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# MICROSTRUCTURE DESCRIPTION FROM THE DIFFERENTIAL AVRAMI FORMULATION

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**Abstract.** A model of microstructural evolution, based only on the original assumptions of the Kolmogorov, Johnson & Mehl, and Avrami model of nucleation and growth kinetics, is presented. It is based on the computation of the average grain size of all grains born at the same time along the transformation, neglecting the dispersion of the grain size around this value. The model is computationally simple and inexpensive, and gives a good description of the grain size distribution along the transformation as well as all its distinctive features.

## 1. INTRODUCTION

Nucleation and growth phase transformations are widely found in Materials Science. The description of the size distribution of the emerging phase is of large interest, as its macroscopic properties are in most cases determined by its microstructure.

Previous works on the subject were based on the definition of an effective radius and allowed to obtain discrete [1] and continuous [2] formulations that allow to compute the grain size distribution along the transformation provided that the kinetic parameters (nucleation and growth rates) are known. These models were checked against Monte Carlo simulations giving excellent results. However, both models are mathematically complex, and its numerical computation is far of being simple. Being a subject of application in the analysis of experimental data, a simpler model would be welcome, even at the price of losing some accuracy in the results. Here we present an extremely simple model, based solely in the assumptions of the Kolmogorov [3], Johnson & Mehl [4], and Avrami [5] model of nucleation and growth kinetics, that allows to compute a good approximation to the grain size distribution along a transformation.

## 2. MODEL

The evolution of the emerging phase in nucleation and growth transformations was described by Kolmogorov, Johnson & Mehl, and Avrami in terms of the transformed - $x(t)$ - and extended - $\tilde{x}(t)$ - volume fractions, through the equation

$$\frac{dx}{d\tilde{x}} = 1 - x(t) \tag{1}$$

whose validity has been checked by Monte Carlo simulations [6]. Being a phase transformation a kinetic process, the proper form of Eq. (1) must include the time dependence, that is

$$dx(t) = [1 - x(t)]d\tilde{x}(t). \tag{2}$$

In order to give a description of the developed microstucture, we will focus our attention on the

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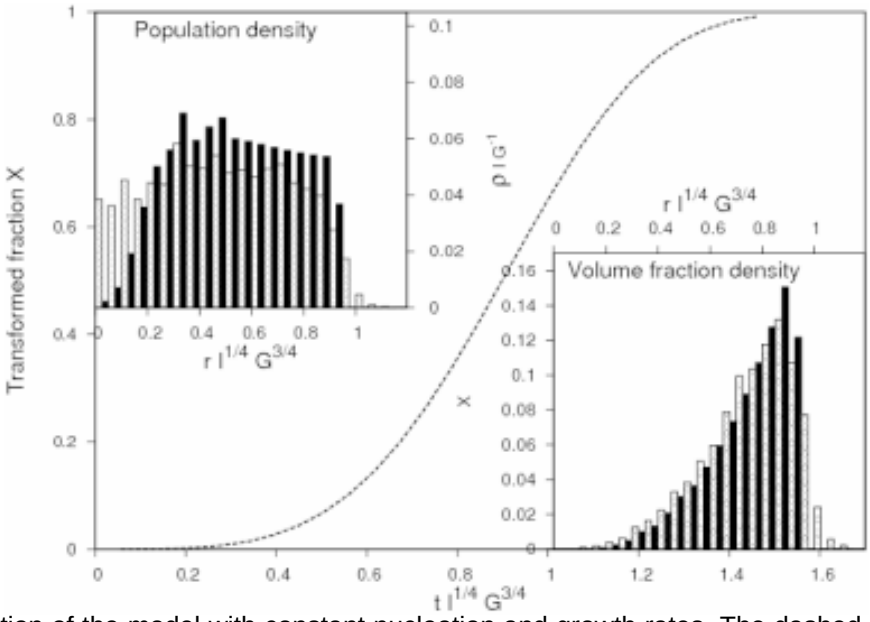


**Fig. 1.** Integration of the model with constant nucleation and growth rates. The dashed line shows the time evolution of the transformed fraction. The left inset shows the grain size distribution, that is the density of grains ρ having radius between *r* and the *r* + *dr*- as a function of *r*, given by the model (solid bars) compared to the distribution obtained from Monte Carlo simulations, both at the end of the transformation. The right inset shows the transformed fraction density also at the end of the transformation as a function of the average grain radius. All magnitudes are given in dimensionless form, related to the kinetic parameters *I* and *G*.

transformed and extended fractions occupied at time *t* by the grains nucleated between τ and τ +*d*τ, that we will call differential transformed and extended fractions and define as *y* (*t*,τ) and $\tilde{y}$ (*t*,τ) respectively. Its relationship with the previously defined transformed fractions is given by

$$x(t) = \int_0^t y(t,\tau)d\tau, \quad \tilde{x}(t) = \int_0^t \tilde{y}(t,\tau)d\tau. \tag{3}$$

Already in the initial works of Avrami [5], it was shown that these fractions have the same relationship than that one, which is

$$\frac{\partial y(t,\tau)}{\partial t} = \left[1 - x(t)\right]\frac{\partial \tilde{y}(t,\tau)}{\partial t} \tag{4}$$

and, taking into account the fact that the differential extended fraction can be easily computed - in this example, for isotropic growth in a three dimensional space with a variable nucleation rate *I*(τ)- from

$$\tilde{y}(t,\tau) = I(\tau)\frac{4}{3}\pi\tilde{r}^3(t,\tau)d\tau \tag{5}$$

allows to determine the behaviour of the differential transformed fraction for any value of the nucleation time *t*. Here, the extended radius $\tilde{r}(t, \tau)$ is the radius of a grain growing in isolation. Additionally, as the density *n* of grains nucleated between t and τ + *d*τ can be also computed from

$$n(\tau, d\tau) = I(\tau)\left[1 - x(\tau)\right]d\tau \tag{6}$$

the average grain size of the grains nucleated between τ and τ + dτ can be easily computed from

$$\left\langle r\langle t,\tau\rangle\right\rangle = \sqrt[3]{\frac{3}{4\pi}\frac{y(t,\tau)d\tau}{n(\tau,d\tau)}}. \tag{7}$$

This computation neglects the dispersion of the grains around their average value, so the grain size distribution obtained will be an approximation to the actual one. However, numerical implementation of the procedure above exposed is really simple, by taking constant nucleation time steps between the beginning of the transformation and the desired time and computing the corresponding differential volume fractions. The whole computa-

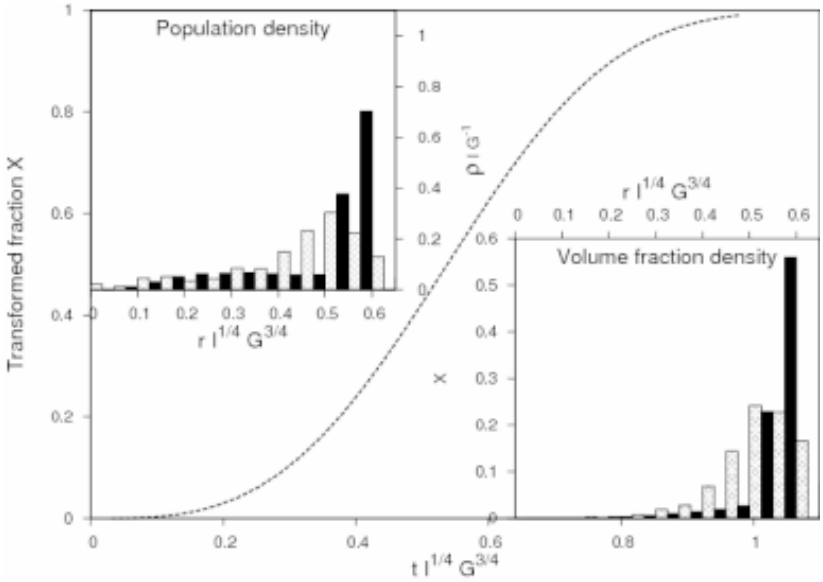


**Fig. 2.** Integration of the model for a process with an initial nucleation followed by constant nucleation, and constant growth rate. Same captions than in Fig. 1.

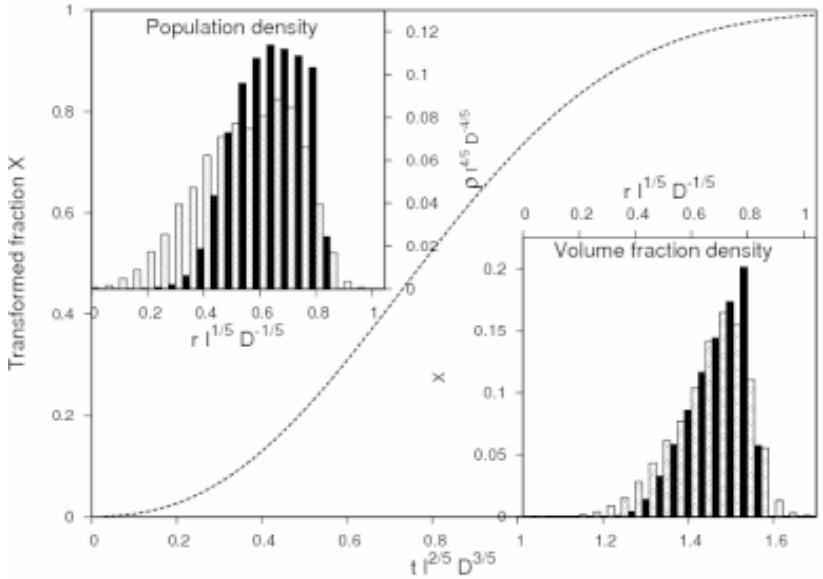


**Fig. 3.** Integration of the mode for a process with constant nucleation rate and diffusion controlled growth. Same captions than in Fig. 1.

tion took less than 100 lines of computer code and a negligible computation time in a personal computer.

## 3. RESULTS

The above model was checked against Monte Carlo simulations in three cases representative of different kinetic processes. The first considered case was the classical problem considered by Avrami, with constant nucleation rate *I* and constant growth rate *G*, physically corresponding to interface controlled grain growth. The relevant physical magnitudes of the process, defined above, are easily computed from

**Table 1.** Average radius <*r*> and standard deviation σ computed from the model and MC simulations in the three cases considered. Numerical values are referred to the natural length scale.

| | Length scale | $\langle r\rangle_{model}$ | $\langle r\rangle_{MC}$ | $\sigma_{\langle r\rangle,model}$ | $\sigma_{\langle r\rangle,MC}$ |
|---|---|---|---|---|---|
| $I=ct$, $G=ct$ | $I^{-1/4}G^{-3/4}$ | 0.556 | 0.526 | 0.232 | 0.279 |
| $I(t) = Nd(t) + I$, | $G=ct\ I^{-1/4}G^{-3/4}$ | 0.505 | 0.503 | 0.179 | 0.156 |
| $I=ct$, $G = D/r$ | $I^{-1/5}G^{1/5}$ | 0.642 | 0.620 | 0.119 | 0.172 |

$$\tilde{r}(r,\tau) = G(t-\tau),$$
$$\tilde{x}(t) = \frac{1}{3}\pi I G^3 t^4,$$
$$n(\tau,d\tau) = I\exp\left(-\frac{1}{3}\pi I G^3\tau^4\right)d\tau, \qquad (8)$$
$$d\tilde{y}(t,\tau,d\tau) = 4\pi I\left[G(t-\tau)\right]^2 d\tau.$$

The result of the integration of the model, compared to Monte Carlo simulation, are shown in Fig. 1. The grain size distribution computed by the model has qualitatively the same shape than that obtained from MC simulation. Slight differences are observed at both tails of the distribution, where the values given by the model underestimate those obtained from MC simulation. This fact is also observed in the standard deviation given by the model (see Table 1), which is lower than the one observed in the MC simulation by 17%, while the average grain size obtained from the model is correct within a 6%.

The second case under consideration is a transformation with initial nucleation of *N* nuclei per unit volume (pre-existing nuclei) and constant nucleation rate *I* afterwards, and with constant growth rate. The corresponding equations are

$$I(t) = N\delta(t) + I,$$
$$\tilde{r}(t,\tau) = G(t-\tau),$$
$$\tilde{x}(t) = \frac{4}{3}\pi N G^3 t^3 + \frac{1}{3}\pi I G^3 t^4,$$
$$n(\tau,d\tau) = N\delta(t) + I\exp\left(-\frac{4}{3}\pi N G^3 t^3 - \frac{1}{3}\pi I G^3 t^4\right), \qquad (9)$$
$$d\tilde{y}(t,\tau,d\tau) = 4\pi\left\{N\delta(t)G^2t^2 + I\left[G(t-\tau)\right]^2 d\tau\right\},$$

where $\delta(t)$ is the Dirac delta function.

The value of *N* was chosen arbitrarily to give the same natural length scale that the continuous nucleation process, that is $N^{-1/3} = I^{-1/4}G^{-3/4}$. Results of the integration of the model are displayed in Fig. 2, showing that the dispersion on the grain size of the pre-existing nuclei is underestimated by the model. This fact is also responsible for the overestimation of the standard deviation of the distribution, although the computed average grain radius is correct within a 1%.

For the third study case we considered constant nucleation rate *I* and diffusion controlled growth (with diffusion coefficient *D*), with equations

$$\tilde{r}(t,\tau) = \lambda\sqrt{D(t-\tau)},$$
$$\tilde{x}(t) = \frac{16}{15}\pi I\sqrt{2D^3t^5},$$
$$n(\tau,d\tau) = I\exp\left(-\frac{16}{15}\pi I\sqrt{2D^3t^5}\right)d\tau, \qquad (10)$$
$$d\tilde{y}(t,\tau,d\tau) = \frac{4}{3}\pi I\left[2D(t-\tau)\right]^{3/2}d\tau$$

with λ = 0,9082959626 for 3-D growth [7]. The results obtained are displayed in Fig. 3. The shape of the distribution is again representative of the one computed by MC simulations. The computed average radius is correct to a 4%, and the standard deviation is lower to the determined in the MC simulations reflecting the fact that the populations at the tails are underestimated.

## 4. CONCLUSIONS

The model presented here allows the determination of the grain size distribution at any stage of a nucleation and growth phase transformation, taking from input data the kinetic parameters of the transformation. The model makes no empiric assumptions and is based solely in the grounds of the Kolmogorov, Johnson & Mehl, and Avrami model, and in the determination of the average grain size of all grains born at the same time along

the transformation. Although this assumption neglects the dispersion of the grain size around the corresponding mean value, comparison to Monte Carlo simulations shows that the model gives a good approximation to the actual grain size distribution and a very accurate estimation of the average radius. However, the grain density is slightly underestimated at the tails, giving usually a standard deviation smaller than that of the actual one.

## ACLNOWLEDGEMENTS

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