N} = -\alpha\partial f/\partial R$ and cannot be imposed to the system as an external parameter.

3. Evolution of critical radius $R_c(t)$ and shape function $g(\rho, t)$

3.1. Evolution of R_c

The rate $\dot{R}_c$ is calculated from Eq. (5) as derivative of R_c with respect to t as

$$\dot{R}_c = \frac{\int_0^\infty \tilde{R}^2\frac{\partial f}{\partial t}\mathrm{d}\tilde{R}\cdot\int_0^\infty \tilde{R}f\mathrm{d}\tilde{R} - \int_0^\infty \tilde{R}\frac{\partial f}{\partial t}\mathrm{d}\tilde{R}\cdot\int_0^\infty \tilde{R}^2 f\mathrm{d}\tilde{R}}{\left(\int_0^\infty \tilde{R}f\mathrm{d}\tilde{R}\right)^2}. \tag{12}$$

Utilizing Eq. (1) and keeping in mind that the total volume V,

$$V = \int_0^\infty \tilde{R}^3 f\left(\tilde{R}, t\right)\mathrm{d}\tilde{R} = \int_0^\infty \tilde{\rho}^3 g(\tilde{\rho}, t)\ \mathrm{d}\tilde{\rho}, \tag{13}$$

is constant and obtains a finite value, it follows that $\rho^n g \to 0$ for $\rho \to \infty$ and $0 \le n \le 3$. Moreover, with $g = 0$ for $\rho = 0$ integration per parts and using Eq. (11) allow calculating