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Concurrent growth of two phases in 2D space

A.A. Burbelko, W. Kapturkiewicz*, E. Fraś
Faculty of Foundry Engineering, AGH University of Science and Technology, Reymonta 23, 30-059 Krakow, Poland
*Corresponding author. E-mail address: kaptur@agh.edu.pl

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Abstract

The kinetics of phase transformations has been studied within the framework of the Kolmogorov-Johnson-Mehl-Avrami (KJMA) theory. This theory accurately describes only the parallel growth of anisotropic products with identical convex shape. The identical growth velocity distribution at an interface is the indispensable condition for the above restriction. The proposed earlier extension of KJMA theory (statistical theory of the screened growth) enlarges the scope of its application and eliminates the above limitation. The results of the application of this extension were compared with the results obtained during modelling of the concurrent growth of the two types of circular particles on a plane, where the said particles were characterised by different growth rates and modelling was carried out by the method of cellular automata (CA).

Keywords: KJMA theory, Concurrent growth, Screening

1. Introduction

The mechanism that drives numerous processes changing the state of matter is the nucleation and growth of single elementary objects of a new substance within the substance subject to transformations. The phenomena of this type are numerous and include crystal physics, metallurgy, polymer physics, ferroelectric domain switching, magnetization and metastability in statistical physics models, phase transitions in particle physics as well as ecological landscapes [1]. No matter how much these phenomena may differ, changes in the volume of the transformed fractions are described by the same statistical theory. The theoretical fundamentals of the mathematical formulae used nowadays were developed by Kolmogorov [2]. Comprehensive case studies of the transformations are described in publications written by Johnson and Mehl [3] and Avrami [4]. This article discusses the case disregarded by the classical statistical theory. This is the case of a concurrent growth of particles, when each of them has a different velocity of growth.

2. Extended range of application of the statistical KJMA theory

The general equation of the statistical theory of solidification, called the Kolmogorov equation, enables us to predict the real transformed fraction volume from the, so called, extended specific volume (Ω)

$$V(t) = 1 - \exp(-\Omega(t)) \tag{1}$$

where: t – the time.

The value of Ω is calculated from some geometrical rules, allowing for the shape, size and quantity of particles in a unit volume but disregarding certain limitations resulting from their interaction [2]. One of the conditions indispensable to satisfy the above mentioned equation is to have equal velocities of growth of all the grains in a given direction and at a given time instant. In reality, this condition is not always satisfied, and actual kinetics of the process differs from that determined by equation (1).

Numerous attempts are known that aim at an improvement of the statistical theory of phase transformations to describe in a correct way the kinetics of these transformations in situations when the above mentioned conditions are not satisfied. Yet, as reported by Koi [5], all these improvements are not of a general character, but refer to some specific cases only.

It has been proven [6] that the most frequent cause of deviations is the effect of screening. The solution presented in further part of this study is based on the statistical theory of the screened growth [7-8]. This study discusses the example of a simultaneous, concurrent growth of the circular grains of two types on the plane when each of them has a different growth velocity.

It has been assumed that we know the function $S(u,t)$, determining the field of an external boundary of the extended grains, the growth of which at a given time instant t takes place at a velocity not greater than u. For the faceted and spherical grains, this function is continuous in intervals, while for other non-faceted grains, it is of a continuous character. In its continuous intervals $S(u,t)$, the function $S'(u,t)$ is equal to its partial derivative $\partial S(u,t)/\partial u$, and at the points of discontinuity, where $S(u,t)$ has a jump equal to the length of the respective crystal facets $\Delta S(u_F,t)$, this function assumes the value:

$$S'(u_F,t)=\Delta S(u_F,t)/u_F \tag{2}$$

where: u_F – the respective growth velocity on the surface.

The velocity of the extended grain surface growth can be expressed with Stieltjes integral:

$$\frac{\partial\Omega}{\partial t}=\int_0^{u_m} uS'(u,t)du+\sum_i u_{Fi}^2 S'(u_{Fi},t) \tag{3}$$

where the second term allows for the faceted or spherical growth velocity, while the first term allows for the non-faceted growth velocity.

The extended volume is determined by the integration of equation (3) after the time:

$$\Omega(t)=\int_0^t\left(\int_0^{u_m} uS'(u,\tau)du+\sum_i u_{F_i}^2 S'(u_{F_i},\tau)\right)d\tau \tag{4}$$

where: u_m – the maximum migration velocity of the boundary.

The screening rate in the case of one-, two-, and three-dimensional growth is given in papers [7, 8] If, within the integration range, there are points of discontinuity of the function S(u), Stieltjes integral applies, and in 2D space the screening rate is:

$$\frac{\partial \ln S'(u_2,t)}{\partial t}=$$
$$=-\frac{u_2}{\pi}\left(\int_{u_{\min}}^{u_2}\left(\sqrt{1-\left(\frac{u_1}{u_2}\right)^2}-\left(\frac{u_1}{u_2}\right)\arccos\left(\frac{u_1}{u_2}\right)\right)S'(u_1,t)\mathrm{d}u_1+\right.$$
$$\left.+\sum_i\left(\sqrt{1-\left(\frac{u_{F_i}}{u_2}\right)^2}-\left(\frac{u_{F_i}}{u_2}\right)\arccos\left(\frac{u_{F_i}}{u_2}\right)\right)S'(u_{F_i},t)u_{F_i}\right) \tag{5}$$

where: u_2 – the velocity of growth of the screened surface, u_1 – the integration variable.

3. Concurrent growth of the circular grains on plane

Let us consider the growth of the circular particles of two types, i.e. A and B, proceeding at different velocities in 2D. It is assumed that the nuclei of these particles are formed at the same time instant t=0 in a number n_A and n_B. Let particles grow at constant velocities u_A and u_B, and let $u_A > u_B$. In the case under consideration and according to definition (2), for the slow growth (B) screening does not occur. The rate of screening the surface of grains A is:

$$\frac{\partial \ln S'(u_A,t)}{\partial t}=$$
$$=-\frac{u_A}{\pi}\left(\sqrt{1-\left(\frac{u_B}{u_A}\right)^2}-\left(\frac{u_B}{u_A}\right)\arccos\left(\frac{u_B}{u_A}\right)\right)S_B(t) \tag{6}$$

where: $S_B(t)$ – the total field of the surfaces of all the extended B type grains in time t.

A more rapid growth of grains A may be screened on the extended boundary of grains B, with the size of the boundary assuming a value equal to:

$$S_B(t)=n_B\cdot 2\pi(u_B t) \tag{7}$$

The boundary $S_A(t)$ of the extended grains A is growing with the growing radius of these grains, and from geometrical relations for the partially screened grains follows:

$$\partial S_A(t)/\partial R_A=S_A(t)/u_A t \tag{8}$$

Since in the examined case the velocities are time-independent, equation (4) for circular particles in 2D is reduced to the following form:

$$\Omega(t)=u_A^2\int_0^t S'(u_A,\tau)\mathrm{d}\tau+n_B\pi(u_B t)^2 \tag{9}$$

Differentiating function S' for grains of type A along their radius, we obtain:

$$\partial S'(u_A,t)/\partial R_A = S'(u_A,t)/u_A t \tag{10}$$

The rate of changes in $S'(u_A,t)$ depends on the two competitive processes, i.e. an increase of the grain dimensions and screening of the surface:

$$\frac{\mathrm{d}S'(u_A,t)}{\mathrm{d}t} = \frac{\partial S'(u_A,t)}{\partial R_A}\frac{\mathrm{d}R_A}{\mathrm{d}t} + S'(u_A,t)\frac{\partial \ln S'(u_A,t)}{\partial t} \tag{11}$$

On substituting to this equation the derivatives (6) and (10) we obtain:

$$\frac{\mathrm{d}S'(u_A,t)}{\mathrm{d}t} = S'(u_A,t)\times \times\left[\frac{1}{t}-\frac{u_A}{\pi}\left(\sqrt{1-\left(\frac{u_B}{u_A}\right)^2}-\left(\frac{u_B}{u_A}\right)\arccos\left(\frac{u_B}{u_A}\right)\right)S_B\right] \tag{12}$$

where from allowing for (2) and (7):

$$\frac{\mathrm{d}\ln S_A(t)}{\mathrm{d}t} = \left[\frac{1}{t}-2n_B u_A u_B t\times \times\left(\sqrt{1-\left(\frac{u_B}{u_A}\right)^2}-\left(\frac{u_B}{u_A}\right)\arccos\left(\frac{u_B}{u_A}\right)\right)\right] \tag{13}$$

An integral of this equation enables calculation of the non-screened boundary of grains A:

$$\ln S_A(t) = \ln t - n_B u_A u_B t^2 \times \times\left(\sqrt{1-\left(\frac{u_B}{u_A}\right)^2}-\left(\frac{u_B}{u_A}\right)\arccos\left(\frac{u_B}{u_A}\right)\right)+C \tag{14}$$

Since at the instant of nucleation, due to a small size of the grain boundaries, screening can be neglected, we have:

$$\lim_{t\to 0} S_A(t) = 2\pi n_A u_A t \tag{15}$$

and it is possible to determine the integration constant C:

$$C = \ln(2\pi n_A u_A) \tag{16}$$

Finally, the non-screened boundary of grains A will be calculated from the equation:

$$S_A(t) = 2\pi n_A u_A t \times \times\exp\left[-n_B u_A u_B\left(\sqrt{1-\left(\frac{u_B}{u_A}\right)^2}-\left(\frac{u_B}{u_A}\right)\arccos\left(\frac{u_B}{u_A}\right)\right)t^2\right] \tag{17}$$

The total extended volume of the products of growth, calculated according to (9), is:

$$\Omega(t) = \Omega_A(t) + \Omega_B(t) \tag{18}$$

where the first term refers to grains of type A, and the second to grains of type B:

$$\Omega_A(t) = 2\pi n_A u_A^2 \times \times\int_0^t \tau\cdot\exp\left[-n_B u_A u_B\left(\sqrt{1-\left(\frac{u_B}{u_A}\right)^2}-\left(\frac{u_B}{u_A}\right)\arccos\left(\frac{u_B}{u_A}\right)\right)\tau^2\right]d\tau \tag{19}$$

$$\Omega_B(t) = n_B\pi(u_B t)^2 \tag{20}$$

Differentiating equation (1) in the case of the growth of two phases, we obtain:

$$\partial V_A/\partial\Omega_A = \exp(-\Omega_A - \Omega_B) \tag{21}$$

The numerical integration of equation (21) using (19) and (20) enables us to analyse the kinetics of transformations in the case under consideration. The computed changes in volume fraction of the grains of types A and B in the function of Ω_B are shown in Fig. 1. Analysis was made for the ratio of growth velocities differing from 1:1 to 1:16. It has been assumed that the growth velocity and the number of grains of type B (blocking) is the same. The growth velocity and the number of grains of type A (screened) was in each individual case calculated from the relation:

$$n_A u_A^2 = n_B u_B^2 \tag{22}$$

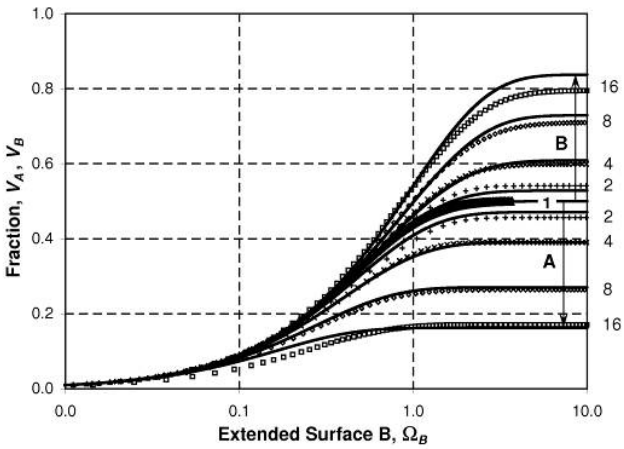
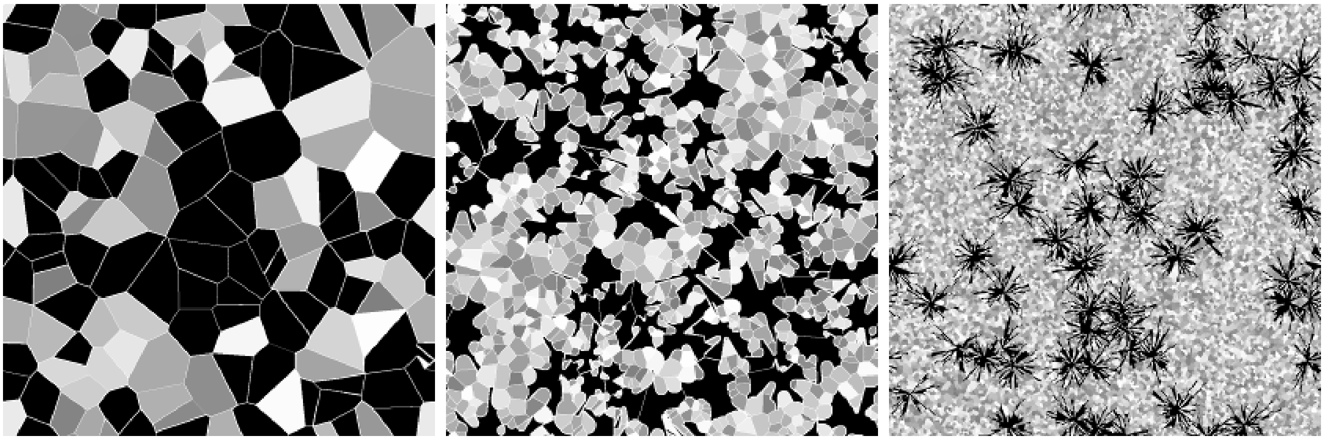


Fig. 1. History of volume fraction for two types of the transformation products A and B with equal extended volumes. Lines – proposed analytical solution; points – the cellular automata modelling; numbers – u_A/u_B

The above results were compared with the data obtained by CA modelling. Final structures obtained for the individual growth rate relations are shown in Fig. 2. Modelling was carried out on a grid of 1024 x 1024 cells with periodic boundary conditions. The technique of determination of the transformation rate in cells for the imposed growth velocity vector is described earlier [9].

The history of changes in the volume fraction of the grains of both phases as a function of Ω_B, as obtained by the CA method, is marked with points in Fig. 1. A good conformity between the results of integration of equation (21) and the results of CA modelling has been obtained.



a) b) c)

Fig. 2. Structure with different relations of the growth rate. Black – A-grains, grey – B-grains, u_A/u_B: a) 1; b) 4, c) 16

4. Conclusions

An example of the application of the statistical theory of the screened growth in description of the concurrent growth of the grains of two phases on a plane (2D) has been presented. The comparison of the results obtained by this method with the results of modelling by the CA method proves the correctness of the statistical theory of the screened growth in this case.

The statistical theory of the screened growth eliminates some limitations of the KJMA theory of phase transformation and extends the field of KJMA theory application.

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