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Transformation kinetics for nucleation on second-phase particles: analytical solution and computer simulation

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ABSTRACT

An analytical solution, based on stochastic geometry concepts, is presented here for transformations in which nuclei are located on the interface between second-phase particles and the parent matrix. The analytical solution aims at the most common situation in which the particles are dispersed within the matrix with a particle volume fraction less than 0.1 so that particle/particle impingement is small. A computer simulation was carried out to compare with the analytical solution. This comparison revealed that in some circumstances the analytical solution may be valid for particle volume fractions well beyond 0.1 when there is a significant amount of impingement. The formalism is valid for particle stimulated nucleation during recrystallization as well as for phase transformations that nucleate on the interface of a previously extant phase and the parent matrix. Detailed determination of the bounds within which the analytical solution is valid is carried out with the help of computer simulation. The reasons for this extended validity of the analytical solution are discussed in depth.

1. Introduction

In their early but still highly influential work, Johnson-Mehl, Avrami and Kolmogorov [1–5] treated nucleation and growth transformations in a formal way. They did not propose specific physical mechanisms for nucleation and growth. Instead they made geometric and kinetic assumptions that described possible nucleation and growth scenarios. In their fundamental work the nucleation sites were uniform randomly located within the parent matrix. Furthermore, the nucleation could take place either with a constant nucleation rate or by site saturation in which all nucleation sites saturated early in the transformation, i. e. all nucleated regions started to grow from the beginning of the transformations. Moreover, they set the growth velocity to be a constant and the new phase to have the shape of spheres. The JMAK equation for site-saturated nucleation will be used later in this paper and is given by

$$V_V(t) = 1 - \exp\left(-\frac{4\pi}{3} N_V G^3 t^3\right) \quad (1)$$

where V_V is the volume fraction, t is time, G is the velocity and N_V is the number of nuclei per unit of volume.

In practice, many situations arise that differ to a great extent from JMAK's original assumptions. Perhaps the simpler deviation is that the velocity might not be a constant during transformation. In this particular case, JMAK findings can be easily generalized by introducing a time dependent velocity. In fact, Avrami herself recognized that deviations from their assumptions could take place and proposed a generalized form of her equation that is known to this day as Avrami's equation [6]:

$$V_V(t) = 1 - \exp(-kt^n) \quad (2)$$

where k and n are adjustable parameters without the meaning they had, for example, in Eq. (1). This equation has been widely used to model many nucleation and growth transformations.

One might say that JMAK work gave birth to two distinct approaches to formal kinetics. On one hand researchers tried to derive JMAK-like analytical expressions by making different assumptions about nucleation and growth. On the other hand researchers have

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taken Eq. (2) as their starting point and developed formal methodologies that are particularly suitable for situations in which detailed information about nucleation and growth is not available. Cahn's paper of nucleation on planes and lines [7] might be considered the first paper of the former approach as he derived exact mathematical equations to model transformations nucleated on random planes and lines. There is a large number of papers based on the latter approach, a comprehensive review can be found in Liu et al. [8].

Many researches have endeavored to pursue JMAK and Cahn's path [7,9]. Owing to the recent developments in Stochastic Geometry [10], a significant number of recent papers have been based on its results. Perhaps the earliest work based on Stochastic Geometry concepts was that of Sekimoto [11]. He provided an expression for the n-point correlation functions describing nucleation and growth in general circumstances. The one-point function is the JMAK result. Building on Sekimoto's approach [11], Rickman et al. [12] presented a general treatment of heterogeneous nucleation.

One of the challenges of formal kinetics is modeling nucleation, particularly, nuclei location within the matrix. One issue is whether nuclei are correlated or uncorrelated [13,14]. Recently, Rickman and Barmak [15] obtained a n-point correlation function for the situations in which correlated and uncorrelated nucleation took place. Moreover, it is worth mentioning an interesting work that models phase transformation taking place in a non-Euclidean space [16].

Rios, Villa and coworkers focused mainly on the nuclei distribution in space and derived exact mathematical expressions to generalize JMAK's to transformations in which nucleation and growth were significantly different from those originally proposed by JMAK [17–27].

As one can see, these diverse approaches are not mutually exclusive and each has significant importance to the theory and practice of transformations in solids depending on the problem to be solved.

In this paper, Rios and Villa previously developed methodology [18–20,23] is applied to the problem of nucleation on the interface between uniform randomly dispersed particles and the parent matrix. Such a nucleation may take place in several circumstances, for instance, in recrystallization one has the so called particle stimulated nucleation (PSN) [28–31] or in an entirely different case nucleation may take place on particles that form within the weld metal [32–34].

In spite of its obvious scientific and technological importance there are not many computacional [35–37] or analytical [38,39] models available for nucleation on particles. The models normally focus on PSN recrystallization and strongly emphasize the texture resulting from nucleation on particles. The present analytical model follows a different path. We use a JMAK-like approach making no specific assumptions about the physical mechanism of nucleation and growth nor about the material. Instead, one provides a phenomenological description of nucleation of new regions on the particles and their subsequent growth. A computer simulation complements the analytical model and follows the same phenomenological approach.

Our analytical model for nucleation at the particle/matrix interface model is based on stochastic geometry. Although exact, the mathematical model makes some assumptions that limit its validity. Therefore, the computer simulation helped to establish within which bounds the present equation may be safely employed.

Therefore, the main objective of this paper is to present an analytical expression that can be used to model nucleation on particle/matrix interfaces specially when particle volume fraction falls within reasonable values, say less than 0.1. A computer simulation generates the microstructures and is compared with the analytical results. Under certain conditions the present formulation can also be used for high particle volume fractions, above 0.1. We fully discuss this point in this paper.

2. Model description

Earlier papers by Rios and Villa [18–20] as well as stochastic geometry books [10,40] contain the necessary mathematical background for the mathematical derivation. For the reader's convenience preliminary definitions and basic stochastic geometry concepts are included in the "Supplementary Material" of this paper.

The derivation starts by considering Φ the underlying homogeneous Poisson point process with intensity λ. Next one defines $Z_0 = Z_0(t)$ to be the typical grain at time t. $Z_0(t)$ is defined to be the transformed region at time t that originates from a birth and growth process on the surface of the ball (i. e. the spherical particles) $B_R(0)$; namely, we assume site saturation and Poissonian homogenous nucleation process on the surface of the ball with mean number of nuclei per ball (per particle) equal to $c>0$, while the grain associated with each nucleus is assumed to grow with constant velocity G outside $B_R(0)$ and zero inside $B_R(0)$. In other words the nucleated region is permitted to grow only within the complement of the ball $B_R(0)$ (the exterior part of the particle), that is, $B_R(0)^C$.

We denote by Θ^t the transformed region at time t. Then Θ^t can be described as a Boolean model driven by a marked Poisson point process $\Phi^t := \{X_i, Z_i(t)\}$, with $\{X_i\} = \psi$ (the homogeneous Poisson point process with intensity λ) and typical grain $Z_0(t)$ as defined above:

$$\Theta^t = \cup_{(X_i, Z_i(t)) \in \Phi^t} X_i + Z_i(t) \tag{3}$$

The resulting transformed region Θ^t is stationary for any $t>0$. It follows that its volume fraction is given by

$$V_V(t) = \mathbb{P}\left(0 \in \Theta^t\right) = 1 - \exp\left\{ -\lambda \mathbb{E}\left[\nu^d\left[Z_0(t)\right]\right]\right\} \tag{4}$$

In order to evaluate $\mathbb{E}[\nu^d[Z_0(t)]$ we consider the auxiliar birth and growth process, say Ξ^t, defined in the same way as Z_0 with the only difference that here the grains are free to grow also inside the particle $B_R(0)$. So, let us denote by Φ_S the Poissonian nucleation process on the sphere with mean number of nuclei per ball equal to $c>0$; then its intensity, say λ_S, is given by (See also [20]).

$$\lambda_S(x) = \frac{c}{4\pi R^2} \delta_{\partial B_R(0)}(x) \tag{5}$$

where $\delta_{\partial B_R(0)}(x)$ is the usual Dirac-delta function on the surface of $B_R(0)$, $\partial B_R(0)$. The transformed region Ξ^t at time t is given by

$$\Xi^t = \cup_{X_i \in \Phi_S} X_i + B_{Gt}(0) \tag{6}$$

Of course Ξ^t is not stationary (since the nucleation takes place only on the sphere); therefore its mean volume density, say $V_{V,\Xi}$, is space and time dependent. Since $\{\Xi^t\}_t$ is a birth and growth process driven by a Poisson point process as nucleation process, it is well known that

$$V_{V,\Xi}(t,x) = 1 - e^{-V_{E,\Xi}(t,x)} \tag{7}$$

where we denoted by $V_{E,\Xi}(t,x)$ the mean extended volume density of Ξ^t at point x. A well known theorem [41] states that $V_{E,\Xi}(t,x)$ is equal to the intensity measure (absolute number of nuclei), Λ_S, of the nuclei located within the causal cone [9,23], $\mathcal{C}(t,x)$, at time t associated to the point x, where $\Lambda_S(\mathrm{d}y) = \lambda_S(y)\mathrm{d}y$ is the intensity measure of the nucleation process Φ_S. It can be seen that