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MATHEMATICAL MODELING OF THE CRYSTAL GROWTH IN BINARY SYSTEM

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This paper is aimed at studying the process of nucleation and crystal growth in binary systems at the intermediate stage of the phase transition with allowance for Meirs kinetics. The mathematical model of this process consists of the kinetic Fokker-Planck equation and the balance equation.

The phase transition process is divided into three main stages. At the first stage, particle growth occurs with constant supercooling. At the second stage, particles grow with the release of the latent heat of the phase transition, which compensates for the overcooling of the system. In the third stage, coalescence and coagulation processes (Ostwald's ripening theory) occur [1, 2]. In this paper, we will consider the processes occurring at the second (intermediate) stage of the phase transition. At this stage, the mathematical model consists of a Fokker-Planck type kinetic equation for the size distribution function of crystals and a balance equation for the degree of supercooling [3, 4].

The crystal-size distribution function $f(r,\tau)$ is described by the kinetic equation:

$$\partial f/\partial\tau+\partial/\partial r\,(dr/d\tau\, f(r,\tau))-\partial/\partial r\,(D\,\partial f/\partial r)=0, \qquad (1)$$

where r is the radius of crystals, τ is time, D is the diffusion coefficient.

The balance equations represent the dependence of various parameters such as concentration σ_l and temperature θ_l on the mixture density ρ_m, heat capacity C_m, latent heat of crystallization L, time τ, etc.

An analytical solution is obtained for a mathematical model that describes the nucleation and growth of crystals at an intermediate stage of a phase transition in a binary melt. The solution took into account the nonlinear crystal growth rate and the Meirs nucleation kinetics. The effect of the nonlinear crystal growth rate changes the degree of supersaturation of the system and the size distribution function of crystals in comparison with the previously used stationary growth rates. Figure 1 shows the solution for various values of the parameter x_0 of the integro-differential system. The graph is a bell-shaped curve that shifts to the right as a function of time. With increasing time, the number of small crystals decreases, and the number of larger crystals increases. This solution of a system with a nonlinear growth rate more accurately describes the real crystallization process.

This theory can be extended to describe crystallization processes taking into account other dynamic laws of growth [5].

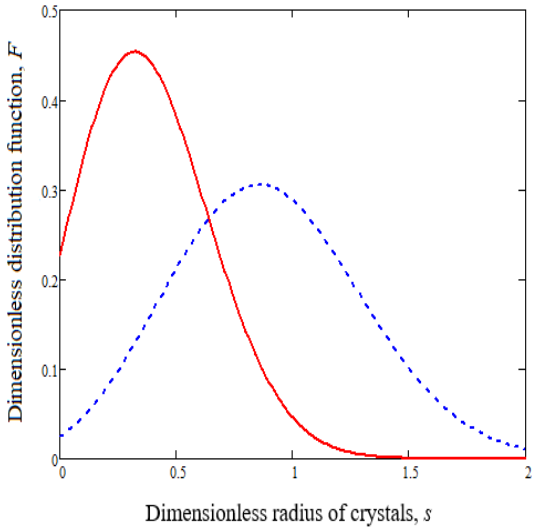

Fig. 1. Dimensionless distribution function F versus dimensionless radius of crystals s at $x_0 = 0.5$- solid line, $x_0 = 1$ - dotted line.

The reported study was funded by RFBR, project number 19-32-90003

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