An Exact Analytical Solution of the Fokker-Planck Type Equation in the Presence of Arbitrary Growth Rates of Nuclei

A. A. Ivanov

Laboratory of Multi-Scale Mathematical Modeling, Ural Federal University
Lenin ave., 51, Ekaterinburg, 620000, Russian Federation

I. G. Nizovtseva

Ural Federal University
Office 607, Turgeneva str. 4, Ekaterinburg, 620075, Russia

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Abstract

A Fokker-Planck type equation for the density distribution function is solved analytically for arbitrary growth rates of nuclei. An exact solution is found in the absence of random fluctuations in the rate of particle growth.

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Let us consider a system of solid spherical particles in a macroscopically homogeneous single-component supercooled liquid or supersaturated solution. The transient behavior of such a two-phase system is described by a kinetic equation for density the $f(r, \tau)$ of particle radius distribution function. Neglecting random fluctuations in the rate of crystal growth, we have

$$\frac{\partial f}{\partial \tau} + \frac{\partial}{\partial r} \left[ V(\tau, r) f(\tau, r) \right] = 0, \quad \tau > 0, \quad r > r_0. \quad (1)$$
where $V$ is the rate of crystal growth, $\tau$ is the time, $r$ is the radius, and $r_*$ is the minimum size of the crystals (radius of critical nuclei). This rate depends upon the crystal size and the supercooling/supersaturation [1]. So, for example, this function can be represented as [2]

$$V(\tau, r) = \frac{\beta \Delta \theta(\tau)}{1 + \beta qr}. \quad (2)$$

where $\beta_*$ is the kinetic parameter, $\Delta \theta(\tau)$ is the supercooling/supersaturation, and $q = \rho_s L/\lambda_i$ in the case of supercooled liquids and $q = C_p/D$ in the case of supersaturated solutions. Here $\rho_s$ is the density of the stable solid phase, $L$ is the latent heat of phase transition per unit mass of substance, $\lambda_i$ is the temperature conductivity coefficient $C_p$ is the concentration at saturation, and $D$ is the diffusion coefficient.

Expression (2) shows that the growth rate is a linear function of the supercooling/supersaturation. In the case of very fine crystals, $r < \left(\beta_*/q\right)^{-1}$, the growth rate is independent of their size. This growth regime is known as “kinetic” because it is fully defined by surface processes. The growth rate for particles whose dimensions exceed markedly the value $\left(\beta_*/q\right)^{-1}$ is controlled by the rate of heat removal. This growth regime is known as “diffusive”. An assumption frequently used by a number of investigators is that the crystal growth rate can be represented as a product of two functions depending solely on the radius and supercooling/supersaturation [1], i.e.

$$V(\tau, r) = R(r) B(\Delta \theta(\tau)). \quad (3)$$

where $R(r)$ and $B(\Delta \theta)$ represent arbitrary functions of $r$ and $\Delta \theta(\tau)$ respectively.

Let us assume that the liquid, which previously did not contain any crystals, is instantaneously cooled at zero time to below the crystallization temperature by the amount $\Delta \theta_0$. Then the boundary conditions can be written as

$$f = 0, \quad \Delta \theta = \Delta \theta_0, \quad \tau = 0. \quad (4)$$

and

$$Vf = I(\Delta \theta), \quad r = r_*. \quad (5)$$

Here $I(\Delta \theta)$ is the frequency of nucleation per unit volume. Note that condition (5) defines the flux of nuclei that have overcome the critical barrier.

Let us introduce the following dimensionless variables and parameters
An exact analytical solution of the Fokker-Planck type equation

\[ F = I^0 \cdot t = \frac{\tau}{\tau_0}, \quad s = \frac{r}{l_0}, \quad w = \frac{\Delta \theta}{\Delta \theta_0}, \quad I_0 = I(\Delta \theta_0), \quad \tau_0 = (\beta \Delta \theta_0)^{-1}, \]

\[ I_0 = (\beta \Delta \theta_0)^{-1} I^0 \cdot R_1(s) = R(s l_0), \quad B_l(w) = B(w \Delta \theta_0), \quad A_l(w) = \frac{B_l(w)}{\beta \Delta \theta_0}, \quad (6) \]

In terms of expressions (6) the problem defined by equations (1), (3)-(5) yields the equations

\[ \frac{\partial F}{\partial x} + \frac{\partial}{\partial z} [R(z) F] = 0, \quad x > 0, \quad z > 0, \quad (7) \]

\[ F = 0, \quad x = 0; \quad F = \frac{\phi(x)}{R_z(0)}, \quad z = 0. \quad \quad (8) \]

\[ \phi(x(t)) = \frac{l^0 I_1(w(t))}{B_l(w(t))}. \]

The exact solution of equations (7), (8) is given by

\[ F(x(t), z) = \frac{1}{R_z(z)} \phi(x(t) - y(z)) \eta(x(t) - y(z)). \quad (9) \]

where \( \eta(h) \) is the Heaviside function, equal to zero or unity at negative or positive values of the argument \( h \), respectively.

Expression (9) represents the key result of the present study. Thus, the density of particle radius distribution function is found in an explicit analytical form for arbitrary laws of growth rates expressed by equation (3). An important point is that the supercooling/supersaturation \( w \) entering in the right-hand side of (9) should be found from the heat or mass balance equation in a metastable media. The exact analytical solution (9) can be used for the description of a lot of phase transition processes with the steady-state [3-5] and transient [6-8] two-phase layer.

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