

RESEARCH ARTICLE

Mathematical modeling of the growth of ellipsoidal crystals in metastable melts and solutions

Margarita A. Nikishina* | Dmitri V. Alexandrov

Department of Theoretical and Mathematical Physics, Laboratory of Multi-Scale Mathematical Modeling, Laboratory of Mathematical Modeling of Physical and Chemical Processes in Multiphase Media, Ural Federal University, Ekaterinburg, Russian Federation

Correspondence

*Margarita A. Nikishina, Department of Theoretical and Mathematical Physics, Laboratory of Mathematical Modeling of Physical and Chemical Processes in Multiphase Media, Ural Federal University, Ekaterinburg, Russian Federation. Email: margarita.a.nikishina@gmail.com

The evolution of individual crystals of ellipsoidal shape in supercooled one-component and binary melts as well as in supersaturated solutions is studied theoretically. The crystal volume growth rate is derived using the prolate ellipsoidal coordinates. We show that this rate is a function of the current crystal volume and supercooling/supersaturation of the ambient liquid. Also, we demonstrate that the particle growth rate increases with increasing the volume of ellipsoidal crystals and supercooling.

KEYWORDS:

mathematical modeling, crystal growth, nucleation, phase transformations, ellipsoidal particles

1 | INTRODUCTION

It is well known that the number of solid-phase elements (nuclei) in a metastable melt determines the final structure of the crystallized material and its properties.^{1–3} Since each crystallite grows from one nucleus, the total number of nuclei characterizes the size of the grains formed during crystallization. To achieve good mechanical properties of materials (for example, strength properties), it is necessary to obtain a fine-grained structure. For this, it is necessary that the largest possible number of crystallization centers appear in the crystallizing melt. As this takes place, the rate of melt cooling should be chosen so that the formed crystallization centers are capable of further growth. The first crystallites formed will grow until they meet with neighboring particles. If the time between the acts of the appearance of crystallization centers is long enough, then the crystallites grow large and during their growth, they can capture a certain number of potential crystallization centers. At large initial supercooling, a significant amount of particles present in the melt can become centers of crystallization before they are captured by neighboring crystals. At the same time, the addition of impurities, which are crystallization centers, makes it possible to control the dynamics of supercooling and the process of nucleation and growth of crystals.⁴

The above shows the importance of mathematical modeling of the process of phase transformation from a metastable state. Since various stages of such a process (initial, intermediate, and concluding) are described by different mathematical models, it is not possible to give a complete theoretical consideration within the framework of one approach. For instance, the initial stage of nucleation proceeds at practically constant supercooling (supersaturation), when the number of nuclei may be small. The intermediate stage of the process is characterized by the simultaneous occurrence of the processes of nucleation of new crystallites and the growth (enlargement) of already existing crystals.^{5–13} At the same time, the growing crystals release the latent heat of phase transformation, which leads to the melt desupercooling. In the absence of heat removal (system cooling), the process smoothly moves to the concluding stage, characterized by low supercooling. At this final stage, the density of crystals

in the melt becomes significant and they interact with each other through the processes of Ostwald ripening, coagulation, and disintegration.^{14–19}

In this work, we investigate the intermediate stage of the phase transformation process, where the individual crystals of ellipsoidal shape evolve. Note that in many real processes the shape of crystals differs from the spherical shape (for example, the shape of crystals can be ellipsoidal^{20–29}), which is a frequently used model approximation. The growth rates of the volumes of ellipsoidal crystals found in this work for supercooled one-component and binary melts, as well as for supersaturated solutions, generalize the previously known growth laws for spherical particles^{30–32} and have the corresponding limiting transition.

2 | THE EVOLUTION OF AN ELLIPSOIDAL PARTICLE IN A METASTABLE LIQUID

For the convenience of the mathematical description of the growth of an ellipsoidal crystal, we use the coordinate system of a prolate ellipsoid³³ (Figure 1)

$$\begin{aligned} x^2 &= a^2 (\sigma^2 - 1) (1 - \tau^2) \cos^2 \varphi, \\ y^2 &= a^2 (\sigma^2 - 1) (1 - \tau^2) \sin^2 \varphi, \\ z &= a\sigma\tau. \end{aligned} \quad (1)$$

Here x , y , and z are the Cartesian coordinates, a is a constant parameter defining the size of growing particle, σ , τ , and φ are the ellipsoidal coordinates satisfying the following inequalities

$$\sigma \geq 1, \quad -1 \leq \tau \leq 1, \quad 0 \leq \varphi \leq 2\pi.$$

Note that the coordinate σ denotes the perpendicular direction to the surface of an ellipsoidal crystal.

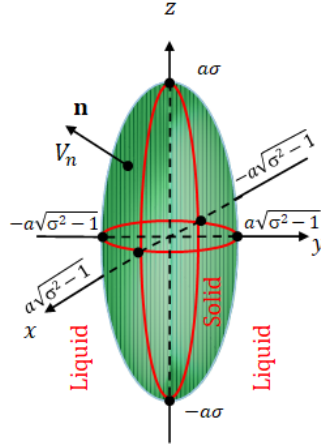


FIGURE 1 An ellipsoidal particle shown in the prolate ellipsoidal coordinates (1).

To write out the heat and mass balance boundary conditions at the surface of an ellipsoidal crystal in coordinates (1), we calculate the Lamé coefficients

$$\begin{aligned} H_\sigma &= \sqrt{\left(\frac{\partial x}{\partial \sigma}\right)^2 + \left(\frac{\partial y}{\partial \sigma}\right)^2 + \left(\frac{\partial z}{\partial \sigma}\right)^2} = a\sqrt{\frac{\sigma^2 - \tau^2}{\sigma^2 - 1}}, \\ H_\tau &= \sqrt{\left(\frac{\partial x}{\partial \tau}\right)^2 + \left(\frac{\partial y}{\partial \tau}\right)^2 + \left(\frac{\partial z}{\partial \tau}\right)^2} = a\sqrt{\frac{\sigma^2 - \tau^2}{1 - \tau^2}}, \\ H_\varphi &= \sqrt{\left(\frac{\partial x}{\partial \varphi}\right)^2 + \left(\frac{\partial y}{\partial \varphi}\right)^2 + \left(\frac{\partial z}{\partial \varphi}\right)^2} = a\sqrt{(\sigma^2 - 1)(1 - \tau^2)}. \end{aligned} \quad (2)$$

For the sake of simplicity, and also based on the corresponding theory of the growth of spherical crystals,^{34–36} everywhere below we use the quasi-stationary approximation for the temperature field and the field of impurity concentration around the growing particle, i.e. $\nabla^2 T = 0$ and $\nabla^2 C = 0$, where T and C stand for the temperature and concentration distributions in the liquid phase (at $\sigma \geq \sigma_0$; σ_0 designates the surface of an ellipsoidal crystal). Also, to find the quasi-stationary solution, we assume that the temperature and concentration distributions depend on only one variable σ , i.e. $T = T(\sigma)$ and $C = C(\sigma)$. In addition, we assume that the temperature field inside the ellipsoidal crystal (in the solid phase) is constant and neglect the diffusion of impurity in the solid phase.

2.1 | Ellipsoidal crystal in a supercooled single-component melt

Let us now consider the growth of an ellipsoidal crystal in one-component melt ($C = 0$), which is caused by its instant cooling. The temperature field satisfies the quasi-stationary thermal conductivity equation, which reads as

$$\frac{d}{d\sigma} \left[(\sigma^2 - 1) \frac{dT}{d\sigma} \right] = 0. \quad (3)$$

The heat balance condition at the surface of an ellipsoidal crystal can be written in the form of

$$\frac{\rho_s L}{\lambda_l} V_n = -\nabla T \mathbf{n}, \quad (4)$$

where ρ_s represents the density of the solid material, L is the latent heat parameter, λ_l is the thermal conductivity of liquid, V_n is the normal growth velocity, and \mathbf{n} is the normal vector to the ellipsoidal surface.

Taking into account that the normal velocity can be expressen in terms of the growth rate $\dot{\sigma}_0$ of the surface coordinate $\sigma = \sigma_0$ as $V_n = H_\sigma \dot{\sigma}_0$, and rewriting ∇ in the ellipsoidal coordinates, we arrive at

$$\dot{\sigma} = -\frac{\lambda_l}{a^2 \rho_s L} \frac{dT}{d\sigma} = \frac{\beta_*}{a} (T_p - T), \quad \sigma = \sigma_0, \quad (5)$$

where T_p represents the phase transition temperature, β_* is the kinetic coefficient, and

$$(\nabla T)_\sigma = \frac{1}{a} \sqrt{\frac{\sigma^2 - 1}{\sigma^2 - \tau^2}} \frac{\partial T}{\partial \sigma}.$$

The second (kinetic) boundary condition (5) shows that the growth rate $\dot{\sigma}$ at $\sigma = \sigma_0$ is defined by the crystallization driving force $T_p - T$.

To close the problem, we also assume that the temperature is fixed at a large distance from the ellipsoidal particle, i.e.

$$T \rightarrow T_l, \quad \sigma \gg 1. \quad (6)$$

Solving the problem (3)-(6), we come to the temperature profile $T(\sigma)$ in the liquid phase and the crystal growth rate $\dot{\sigma}_0$ in the form of

$$\begin{aligned} T(\sigma) &= T_l + C_1 \ln \left(\frac{\sigma - 1}{\sigma + 1} \right), \quad C_1 = \frac{(\beta_*/a) (T_p - T_l)}{(\beta_*/a) \ln \left(\frac{\sigma_0 - 1}{\sigma_0 + 1} \right) - \frac{2\varepsilon_1}{\sigma_0^2 - 1}}, \\ \dot{\sigma}_0 &= \frac{-2\varepsilon_1}{\sigma_0^2 - 1} \frac{(\beta_*/a) (T_p - T_l)}{(\beta_*/a) \ln \left(\frac{\sigma_0 - 1}{\sigma_0 + 1} \right) - \frac{2\varepsilon_1}{\sigma_0^2 - 1}}, \quad \varepsilon_1 = \frac{\lambda_l}{a^2 \rho_s L}. \end{aligned} \quad (7)$$

The volume V of an ellipsoidal particle and its growth rate dV/dt can be easily found with allowance for the crystal semiaxes $a\sqrt{\sigma_0^2 - 1}$ and $a\sigma_0$ (Figure 1) and read as

$$V = \frac{4}{3} \pi a^3 (\sigma_0^2 - 1) \sigma_0, \quad \frac{dV}{dt} = \frac{4}{3} \pi a^3 (3\sigma_0^2 - 1) \dot{\sigma}_0. \quad (8)$$

Analysing expressions (7) we see that $\dot{\sigma}_0 = \dot{\sigma}_0(\sigma_0, \Delta T)$, where $\Delta T = T_p - T_l$ stands for the melt supercooling. In addition, expression (8) demonstrates that $\sigma_0 = \sigma_0(V)$. This dependence is defined by the cubic equation

$$\sigma_0^3 - \sigma_0 = \frac{3V}{4\pi a^3}. \quad (9)$$

Keeping this in mind we express the crystal volume growth rate dV/dt in terms of two variables V and ΔT in the form of

$$\frac{dV}{dt} = \frac{4}{3}\pi a^3 [3\sigma_0^2(V) - 1] \dot{\sigma}_0(\sigma_0(V), \Delta T), \quad \Delta T = T_p - T_l. \quad (10)$$

For the convenience of analyzing the dynamics of the growth rate (10), we introduce the dimensionless variables and parameters

$$V_1 = \frac{3V}{4\pi a^3}, \quad \Delta_1 = \frac{T_p - T_l}{T_l}, \quad t_1 = \frac{\beta_* T_l t}{a}, \quad \alpha_1 = \frac{\beta_*}{2a\epsilon_1},$$

$$G_R(V_1, \Delta_1) = \frac{dV_1}{dt_1} = \frac{(3\sigma_0^2 - 1)\Delta_1}{1 - \alpha_1(\sigma_0^2 - 1) \ln\left(\frac{\sigma_0 - 1}{\sigma_0 + 1}\right)},$$

where V_1 , Δ_1 , t_1 , and G_R represent the dimensionless volume, supercooling, time, and volume growth rate. This rate is shown in Figure 2 as a function of crystal volume V_1 for different supercoolings Δ_1 . As would be expected, the crystal volume growth rate increases with increasing V_1 and Δ_1 .

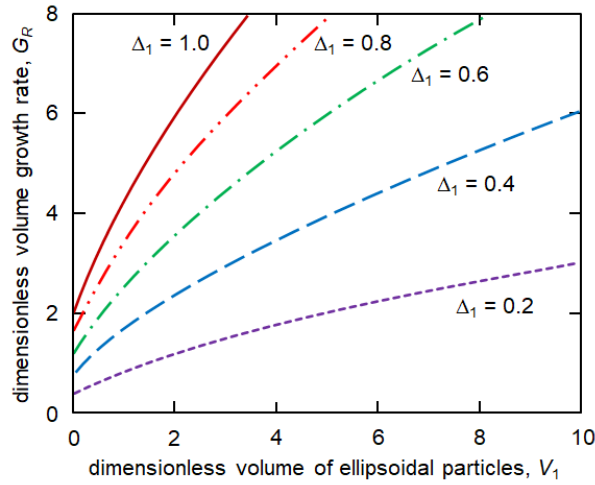


FIGURE 2 The dimensionless volume growth rate G_R of ellipsoidal crystals at fixed dimensionless supercoolings Δ_1 . Parameters used in calculations are:³⁴ $\lambda_l = 63 \text{ J m}^{-1} \text{ K}^{-1} \text{ s}^{-1}$, $L_V = \rho_s L = 7 \cdot 10^9 \text{ J m}^{-3}$, $a = 1.26 \cdot 10^{-9} \text{ m}$, $\beta_* = 10^{-26} \text{ m s}^{-1} \text{ K}^{-1}$.

2.2 | Ellipsoidal crystal in a supercooled binary melt

Let us now analyze the growth of an ellipsoidal crystal in a binary melt where the phase transition temperature depends on the impurity concentration C . In this case, the moving-boundary problem in the steady-state approximation becomes³²

$$\frac{d}{d\sigma} \left[(\sigma^2 - 1) \frac{dT}{d\sigma} \right] = 0, \quad \frac{d}{d\sigma} \left[(\sigma^2 - 1) \frac{dC}{d\sigma} \right] = 0, \quad (11)$$

$$\dot{\sigma} = -\frac{\lambda_l}{a^2 \rho_s L} \frac{dT}{d\sigma} = \frac{\beta_*}{a} (T_p - mC - T), \quad (1 - k_0)C\dot{\sigma} = -\frac{D}{a^2} \frac{dC}{d\sigma}, \quad \sigma = \sigma_0, \quad (12)$$

$$T \rightarrow T_l, \quad C \rightarrow C_l, \quad \sigma \gg 1. \quad (13)$$

where k_0 and m are the equilibrium partition coefficient and the liquidus slope, D is the diffusion coefficient of impurity dissolved in the melt, and C_l is a constant impurity concentration far from the growing particle.

The solution to the problem (11)-(13) reads as

$$T(\sigma) = T_l + C_1 \ln \left(\frac{\sigma - 1}{\sigma + 1} \right), \quad C(\sigma) = C_l + C_2 \ln \left(\frac{\sigma - 1}{\sigma + 1} \right), \quad \dot{\sigma}_0 = \frac{-2\varepsilon_1 C_1}{\sigma_0^2 - 1}, \quad (14)$$

$$C_1 = \frac{\frac{\beta_*}{a} \left[T_p - T_l - mC_l - mC_2 \ln \left(\frac{\sigma_0 - 1}{\sigma_0 + 1} \right) \right]}{\frac{\beta_*}{a} \ln \left(\frac{\sigma_0 - 1}{\sigma_0 + 1} \right) - \frac{2\varepsilon_1}{\sigma_0^2 - 1}} = \frac{DC_2}{a^2 \varepsilon_1 (1 - k_0) \left[C_l + C_2 \ln \left(\frac{\sigma_0 - 1}{\sigma_0 + 1} \right) \right]}, \quad (15)$$

where C_2 is defined by the following quadratic equation

$$\alpha C_2^2 + \beta C_2 + \gamma = 0, \quad (16)$$

$$\alpha = \beta_* m a \varepsilon_1 (1 - k_0) \ln^2 \left(\frac{\sigma_0 - 1}{\sigma_0 + 1} \right), \quad \gamma = -\beta_* (T_p - T_l - mC_l) a \varepsilon_1 (1 - k_0) C_l,$$

$$\beta = \beta_* \ln \left(\frac{\sigma_0 - 1}{\sigma_0 + 1} \right) \left[mC_l a \varepsilon_1 (1 - k_0) + \frac{D}{a} - (T_p - T_l - mC_l) a \varepsilon_1 (1 - k_0) \right] - \frac{2\varepsilon_1 D}{\sigma_0^2 - 1}.$$

An important point is that $\dot{\sigma}_0$ is a function of σ_0 and the melt supercooling $\Delta = T_p - T_l - mC_l$ for a binary system, i.e. $\dot{\sigma}_0 = \dot{\sigma}_0(\sigma_0, \Delta T)$ (see, for details, expressions (14)-(16)). Then, by analogy with expression (10), the crystal volume growth rate dV/dt represents a function of two variables V and ΔT

$$\frac{dV}{dt} = \frac{4}{3} \pi a^3 [3\sigma_0^2(V) - 1] \dot{\sigma}_0(\sigma_0(V), \Delta T), \quad \Delta T = T_p - T_l - mC_l, \quad (17)$$

where $\sigma_0(V)$ is a root of the cubic equation (9) and $\dot{\sigma}_0 = \dot{\sigma}_0(\sigma_0(V), \Delta T)$ is defined by expressions (14)-(16).

2.3 | Ellipsoidal crystal in a supersaturated solution

Now we consider the evolution of an ellipsoidal crystal in a supersaturated solution. In this case, the mass transfer boundary-value problem takes the form

$$\frac{d}{d\sigma} \left[(\sigma^2 - 1) \frac{dC}{d\sigma} \right] = 0, \quad (18)$$

$$\dot{\sigma} = -\frac{D}{a^2(1 - k_0)C} \frac{dC}{d\sigma} = \frac{\beta_*}{a} (C - C_p), \quad \sigma = \sigma_0, \quad (19)$$

$$C \rightarrow C_l, \quad \sigma \gg 1. \quad (20)$$

Here C_p stands for the concentration at saturation, and β_* represents the kinetic coefficient, which is measured in other units than the previously introduced kinetic coefficient for crystal growth in melts.

The boundary-value problem (18)-(20) takes the following solution

$$C(\sigma) = C_l + C_3 \ln \left(\frac{\sigma - 1}{\sigma + 1} \right), \quad \dot{\sigma}_0 = \frac{\beta_*}{a} \left[\Delta C + C_3 \ln \left(\frac{\sigma_0 - 1}{\sigma_0 + 1} \right) \right], \quad (21)$$

where C_3 is defined by the quadratic equation

$$\ln^2 \left(\frac{\sigma_0 - 1}{\sigma_0 + 1} \right) C_3^2 + bC_3 + C_l \Delta C = 0, \quad (22)$$

$$b = C_l \ln \left(\frac{\sigma_0 - 1}{\sigma_0 + 1} \right) + \Delta C \ln \left(\frac{\sigma_0 - 1}{\sigma_0 + 1} \right) + \frac{2D}{a\beta_*(1 - k_0)(\sigma_0^2 - 1)},$$

and $\Delta C = C_l - C_p$ is the supersaturation.

It is significant to note that $\dot{\sigma}_0$ is a function of σ_0 and the supersaturation ΔC , i.e. $\dot{\sigma}_0 = \dot{\sigma}_0(\sigma_0, \Delta C)$ (see, for details, expressions (21) and (22)). In this case, the crystal volume growth rate dV/dt represents a function of two variables V and ΔC and reads as

$$\frac{dV}{dt} = \frac{4}{3} \pi a^3 [3\sigma_0^2(V) - 1] \dot{\sigma}_0(\sigma_0(V), \Delta C), \quad \Delta C = C_l - C_p, \quad (23)$$

where $\sigma_0(V)$ is a root of the cubic equation (9) and $\dot{\sigma}_0 = \dot{\sigma}_0(\sigma_0(V), \Delta C)$ is defined by expressions (21) and (22).

Let us especially highlight that the analytical solutions (9), (10), (17) and (23) describing the ellipsoidal particles correspond to the case of spherical crystals if $\sigma_0 \gg 1$.³⁷ Indeed, the larger the volume of an ellipsoidal crystal, the less it differs from a spherical particle (Figure 3). This means that the greatest difference in the growth dynamics of ellipsoidal crystals from spherical ones occurs at the initial stages when the particle sizes are small enough and the contribution from their ellipsoidal shape is significant.

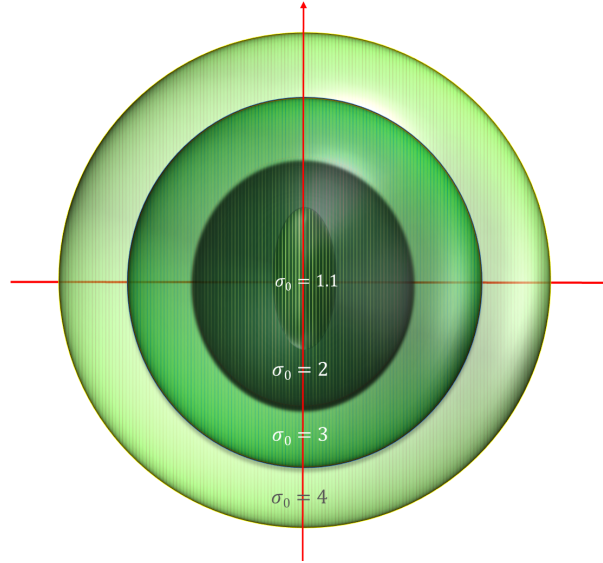


FIGURE 3 Cross-sections of ellipsoidal crystals with different surfaces $\sigma = \sigma_0$.

3 | CONCLUSION

In summary, new expressions for crystal volume growth rates (10), (17) and (23) describing the evolution of individual aggregates in supercooled one-component and binary melts as well as in supersaturated solutions are derived with allowance for the prolate ellipsoidal coordinates. These steady-state expressions determine the volume growth rate dV/dt as a function of current particle volume V and supercooling ΔT (supersaturation ΔC). As this takes place the liquid supercooling (supersaturation) should be different for each of the metastable systems under consideration. To study the evolution of a particulate ensemble of ellipsoidal crystals using the growth rates (10), (17), or (23), we need to analyze an integro-differential system of kinetic and balance equations for the crystal-volume distribution function and liquid metastability (supercooling or supersaturation). Such a model can be formulated by analogy with the previously known model of the evolution of an ensemble of spherical crystals.^{5,37} In addition, to study a simultaneous occurrence of the directional and bulk crystallization a mushy layer theory describing the growth of dendrite-like structures and nucleation of crystals should be taken into consideration.^{38–45} These tasks form the directions of future research, taking into account the ellipsoidal shape of crystals.

ACKNOWLEDGMENTS

This work was supported by the Russian Science Foundation (grant no. 18-19-00008).

Author contributions

The authors contributed equally to the present research article.

Conflict of interest

The authors declare no potential conflict of interests.

ORCID

Margarita A. Nikishina <https://orcid.org/0000-0001-5408-4498>

Dmitri V. Alexandrov <https://orcid.org/0000-0002-6628-745X>

References

1. WC Winegard. *An Introduction to the Solidification of Metals*. London: Institute of Metals; 1964.
2. DM Herlach. *Phase Transformations in Multicomponent Melts*. Weinheim: Wiley-VCH; 2008.
3. Galenko PK, Alexandrov DV. From atomistic interfaces to dendritic patterns. *Phil. Trans. R. Soc. A*. 2018;376:20170210.
4. Alexandrov DV. Nucleation and crystal growth in binary systems. *J. Phys. A: Math. Theor.*. 2014;47:125102.
5. Alexandrov DV, Nizovtseva IG. On the theory of crystal growth in metastable systems with biomedical applications: Protein and insulin crystallization. *Phil. Trans. R. Soc. A*. 2019;377:20180214.
6. Ivanov AA, Alexandrova IV, Alexandrov DV. Phase transformations in metastable liquids combined with polymerization. *Phil. Trans. R. Soc. A*. 2019;377:20180215.
7. Buyevich YuA, Mansurov VV. Kinetics of the intermediate stage of phase transition in batch crystallization. *J. Cryst. Growth*. 1990;377:861–867.
8. Buyevich YA, Goldobin YM, Yasnikov GP. Evolution of a particulate system governed by exchange with its environment. *Int. J. Heat Mass Trans.*. 1994;37:3003–3014.
9. Alexandrov DV. Nonlinear dynamics of polydisperse assemblages of particles evolving in metastable media. *Eur. Phys. J. Special Topics*. 2020;229:383–404.
10. Makoveeva EV, Alexandrov DV. A complete analytical solution of the Fokker-Planck and balance equations for nucleation and growth of crystals. *Phil. Trans. R. Soc. A*. 2018;376:20170327.
11. Makoveeva EV, Alexandrov DV. Effects of nonlinear growth rates of spherical crystals and their withdrawal rate from a crystallizer on the particle-size distribution function. *Phil. Trans. R. Soc. A*. 2019;377:20180210.
12. Buyevich YA, Alexandrov DV. On the theory of evolution of particulate systems. *IOP Conference Series: Materials Science and Engineering*. 2017;192:012001.
13. Alexandrov DV. Nucleation and crystal growth kinetics during solidification: The role of crystallite withdrawal rate and external heat and mass sources. *Chem. Eng. Sci.*. 2014;117:156–160.
14. Lifshitz EM, Pitaevskii LP. *Physical Kinetics*. Oxford, UK: Pergamon; 1981.
15. Alyab'eva AV, Buyevich YuA, Mansurov VV. Evolution of a particulate assemblage due to coalescence combined with coagulation. *J. Phys. II France*. 1994;4:951–957.
16. Lifshitz IM, Slyozov VV. The kinetics of precipitation from supersaturated solid solutions. *J. Phys. Chem. Solids*. 1961;19:35–50.
17. Slezov VV. *Kinetics of First-Order Phase Transitions*. Weinheim, Germany: Wiley, VCH; 2009.
18. Alexandrov DV. On the theory of Ostwald ripening in the presence of different mass transfer mechanisms. *J. Phys. Chem. Solids*. 2016;91:48–54.

19. Alexandrov DV, Alexandrova IV. From nucleation and coarsening to coalescence in metastable liquids. *Phil. Trans. R. Soc. A*. 2020;378:20190247.
20. Martin S, Kauffman P. The evolution of under-ice melt ponds, or double diffusion at the freezing point. *J. Fluid Mech.* 1974;64:507–527.
21. Ovsienko DE, Alfintsev GA. Kinetics and shape of crystal growth from the melt for substances with low L/kT values. *J. Cryst. Growth*. 1974;26:233–238.
22. Nestler B, Danilov D, Galenko P. Crystal growth of pure substances: phase-field simulations in comparison with analytical and experimental results. *J. Comput. Phys.* 2005;207:221–239.
23. Gasser U, Weeks ER, Schofield A, Pusey PN, Weitz DA. Real-space imaging of nucleation and growth in colloidal crystallization. *Science*. 2001;292:258–262.
24. Prieler R, Hubert J, Li D, Verleye B, Haberkern R, Emmerich H. An anisotropic phase-field crystal model for heterogeneous nucleation of ellipsoidal colloids. *J. Phys.: Condens. Matter*. 2009;21:464110.
25. Alexandrov DV, Galenko PK. The shape of dendritic tips. *Phil. Trans. R. Soc. A*. 2020;378:20190243.
26. De Yoreo JJ, Vekilov PG. Principles of crystal nucleation and growth. *Rev. Mineral. Geochem.* 2003;54:57–93.
27. Mann S. *Bioinorganic Materials Chemistry: Principles and Concepts in Bioinorganic Materials Chemistry*. New York: Oxford University Press; 2001.
28. Thieme K, Avramov I, Rüssel C. The mechanism of deceleration of nucleation and crystal growth by the small addition of transition metals to lithium disilicate glasses. *Sci. Rep.* 2016;6:25451.
29. Ocaña M, Morales MP, Serna CJ. The growth mechanism of $\alpha - \text{Fe}_2\text{O}_3$ ellipsoidal particles in solution. *J. Colloid Int. Sci.* 1995;171:85–91.
30. Alexandrov DV. Nucleation and evolution of spherical crystals with allowance for their unsteady-state growth rates. *J. Phys. A: Math. Theor.* 2018;51:075102.
31. Alexandrov DV, Nizovtseva IG, Alexandrova IV. On the theory of nucleation and nonstationary evolution of a polydisperse ensemble of crystals. *Int. J. Heat Mass Trans.* 2019;128:46–53.
32. Alexandrov DV, Alexandrova IV. On the theory of the unsteady-state growth of spherical crystals in metastable liquids. *Phil. Trans. R. Soc. A*. 2019;377:20180209.
33. Korn GA, Korn TM. *Mathematical Handbook for Scientists and Engineers: Definitions, Theorems, and Formulas for Reference and Review*. New York: McGraw-Hill Book Company; 1968.
34. Alexandrov DV, Malygin AP. Transient nucleation kinetics of crystal growth at the intermediate stage of bulk phase transitions. *J. Phys. A: Math. Theor.* 2013;46:455101.
35. Alexandrov DV. Nucleation and growth of crystals at the intermediate stage of phase transformations in binary melts. *Phil. Mag. Lett.* 2014;94:786–793.
36. Alexandrov DV, Makoveeva EV. The Gibbs-Thomson effect in the evolution of particulate assemblages in a metastable liquid. *Phys. Lett. A*. 2020;384:126259.
37. Alexandrova IV, Alexandrov DV. Dynamics of particulate assemblages in metastable liquids: a test of theory with nucleation and growth kinetics. *Phil. Trans. R. Soc. A*. 2020;378:20190245.
38. Huppert HE. The fluid mechanics of solidification. *J. Fluid Mech.* 1990;212:209–240.
39. Hills RN, Loper DE, Roberts PH. A thermodynamically consistent model of a mushy zone. *Q. J. Appl. Maths.* 1983;36:505–539.

40. Alexandrov DV, Ivanov AA, Alexandrova IV. Analytical solutions of mushy layer equations describing directional solidification in the presence of nucleation. *Phil. Trans. R. Soc. A.* 2018;376:20170217.
41. Nizovtseva IG, Alexandrov DV. The effect of density changes on crystallization with a mushy layer. *Phil. Trans. R. Soc. A.* 2020;378:20190248.
42. Fowler AC. The formation of freckles in binary alloys. *IMA J. Appl. Math.*. 1985;35:159–174.
43. VT Borisov. *Theory of Two-Phase Zone of a Metal Ingot*. Moscow, Russia: Metallurgiya Publishing House; 1987.
44. Alexandrov DV, Bashkirtseva IA, Ryashko LB. Nonlinear dynamics of mushy layers induced by external stochastic fluctuations. *Phil. Trans. R. Soc. A.* 2018;376:20170216.
45. Alexandrov DV, Bashkirtseva IA, Malygin AP, Ryashko LB. Sea ice dynamics induced by external stochastic fluctuations. *Pure Appl. Geophys.*. 2013;170:2273–2282.

How to cite this article: Nikishina M.A. and Alexandrov D.V. (2020), Mathematical modeling of the growth of ellipsoidal crystals in metastable melts and solutions, *Math Meth Appl Sci.*,