



Selection criterion of a stable dendrite growth in rapid solidification



D.V. Alexandrov^a, D.A. Danilov^{b,*}, P.K. Galenko^c

^a Ural Federal University, Department of Mathematical Physics, Ekaterinburg, 620000, Russian Federation

^b Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology (INT), 76344 Eggenstein-Leopoldshafen, Germany

^c Friedrich-Schiller-Universität-Jena, Physikalisches-Astronomische Fakultät, 07743 Jena, Germany

ARTICLE INFO

Article history:

Received 21 March 2016

Accepted 18 May 2016

Keywords:

Solidification
Interface
Crystal
Dendrite
Solute
Non-Fickian diffusion

ABSTRACT

We present an analysis of a free dendrite growing in a binary mixture under non-isothermal conditions. The stable growth mode is analyzed through the solvability condition giving the stability criterion for the dendrite tip as a function of the thermal Péclet number, Pe_T , and ratio, $W = V/V_D$, of the dendrite velocity V and solute diffusion speed V_D in bulk liquid. We extend previous studies limited to small values of the Péclet numbers, by considering the effect of the anisotropy of surface energy for the needle-like dendrite growing at arbitrary Péclet numbers and under local non-equilibrium solute diffusion described by a hyperbolic type of transport equation. Transitions in growth regimes, namely, from solute diffusion-limited to thermo-solutal regime and, finally, to pure thermally controlled regime of the anisotropic dendrite are derived and revealed. Limiting cases of known criteria for anisotropic dendrite growing at small and high growth Péclet numbers are provided. A comparison with the previously obtained criterion of marginal stability of rapidly growing dendrite is made.

© 2016 Elsevier Ltd. All rights reserved.

1. Introduction

Solidification processes from supersaturated or undercooled mixtures (suspensions, liqueurs, solutions and melts) exhibit formation of dendritic patterns due to the Mullins–Sekerka instability [1–4]. For description of crystal's forms, classical Ivantsov's solutions [5–9] of the dendritic problem were obtained for needle-like shapes of dendrites in the limit of zero surface tension. The Ivantsov solution depends only on the Péclet number and in that way it provides the first relationship between the dendrite tip velocity V and the tip diameter ρ . Because the Ivantsov solution does not provide information on V and ρ separately, a second condition for these both parameters has been suggested in the form of stability criterion [2]. This criterion follows from a solvability theory which predicts the marginal mode of the dispersion relation for perturbations on the anisotropic surface of dendrite [10,11]. Mathematically, the criterion allows for selecting a stable growth mode from the continuous family of all available Ivantsov solutions for a given Péclet number. As a result, the solvability theory predicts the second combination of parameters in the following form

$$\sigma^* = \frac{2d_0D_T}{\rho^2V}, \quad (1)$$

where D_T is the thermal diffusivity, d_0 is the capillary length and σ^* is the dimensionless scaling factor defined in the case of thermal problem by the crystalline anisotropy as

$$\sigma^* \propto \begin{cases} \beta^{7/4}, & \text{small Peclét numbers [10, 11], } Pe \ll 1, \\ \frac{\beta^{7/4}}{(1+a_1\sqrt{\beta Pe})^2}, & \text{arbitrary Peclét numbers [12, 13],} \end{cases} \quad (2)$$

with $Pe = \rho V/(2D_T)$ the Peclét number, β the stiffness (small anisotropy parameter), and a_1 is a constant. Thus, the solutions of the Ivantsov-type and the criterion of stable growth mode give a system of equations that defines a unique combination of V and ρ for a given undercooling or temperature gradient. Such predictions were intensively tested against experimental data during past decades [3,4,14,15].

Criteria (1), (2) of stable dendrite growth include crystalline anisotropy of solid–liquid interface for the dendrite growth in a pure (one-component) system. These criteria can be tested in a computational experiment in which specially created conditions are suitable only for the considered concrete limiting case [16,17]. Additionally, a combination of two or more processes having different length scales exists in real experimental conditions of crystal growth. For example, influence of external electromagnetic or gravitational fields, as well as transport processes in non-isothermal multi-component mixtures, may drastically change the crystal growth kinetics [18,15]. These processes should be taken into account in the theory to predict formation of realistic

* Corresponding author.

E-mail address: denis.danilov@kit.edu (D.A. Danilov).

crystal patterns originating under influence of predominant heat and mass transfer [19,20]. Indeed, bulk transport of heat and mass together with interfacial properties (anisotropy of surface energy and growth kinetics) drastically affect on the shape of dendritic crystals in inorganic and organic mixtures [21,22]. As experiments show, anisotropy of crystalline growth controls formation of dendritic nanostructures and highly ordered fractal-like aggregates [23,24]. Control of growing nano-crystals may also be provided in suspensions by changing the chemical content and chemical reactions together with anisotropy of growth [25–29]. Also, it is important to note that modern experimental techniques for inorganic samples allow access large undercoolings, high temperature and concentration gradients as well as fast velocities of phase transformations. For example, in observation and evaluation of crystal growth kinetics during experimentation with levitated melt droplets [30,31], the interface velocity reaches the values of 10–100 m/s and the liquid phase can be undercooled in a wide range from 10 to 400 K below the liquidus temperature [32]. For the large driving forces connected with such undercoolings and with increasing crystal growth velocity, deviations from local thermodynamic equilibrium occur at the advancing solid–liquid interface, and metastable states can be retained in the bulk phases [18]. More specifically, the formation of metastable supersaturated solid solutions has been evidenced for the case of rapid dendritic growth [31]. Theoretical predictions of the formation of metastable phases are based on models that include deviations from local thermodynamic equilibrium at the dendritic interface and in diffusion field which result in hyperbolic mass transport equation for solute diffusion [33,34]. The validity of hyperbolic type models has been verified in molecular dynamics simulations of solute trapping effect by the rapidly moving fronts [35] and by coarse graining derivations of equations of fast phase transitions [36]. Therefore, the main goal of the present work is to advance the theory of crystal growth for simultaneous inclusion of significant effects which may manifest in a wide range of solid–liquid interface velocity.

The focus of the present work lies in description of a whole measurable range [32,18] of undercoolings, temperature gradients, cooling rates and solidification velocities on the basis of unified approach to dendritic growth phenomenon. Such motivation requires a development of a theory for the stable mode of the non-isothermal dendrite growing in a chemically binary system with anisotropy of the solid–liquid interface.

2. Statement of the problem

Consider the growth of a parabolic dendrite in a binary undercooled liquid under local non-equilibrium conditions. In the case of isotropic shape of dendrite, such system was analyzed in Refs. [33,34]. In the present work, we re-formulate equations for the same local non-equilibrium system additionally to the anisotropic dendrite growth.

Neglecting the diffusion in the solid phase (due to much slower diffusion transport in comparison with diffusion in the liquid phase) and convection of the liquid, the concentration field is governed by

$$\tau_D \frac{\partial^2 C_l}{\partial t^2} + \frac{\partial C_l}{\partial t} = D_C \nabla^2 C_l, \quad (3)$$

where C_l is the solute concentration in the liquid, D_C is the diffusion coefficient of a solute, t is the time and τ_D is the time of the local diffusion relaxation of the mass flux to its steady-state value.

Because a characteristic relaxation time of the temperature field is much faster than a relaxation time of the solute concentration, the heat transfer in both phases is described by the parabolic equations:

$$\frac{\partial T_l}{\partial t} = D_T \nabla^2 T_l, \quad \frac{\partial T_s}{\partial t} = D_T \nabla^2 T_s, \quad (4)$$

where T_l and T_s are the temperatures in the liquid and solid phases, respectively, and D_T stands for the thermal diffusivity equals in both phases.

At the dendritic interface, conservation of mass and energy gives the boundary conditions of the form

$$\tau_D \frac{\partial}{\partial t} [(C_l - C_s) \vec{v} \cdot \vec{n}] + (C_l - C_s) \vec{v} \cdot \vec{n} + D_C \nabla C_l \cdot \vec{n} = 0, \quad (5)$$

$$T_Q \vec{v} \cdot \vec{n} = D_T (\nabla T_s - \nabla T_l) \cdot \vec{n}, \quad (6)$$

where \vec{n} is the unit vector normal to the dendrite interface, \vec{v} is the interface velocity, k_v is the interface velocity dependent coefficient of the solute distribution,

$$C_s = k_v C_l \quad (7)$$

is the concentration in the solid phase at the dendritic interface, $T_Q = Q/c_p$ is the temperature for adiabatic crystallization (or the measure of hypercooling limit), Q is the latent heat released per unit volume of solid and c_p is the specific heat at a constant pressure.

The temperature at the dendrite interface $T_i = T_l = T_s$ is a function of the crystallization temperature T_M of a pure liquid, velocity-dependent liquidus slope m_v , solute concentration C_l , anisotropic capillary length $d(\theta, \phi)$ and the local curvature $1/R$ of the front

$$T_i = T_M - m_v C_l - T_Q R^{-1} d(\theta, \phi). \quad (8)$$

Here θ and ϕ are the spherical angles which define the orientation of the normal to the dendrite interface to its growth direction.

In the case of the cubic symmetry, the capillary length $d(\theta, \phi)$ is described by

$$d(\theta, \phi) = d_0 \left\{ 1 - \beta \left[\cos^4 \theta + \sin^4 \theta \left(1 - 2 \sin^2 \phi \cos^2 \phi \right) \right] \right\}, \quad (9)$$

where d_0 is the capillary constant and β stands for the stiffness which depends on a small anisotropy parameter ε_c of surface energy. Considering a case of axisymmetric needle-like crystal, Eq. (9) can be reduced by averaging over ϕ to the following form (see Ref. [37])

$$d(\theta) = d_0 \{ 1 - \beta \cos(4\theta) \}, \quad (10)$$

in which the stiffness is given by $\beta = 15\varepsilon_c$ for cubic crystals. We assume that the selection criterion σ^* , which will be obtained in the following analysis, must have the scaling $\sigma^* \propto \beta^n$ with the same exponent n and the same general form [see, for example, Eq. (2)] if the anisotropy (9) or (10) are taken into account. An existence of the same scalings in these cases has been shown in Refs. [38,39] in which a difference consists only in a constant of proportionality for the scaling $\sigma^* \propto \beta^n$. Therefore, for obtaining selection criterion σ^* we shall use the case of simplest form of anisotropy (10) under the assumption that the final scaling might be applied to the three dimensional case of dendrite growth.

The velocity-dependent functions of kinetic liquidus slope m_v and non-equilibrium solute partitioning k_v are defined, respectively, as [40,41]

$$m_v(V) = \frac{m_e}{1 - k_e} \left\{ 1 - k_v + \ln \left(\frac{k_v}{k_e} \right) + (1 - k_v)^2 \frac{V}{V_D} \right\}, \quad V < V_D, \\ m_v = \frac{m_e \ln k_e}{k_e - 1}, \quad V \geq V_D, \quad (11)$$

and

$$k_v(V) = \frac{(1 - V^2/V_D^2)[k_e + (1 - k_e)C_\infty] + V/V_{Dl}}{1 - V^2/V_D^2 + V/V_{Dl}}, \quad V < V_D,$$

Download English Version:

<https://daneshyari.com/en/article/7055389>

Download Persian Version:

<https://daneshyari.com/article/7055389>

[Daneshyari.com](https://daneshyari.com)