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Materials

Derivation of Hillert-type 3D grain growth rate model with topological considerations and discussion on its grain size parameter

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Abstract: A Hillert-type three-dimensional grain growth rate model was derived through the grain topology-size correlation model, combined with a topology-dependent grain growth rate equation in three dimensions. It shows clearly that the Hillert-type 3D grain growth rate model may also be described with topology considerations of microstructure. The size parameter bearing in the model is further discussed both according to the derived model and in another approach with the aid of quantitative relationship between the grain size and the integral mean curvature over grain surface. Both approaches successfully demonstrate that, if the concerned grains can be well approximated by a space-filling convex polyhedra in shape, the grain size parameter bearing in the Hillert-type 3D grain growth model should be a parameter proportional to the mean grain tangent radius.

Key words: 3D grain growth; theoretic model; topology; grain size parameter

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1 Introduction

By adapting the "LSW" (Lifshitz-Slyozov-Wagner) theory of particle coarsening and based on the assumption that the grain boundary velocity is inversely proportional to its radius of curvature, Hillert [1,2] established his classical "mean field theory" of two- and three- dimensional grain growth (2DGG and 3DGG). However, the physical definition of the " grain size" in the model was not clearly specified, though many different definitions for "grain size" are possible for real polycrystals [3,4].

In the present work, according to above-mentioned Hillert's original assumption and the quantitative relationship of the average mean curvature over grain boundary with grain size, the grain size parameter in the classical 3DGG theory is first assumed as the mean tangent radius other than the size parameters used conventionally. A derivation of the 3DGG rate equation again gives the same conclusion. The physical definitions of other parameters bearing in the model are also discussed.

2 Discussion on the grain size parameter directly based on Hillert's original assumption

The original Hillert basic rate equation (equation (6) in reference [1]) for the growth rate of grains of size R is written as

$$dR/dt = \alpha M\sigma \cdot (R_{cr}^{-1} - R^{-1}) \quad (1)$$

where $\alpha \cong 1$ for three-dimensional grain growth, σ is the specific grain boundary energy, M may be regarded as the mobility of the grain boundary, while R_{cr} is the critical grain size defined as that below which grains shrink and above which grains grow.

In generating equation (1), a central problem is to find the value of $(\rho_1^{-1} + \rho_2^{-1})$ averaged over the surface of a grain or all the grains of each size R, where ρ_1 and ρ_2 are the principal radii of curvature [1]. To avoid to solve the related complex geometric problem in a rigorous way, Hillert simply chose the assumption that the $(\rho_1^{-1} + \rho_2^{-1})_{average}$ is proportional to $(R_{cr}^{-1} - R^{-1})$, stating that the final justification for the choice may have to await further tests of the predicted characteristics of grain growth [1], leaving the exact definition of "grain size" un-specified.

It is known that the local mean surface curvature, H, at a given point on a surface can be defined as the average of the principal curvatures:

$$H=(\rho_1^{-1}+\rho_2^{-1})/2 \quad (2)$$

Thus, the value of $(\rho_1^{-1} + \rho_2^{-1})/2$ averaged over the

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surface of a grain or the average mean curvature of grain faces would be:

$$(\rho_1^{-1}+\rho_2^{-1})_{average}/2=<H>=K_m/\iint dS \quad (3)$$

where

$$K_m=\iint H dS \quad (4)$$

is the integral mean curvature over the surface [5]. For a group of grains with the same size R, $(\rho_1^{-1}+\rho_2^{-1})_{average}$ should be the corresponding value averaged over the grain faces of all the concerned grains.

It has been already demonstrated that the three-dimensional grains may be well approximated as convex polyhedra [6]. For convex polyhedra [7,8],

$$K_m=2\pi<D_t> \quad (5)$$

where $<D_t>$ is the mean tangent diameter (the mean distance between parallel tangent planes). Thus, it is clearly shown by equations (2)-(5) that the value of $(\rho_1^{-1} + \rho_2^{-1})_{average}$ in Hillert's 3DGG theory is directly proportional to the mean tangent radius.

3 Derivation of the Hillert-type rate equation and defining its grain size parameter

No derivation of Hillert's basic growth rate equation was given in reference [1]. An attempt of such a derivation is given below based on some of our previous results [4,6,9].

First, a relationship between the growth kinetics and the topology of individual grains in three dimensions was established [9] based on the following widely accepted assumptions: the structure results from the interaction between the equilibrium angles of grain junction and the inescapable topology; grain growth results from the curvature-driven grain boundary motion only; no texture effects are considered.

The relationship so established theoretically depicts that the changing rate of the grain surface area is linearly related to the number of grain faces [9]:

$$dS/dt=kM\sigma\cdot(F-F_{cr}) \quad (6)$$

where dS/dt is the changing rate of the total surface area S of an individual F-faced grain during three-dimensional normal grain growth process; $k\cong1.1026$, M and σ denote the mobility of triple grain edges and the specific energy of grain edges, respectively. F_{cr} is the critical number of grain faces, defined as the number of faces below which grains shrink and above which grains grow. It is theoretically found that F_{cr} should be the number of faces per grain averaged over all the grains in the polycrystal considered, approaching to a constant value of 13.3973 when the equilibrium angles of grain junction have been reached.

A modified Monte Carlo Potts simulation algorithm [10] was used to simulate the 3DGG process appropriately so that equation (6) can be tested. The following experimental relationship was obtained by fitting the data of 300 individual grains in simulation using the least square method [9]:

$$dS/dt=0.09\cdot(F-12.95) \quad (7)$$

with a correlation coefficient of 0.92. The data used to equation (7) were measured in each 25 Monte-Carlo-Step interval within the time scope of 10-1200 Monte-Carlo-Steps, when the average number of faces per grain F increases within the ranges of 10.8-13.3. On the other hand, the simulated 3DGG process obeys the grain growth power law kinetics with its growth exponent approaching 0.5, and quantitatively agrees well with the experimental observations of topological evolution during the 3DGG process in real polycrystalline materials found in the literature. Thus, the Monte Carlo Potts simulation results strongly support the validity of theoretical relationship given by equation (6).

On the other hand, based on equation (5) exactly valid for convex polyhedra, the DeHoff-Liu linear model of grain topology-size relationship in three dimensions predicts [4,6]:

$$F=2+(<F>-2)\cdot(D_t/<D_t>) \quad (8)$$

where $<F>$ and $< D_t >$ are respectively the number of faces and the mean tangent diameter averaged over all the grains, F and D_t are respectively the number of faces and the mean tangent diameter of grains of a given size. Such relation exists only possible in statistical sense for the structure as a whole, and the experimental data from real materials agree well with this relationship [4].

Inserting equation (8) into equation (6) and taking $F_{cr} = <F>$, $R_{t,cr} = <R_t>$ as first approximation, one finally obtains

$$dR_t/dt = [(<F>-2)/2\eta]\cdot kM\sigma\cdot(R_{t,cr}^{-1}-R_t^{-1})$$

or simply,

$$dR_t/dt = \alpha M\sigma\cdot(R_{t,cr}^{-1}-R_t^{-1}) \quad (9)$$

where the grain shape factor η is introduced by assuming that $S=\eta(R_t)^2$.

Obviously, equation (9) is exactly the same as equation (1) in form, except for its variable and constant parameters are more clearly specified in their physical meanings.

4 Further discussion on parameters in the Hillert-type grain growth rate model

4.1 Grain size parameter

The mean grain tangent radius is defined rigorously as

$R_t = D_t/2$

With

$$D_t=\frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} D_t(\theta,\varphi)\sin\varphi \mathrm{d}\theta \mathrm{d}\varphi \quad (10)$$

where $D_t(\theta,\varphi)$ is the distance between parallel tangent planes in a particular orientation (θ,φ) of the grain considered, so that D_t is the value averaged over all the possible spatial orientations. When the grain is a perfect sphere, D_t would have the same value as the conventional sphere- (or volume-) equivalent diameter, $D_e=(6V/\pi)^{1/3}$, where V is the grain volume.

For non-spherical grains, however, the exact experimental determination of D_t is much more difficult than that of D_e, if it is not completely impossible. Almost no experimental data of D_t for real and simulated grains available in literature except for our pervious reports [4,6,11]. This earlier experimental work was limited in one-direction measurement of D_t and found that $\langle D_t\rangle \cong 1.38\langle D_e\rangle$ for the aggregate consisting of 1215 austenite grains in a low carbon steel sample [4].

Fortunately, computer simulation of 3DGG makes multi-direction determination of D_t of a large number of 3D grains possible. Based on the data of D_t averaged over three mutually perpendicular directions for each grain in a recent 400^3 lattice grain growth simulation [11], it has been demonstrated that D_t almost linearly related with D_e for individual equiaxed grains, and that $\langle D_t\rangle \cong 1.16\langle D_e\rangle$ for 6 simulated aggregates in quasi-steady stage of 3DGG, respectively consisting of 9997, 9004, 8040, 7057, 6048, and 4998 grains with their $\langle F\rangle$ values varying within a range of 13.87~13.91.

If such kind of D_t-D_e near-proportionality relationship found in the above-mentioned simulation work also exists in real materials, the Hillert-type 3D grain growth equations would be valid for both the mean grain tangent radius and the conventional sphere- (or volume-) equivalent grain radius [12]. Otherwise, the grain size parameter in the model would be better considered as the mean grain tangent radius.

4.2 The parameter α

According to equations (6) and (9), $\alpha = [(\langle F\rangle - 2)/2\eta]\cdot k$, with k being a dimensionless constant close to unity. The value of $\langle F\rangle$ is the same for all the grains in a given polycrystal, while increasing monotonically during normal grain growth [9,13,14], and approaching to its theoretical asymptotical value.

Also, α depends on the grain shape through the shape factor η. Taking the $\eta=4\pi$ for ideal sphere and $\langle F\rangle=13.3973$, one obtains that $2\alpha \cong 2.8493\pi^{-1}\cdot 1.1026 \cong 1.0000$, *i.e.* in this case α is half value of that given for 3DGG by Hillert [1].

The shape factor η varies from grain to grain but probably not far from 4π for essentially equiaxed grains in real materials. On the other hand, $\langle F\rangle$ may be much smaller than the theoretical asymptotical value at early stages of 3DGG process. Its smallest experimental value found in literature so far was about 7.5, then α may become as low as 1/6.

Based on above analysis, α depends not only on the shape of grain(s) of a given size, but also on the global topological characteristics of the polycrystal in which the 3DGG process takes place.

5 Conclusions

(1) Hillert's original assumption that the $(\rho_1^{-1} + \rho_2^{-1})_{average}$ is proportional to $(R_{cr}^{-1}-R^{-1})$ has been justified with the aid of quantitative relationship between the grain size and the integral mean curvature over grain surface, assuming that the grains can be well approximated by space-filling convex polyhedra.

(2) The 3DGG rate model of Hillert's classical type can be derived by combining the grain topology-size model proposed by R.T. DeHoff and Guoquan Liu, with the 3D topology-dependent grain growth rate equation proposed by Guoquan Liu and his coworkers. It means that Hillert-type 3D grain growth rate model may also be described with topology considerations of the concerned microstructure.

(3) Consequently, the grain size in Hillert's classical 3DGG rate model should be a size parameter directly proportional to the mean grain tangent radius (D_t) or simply this size parameter itself. In this case, the "constant" α in the model depends not only on the shape of the grains considered, but also on the global topological characteristics of the polycrystal in which the 3DGG process takes place.

(4) If D_t is proportional to D_e of the concerned grains, however, Hillert-type 3D grain growth equations would be valid for both the mean grain tangent radius and the conventional sphere- (or volume-) equivalent radius (D_e).

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