SELF-SIMILAR SOLUTIONS OF THE STEFAN PROBLEM

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Investigation is made of one of the self-similar regimes in the problem of a crystal growing from a pure melt with an isothermal surface. This regime is shown to exist only in the case of two-dimensional, cylindrical, or spherical geometry of the crystal and also when a two-dimensional crystal grows on a surface isometric to the surface of revolution. Modeling of the spherical crystal growth by two-dimensional crystallization on the surface of revolution is discussed.

The Stefan problem is termed a mathematical model of heat transfer processes (diffusion) accompanied by phase changes in a medium with an unknown position of the phase boundary. The problems of heat flux in a superheated melt (Czochralski, Bridgman, Chalmers crystal growth, ice crystallization, cast solidification), in a supercooled melt (dendritic growth), on diffusion (crystal growth from a solution) fall in this category. One of the trends in the Stefan problem investigation is finding analytical solutions. The known exact solutions corresponding to cylindrical, spherical, paraboloidal, and elliptical forms of growth [3] possess certain symmetries. Therefore it is natural to study solutions with a sufficiently high degree of symmetry (the presence of the latter simplifies the problem) when searching for other geometries of growth.

The present work deals with the case when a family of isotherms in the process of crystal growth (henceforth just this variant is under consideration) remains permanent, with a temperature on each surface varying with time. In other words, there exists a time-independent (n — 1)-parametric group of transforms of a n-dimensional manifold M, in which a crystal is growing, relative to which both the heat conduction equation and the boundary conditions on a phase boundary are invariant. Here temperature distribution is a function of time and some scalar function of a space variable and the problem is reduced to the one-dimensional problem with a movable boundary which essentially simplifies the initial formulation.

Consider a process of crystal growth from a melt with some time interval $\tau \in (\tau_0, \tau_1)$. Assume that at any $\tau \in (\tau_0, \tau_1)$ a crystal surface $\Gamma(\tau)$ is a smooth (n — 1)-dimensional submanifold of an n-dimensional manifold M which subdivides M into two regions, namely, M_1 occupied with a solid phase and M_2 with a liquid phase. The temperature distribution $T = T_i$, $x \in M_1$ satisfies the heat conduction equation

$$c_i(T)\,\partial T/\partial \tau = \operatorname{div}(\varkappa_i(T)\nabla T) \tag{1}$$

and the heat balance condition for $\Gamma(\tau)$

$$(\varkappa_1 \nabla T_1 - \varkappa_2 \nabla T_2)\,\mathbf{n} = Lv. \tag{2}$$

A crystal surface is isothermal

$$T|_{\Gamma(\tau)} \equiv T_0 = \text{const}. \tag{3}$$

Here **n** is the unit normal to $\Gamma(\tau)$, v is the growth rate in the direction of the normal.

In the domain $\bar{M} = \cup\Gamma(\tau) \subseteq M$ the function $\gamma(x)$ is naturally determined as a moment of time γ at which the crystal surface $\Gamma(\gamma)$ goes through the point x. Then $\Gamma(\tau)$ is prescribed by the equation $\gamma(x) = \tau$. We investigate the case when a family of isotherms remains permanent in a solidification process, however a temperature on each surface varies with time. From (3) it follows that the family of isotherms in the region M coincides with the family of surfaces of the level of the function $\gamma(x)$

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and, consequently, in $\bar{M}$ T is a function of (τ, γ). Now we try to elucidate at what conditions T may be represented in the form:

$$T(\tau, x) = t(\tau, \gamma(x)). \tag{4}$$

Substituting $\nabla T_i \cdot n = (\partial t_i/\partial\gamma)(\nabla\gamma \cdot n) = (\partial t_i/\partial\gamma) \; |\nabla\gamma| , \; v = |\nabla\gamma|^{-1}$ into (2) we obtain on $\Gamma(\tau)$

$$|\nabla\gamma|^{-2} = v^2 = \frac{\varkappa_1}{L}\frac{\partial t_1}{\partial\gamma} - \frac{\varkappa_2}{L}\frac{\partial t_2}{\partial\gamma}.$$

The right-hand side of this equality is a function of (τ, γ), while the l.h.s. is a function of x. Therefore, we have

$$|\nabla\gamma(x)| = f(\gamma(x)) \tag{5}$$

on $\Gamma(\tau)$ for some function of f and $\tau \in (\tau_0, \tau_1)$. But at τ running through the segment (τ_0, τ_1) the moving surface $\Gamma(\tau)$ sweeps over the entire region $\bar{M}$. Thus, (5) is valid at all $x \in \bar{M}$.
Substituting (4) and (5) into (1) we arrive at

$$\Delta\gamma = \Big[c(t)\frac{\partial t}{\partial\tau} - f^2(\gamma)\frac{\partial}{\partial\gamma}\Big(\varkappa(t)\frac{\partial t}{\partial\gamma}\Big)\Big] \Big/ \Big[\varkappa(t)\frac{\partial t}{\partial\gamma}\Big].$$

Here the r.h.s. is again the function of (τ, γ) and, consequently, for some function g and $x \in \bar{M}$.

$$\Delta\gamma = g(\gamma). \tag{6}$$

Now we are to find a possible form of the functions $\gamma(x)$ satisfying the conditions (5), (6) and not equal to the constant. For this, we consider the function

$$\rho(\gamma) = \int_{\tau_0}^{\gamma} \frac{d\xi}{f(\xi)}. \tag{7}$$

It is easy to see that $\nabla\rho(\gamma(x)) = n(x)$ is the field of unit normals to $\Gamma(\gamma(x))$ and, consequently, $\rho(\gamma(x))$ is the distance from the point x to $\Gamma_0 = \Gamma(\tau_0)$ and all the points of the surface $\Gamma(\gamma)$ are at the same distance $\rho(\gamma)$ from Γ_0.

From (6) and (7) we find

$$\Delta\rho = g(\gamma)/f(\gamma) - df/d\gamma = h(\rho). \tag{8}$$

Introduce into $\bar{M}$ the structure of the direct product $\Gamma_0 \times \{\rho\}$: make each point $x \in \bar{M}$ juxtapose the pair (u, ρ), where u is the nearest point to x on Γ_0, while ρ, determined by formula (7) is, up to a sign, the distance from x to Γ_0. For arbitrary parametrization of Γ_0 and the parametrizations induced by it, of surfaces of the level ρ

$$h(\rho) = \operatorname{div} n = \frac{\partial}{\partial\rho}\left[\ln \sqrt{\det\left(g_{ij}(u, \rho)\, g^{jk}(u, 0)\right)}\right], \tag{9}$$

where g_{ij} is the first quadratic form of the surface $\rho = \text{const}$. Designate

$$H(\rho) = \exp\Big(\int_0^{\rho} h(\xi)\, d\xi\Big).$$

Integrating (9) yields the next result. For a self-similar solution of the form (4) of the Stefan problem (1)-(3) to exist, it is necessary that coordinates (u^i, ρ) exist on $\bar{M}$, in which the first quadratic form is

$$\begin{pmatrix} g_{ij} & 0 \\ 0 & 1 \end{pmatrix}, \quad \det [g_{ij}(u, \rho) g^{ik}(u, 0)] = H^2(\rho).$$

In this case, the system of equations for the temperature distribution $t(\tau, \rho)$ and unknown boundary $\rho = P(\tau)$, with ρ being the distance from x to Γ_0, takes the following form:

$$c_i(t)\, H(\rho) \frac{\partial t}{\partial \tau} = \frac{\partial}{\partial \rho} \left[\varkappa_i(t)\, H(\rho) \frac{\partial t}{\partial \rho} \right], \tag{10}$$

$$\left. \varkappa_1 \frac{\partial t_1}{\partial \rho} - \varkappa_2 \frac{\partial t_2}{\partial \rho} \right|_{(\tau, P(\tau))} = L \frac{dP}{d\tau}, \tag{11}$$

$$t(\tau, P(\tau)) \equiv T_0. \tag{12}$$

The obtained system may be formally considered as the one-dimensional Stefan problem for a medium with a coordinate-dependent density $H(\rho)$ but in the absence of convection. In our case a surface area ρ = const (if this area is finite) serves as a density.

To illustrate solving the system (10)-(12) for an arbitrary function $H(\rho)$, we consider the inverse Stefan problem when a law of crystallization front displacement $\rho = P(\tau)$ is given and we are to determine the temperature distribution in solid and liquid phases. In the case of constant (probably different) phase thermal diffusivities $\kappa_i(T)/c_i(T) = a_i$ = const, the temperature distribution is described by the following equation

$$\int_{T_0}^{T} c(\xi)\, d\xi = \sum_{k=0}^{\infty} \frac{1}{a_i^{k+1}} \frac{d^k}{d\tau^k} \left[f_k(\rho, P(\tau)) \left(q(\tau) + (i-1) \frac{dP}{d\tau} \right) \right], \tag{13}$$

where

$$f_n(\rho, P) = \int_P^{\rho} H^{-1}(\xi) \int_P^{\xi} H(\zeta) f_{n-1}(\zeta, P)\, d\zeta\, d\xi;$$

$$f_0(\rho, P) = H(P) \int_P^{\rho} H^{-1}(\xi)\, d\xi,$$

and a choice of an arbitrary function $q(\tau)$ may satisfy additional boundary conditions, for instance, the limitedness condition of T at $\rho \to \infty$. Substituting $H \equiv 1$ into (13), we obtain the known solution of the inverse one-dimensional Stefan problem [2].

The boundary conditions (11), (12) may be complicated by considering the surface tension and kinetic supercooling at the crystallization front, for instance, in the following manner [2, 3]

$$\left. \varkappa_1 \frac{\partial t_1}{\partial \rho} - \varkappa_2 \frac{\partial t_2}{\partial \rho} \right|_{(\tau, P(\tau))} = L \left(1 - d_1 \frac{h(P)}{n} \right) \frac{dP}{d\tau}, \tag{14}$$

$$t(\tau, P(\tau)) = T_0 - \Gamma \frac{h(P)}{n} - \Delta T \left(\frac{dP}{d\tau} \right), \tag{15}$$

where $\Delta T(v)$ is the kinetic supercooling as a function of the growth rate; $dP/d\tau$ is the growth rate; $h(P)/n$ is the mean surface curvature of the crystal.

Now consider in detail two important cases, namely, the crystal growth in the Euclidean space and on the two-dimensional surface in R^3.

1. $M = R^n$. In the vicinity of an arbitrary point $u \in \Gamma_0$ introduce coordinates (u^i) on Γ_0 so that in u the main quadratic forms were $g_{ij} = \delta_{ij}$, $h_{ij} = k_i \delta_{ij}$ (k_i are the main curvatures of the surface Γ_0 in u). In these coordinates

$$g_{ij}(\mathrm{u},\ \rho) = \frac{\partial \mathrm{x}}{\partial u^i}\frac{\partial \mathrm{x}}{\partial u^j} = \frac{\partial(\mathrm{u}+\rho\mathrm{n}(\mathrm{u}))}{\partial u^i}\,\frac{\partial(\mathrm{u}+\rho\mathrm{n}(\mathrm{u}))}{\partial u^j} =$$

$$= g_{ij} + 2\rho h_{ij} + h_i^k h_{kj}\rho^2 = (1+\rho k_i)^2\,\delta_{ij},$$

$$\det g_{ij}(\mathrm{u},\ \rho) = \prod_{i=1}^{n-1}(1+\rho k_i)^2, \quad H(\rho) = \prod_{i=1}^{n-1}(1+\rho k_i).$$

Since the set (k_i) is restored unambiguously from the last equation, then the main curvatures of k_i are constants. It is easy to show that Γ_0 is either a plane, a sphere, or a cylinder with the m-dimensional ($1 \le m \le n-1$) sphere in the base.

Thus $\rho(x)$, within the entire region M swept by a crystal surface during motion, is the distance, with an accuracy to the additive constant, between the point x and the prescribed m-dimensional ($0 \le m \le n$) affine surface R^n. The crystal surface will be either a plane, straight circular cylinder, or a sphere and in (10)

$$H(\rho) = \rho^m.$$

For instance, for the growth of a flat crystal in a three-dimensional space $H = 1$, for a cylindrical crystal $H = \rho$, for a spherical crystal $H = \rho^2$.

2. M is the two-dimensional surface in R^n. Introduce a natural parameter u on Γ_0. Then we may write in the coordinates (u, ρ)

$$g_{ij}(u,\ \rho) = \begin{pmatrix} H^2(\rho) & 0 \\ 0 & 1 \end{pmatrix}. \tag{16}$$

Such a surface is isothermal to a surface of revolution specified by the equation

$$r = r_0 H(\rho), \quad \rho = \int_{z_0}^{z} \sqrt{1+(dr/dz)^2}\,dz. \tag{17}$$

Here ρ is the distance along the generatrix.

Thus, a self-similar regime of the form (4) is possible only on a surface satisfying the condition (16) (in particular, on an arbitrary surface of revolution).

As an example, consider modeling of the growth of a spherical crystal in R^3 by the crystal growth on a two-dimensional surface. Substituting $H(\rho) = \rho^2$ into (17), we find the required form of the surface:

$$z/a = \arcsin\sqrt{r/a} + \sqrt{r/a - r^2/a^2}, \quad 0 \leqslant r \leqslant a \tag{18}$$

(a is an arbitrary constant). Therefore, axisymmetric crystallization of a sufficiently viscous (to avoid runoff) thin film on a surface of revolution prescribed by Eq. (18), without heat transfer with the surrounding medium, is the model of spherical crystal growth in the limited region ($\rho \le 2a$). In this case, the temperature and the heat flux across the crystallization front may be given both by Eqs. (11), (12) and (14), (15). The boundary conditions in the first case on the circumference $r = a$ correspond in the second case to the boundary conditions at the boundary of a spherical region $\rho = 2a$. Thus, the three-dimensional Stefan problem is modeled by the two-dimensional one that implies the possibility of direct observation of the crystallization process. Analogously, the spherical crystal growth from a binary alloy, when heat conduction and diffusion processes proceed simultaneously, is modeled as axisymmetric crystallization from a binary alloy on the surface given by (18). Such modeling exists also in other physical processes if interaction in the two-dimensional model occurs only along the surface.

NOTATION

T, t, temperature; $\Gamma(\tau)$, crystal surface; n, normal to $\Gamma(\tau)$; v, growth rate; M, n-dimensional manifold; x, point on M; τ, time; κ_1, thermal conductivity; c_i, heat capacity; L, latent heat of melting; T_0, melting point; Γ, surface tension coefficient. Subscripts i = 1, 2 stand for solid and liquid phases, respectively.

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