On the interface modelling of crystal growth processes
Part II. Uncoupled thermoelastic theory

Dedicated to Professor Franz Ziegler
on the occasion of His 60th birthday

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SOLIDIFICATION of an elastic sphere from melt in a quasi-static formulation has been investigated in "singular surface approach" and in "finite slab approach". Thermal stresses in the solid phase are derived for both approaches due to the uncoupled thermoelastic quasi-static theory. In the interfacial layer, which has been regarded as a boundary layer between the liquid and the solid phase, special constitutive relations for the purely mechanical problem are posed in order to have a continuous change from the liquid to solid phase. It has been found that the solutions corresponding to the "singular surface approach" are the zero order terms of the asymptotic expansions in the small parameter of the "finite slab approach" solutions.

1. Introduction

IN THE FIRST PART of the present paper [1] the different approaches treating the interface modelling during phase-change process (solidification or melting) are listed. A comparison between the two approaches: the "singular surface approach" and the "finite slab approach" is presented there. It is shown that under some physical hypotheses, the interfacial layer could be regarded as a "phase-change" boundary layer and its thickness depends only on the solidification mechanism specific for a given material. The surface fields (internal energy, density, evolution time) in the "singular surface approach" are obtained to be the zero order terms in the asymptotic expansion (in a small parameter related to the layer thickness) of the correspondent fields in the "finite slab approach". In the same paper, as a particular case, the quasi-static solidification of a sphere and its interface evolution in time is observed. In the "finite slab approach" an averaging procedure is applied, in which integration along the thickness is performed to get mean quantities defined as surface fields, and some preliminary phenomenological assumptions are necessary to obtain the field quantities. In some aspect this is shown in [1] for the internal energy and temperature distribution in the layer.

The aim of the present paper is to continue the comparison between the "singular surface approach" and the "finite slab approach" for the quasi-static axisymmetrical growth of an elastic sphere from a liquid phase. In the framework of the quasi-static uncoupled thermoelastic theory, the results obtained in [1]

for the thermal problem will be used when solving the purely mechanical problem. For the case of solidification discussed here, it is appropriate to apply the uncoupled quasi-static thermoelastic theory [3]. The extension of the model to the thermal stresses necessitates the assumption of some constitutive law for the thermal stresses inside the layer. It will be shown that the solutions for the deformations, stresses and pressure corresponding to the "singular surface approach" are the zero order terms of the asymptotic expansion in a small parameter of the solutions obtained from the "finite slab approach".

2. Formulation of the problem

The crystal growth of an elastic sphere $\widehat{G}_t^-$ with radius R in a spherical container with radius R^* filled with its melt $\widehat{G}_t^+$ is considered as in [1]. The phase change process is due to a continuous negative heat flux $Q_0 < 0$ from a crystal seed of radius ε concentric with the spherical container. The solid and liquid phases are supposed to be at thermostatic equilibrium, isotropic, and the liquid phase is incompressible and ideal. A spherical coordinate system (r, φ, θ) is introduced connected with the container. The problem is 1D due to the symmetry with respect to φ and θ if the problem boundary conditions are independent of φ and θ. The interface evolution in time is $r = R(t)$ and the interface coordinates are $l^1 := \varphi$, $l^2 := \theta$. The second fundamental tensor of the surface is $b_{11} = -R \sin^2 \theta$, $b_{22} = -R$, $b_{12} = b_{21} = 0$ and the mean and Gauss curvatures are $H = -1/R$ and $K = 1/R^2$ and $\mathrm{div}_s = 0$ (all the notations are the same as those in [1]).

The solidification process is treated in the solidification time scale, i.e., it is assumed to be quasi-static. The uncoupled quasi-static theory of thermoelasticity is applied for the solid phase. Then for both media the general balance laws for mass and momentum [1] give:

$$(2.1) \qquad \varrho_l = \varrho^+ = \text{const}, \qquad \varrho_s = \varrho_s(r),$$

where ϱ_l and ϱ_s are the liquid and solid densities,[1] respectively;

$$(2.2) \qquad \mathrm{div}\,\mathbf{T}_l = 0, \qquad \mathrm{div}\,\mathbf{T}_s = 0,$$

where $\mathbf{T}$ is the stress tensor. For the liquid phase, $\mathbf{T}_l = -p\mathbf{I}$, where $p = p(r)$ is the pressure and $\mathbf{I}$ is the identity tensor. From fluid incompressibility it follows that $\mathrm{div}\,\mathbf{u}_l = 0$, where $\mathbf{u}_l = (u_{l_r}, 0, 0)$ are the displacements in the fluid. For the solid phase as in [3], $\mathbf{T}_s = \lambda_s \mathrm{tr}\,\mathbf{E}_s\mathbf{I} + 2\mu_s\mathbf{E}_s - (3\lambda_s + 2\mu_s)\alpha_s(\theta_s - \theta_a)\mathbf{I}$, where λ_s, μ_s and α_s are the material constants, $\mathbf{E}_s$ is the deformation tensor with components

$$\varepsilon_{s_{rr}} = \frac{\partial u_{s_r}}{\partial r}, \qquad \varepsilon_{s_{\varphi\varphi}} = \varepsilon_{s_{\theta\theta}} = \frac{u_{s_r}}{r}, \qquad \varepsilon_{s_{r\varphi}} = \varepsilon_{s_{r\theta}} = \varepsilon_{s_{\varphi\theta}} = 0,$$

[1] Everywhere in the text index l refers to the liquid phase and index s – to the solid.

$u_{s_r} = u_{s_r}(r)$ is the radial displacement and θ_a is some reference temperature, e.g. $\theta_a = \theta|_{r=\varepsilon}$.

The boundary conditions for the unknown functions have to be imposed on $\partial \widehat{G}_t^-$, $\partial \widehat{G}_t^+$ and on S_t – the interface boundary – for the "singular surface approach", or on S_t^- and S_t^+ – the two interface boundaries – for the "finite slab approach". Then on $\partial \widehat{G}_t^-$, which means $r = \varepsilon$ and ε – greater than the critical radius of a crystal nucleus [4]:

$$
(2.3) \qquad
\begin{aligned}
\varrho_s &= \varrho_{s_0} = \text{const}, \\
u_{s_r} &= 0.
\end{aligned}
$$

On $\partial \widehat{G}_t^+$, i.e., $r = R^*$:

$$
(2.4) \qquad p = p_\infty.
$$

3. Singular surface approach

The interface $S_t : F = r - R(t) = 0$, is defined as the isotherm $\theta = \theta_m$ and the surface normal velocity is $c_n = \dot{R}$. On that surface the density and displacement are continuous, while the stress tensor suffers a jump [2]:

$$
(3.1) \qquad
\begin{aligned}
\varrho_s &= \varrho^+, \\
u_{l_r} &= u_{s_r}, \qquad \mathbf{T}_s \cdot \mathbf{n} - \mathbf{T}_l \cdot \mathbf{n} = \sigma H \mathbf{n},
\end{aligned}
$$

where σ is the solid/liquid surface tension, and $\mathbf{n} = (1, 0, 0)$ is the unit normal.

The uncoupled thermoelastic problem (2.2) with (2.3)$_2$, (2.4), (3.1)$_2$, and with the expressions (4.4) and (4.3) for θ_l and θ_s found in [1], has the following solutions in $\widehat{G}_t^+$:

$$
(3.2) \qquad
\begin{aligned}
p &= p_\infty, \\
u_{l_r} &= \frac{C}{r^2};
\end{aligned}
$$

and in $\widehat{G}_t^-$

$$
(3.3) \qquad
\begin{aligned}
u_{s_r} &= b_0 + b_1 r + \frac{b_2}{r^2}, \\
\tau_{s_{rr}} &= 2(\lambda_s + \mu_s)\left(\frac{b_0}{r} + b_1\right) - 4\mu_s \frac{b_2}{r^3} + \lambda_s b_1 + A, \\
\tau_{s_{\varphi\varphi}} &= \tau_{s_{\theta\theta}} = 2(\lambda_s + \mu_s)\left(\frac{b_0}{r} + b_1\right) + 2\mu_s \frac{b_2}{r^3} + \lambda_s b_1 + A,
\end{aligned}
$$

where

$$A = -(3\lambda_s + 2\mu_s)\alpha_s\left[\theta_m - \theta_a - \frac{Q_0}{4\pi\kappa_s}\left(\frac{1}{R} - \frac{1}{r}\right)\right], \quad b_0 = \frac{(3\lambda_s + 2\mu_s)\alpha_s Q_0}{8\pi\kappa_s(\lambda_s + 2\mu_s)},$$

$$C = C' = b_0\left(R^2 - \varepsilon^2\right) + b_1\left(R^3 - \varepsilon\right), \qquad b_2 = -b_0\varepsilon^2 - b_1\varepsilon,$$

$$b_1 = b_1' = \frac{-\dfrac{\sigma}{R} - p_\infty - \left[\dfrac{2\lambda_s}{R} + \dfrac{4\mu_s}{R^3}\varepsilon^2\right]b_0 + (3\lambda_s + 2\mu_s)\alpha_s(\theta_m - \theta_a)}{3\lambda_s + 2\mu_s + \dfrac{4\mu_s}{R^3}\varepsilon}.$$

Here b_1' and C' correspond to the "singular surface approach". In the next section dealing with the "finite slab approach" we shall give another value of b_1.

4. Finite slab approach

In this approach the two subregions $\hat{G}_t^{\pm}$ are divided by a narrow layer Z_t with regular surface boundaries $S_t^{\pm}$, and a reference surface S_t is located between them, to which the mean interfacial fields will be referred. The surface boundaries $S_t^{\pm}$ are defined as $S_t^- : r = R + z^-$ and $S_t^+ : r = R + z^+$ and a coordinate $l \in [z^-, z^+]$ is ascribed to the layer, such that $r = R + l$.

Suppose that the physical assumptions i) – vi) from [1] hold. Therefore, the interfacial layer is a phase change boundary layer between the liquid and the solid phase with thickness $\delta R_0 \ll 1$ and $z^+ - z^- = \delta R_0$, where δ is a small parameter. Moreover, from (4.14) of [1] the quantities z^+ and z^- depend only on the thermal properties of the media in contact. All the interfacial fields are represented as polynomial functions of l, while their corresponding mean values F – in an asymptotic expansion of the small parameter δ:

(4.1) $F = F_0 + \delta F_1 + \delta^2 F_2 + \ldots,$

where F_0 relates to the "singular surface approach" solution.

As a result, for the density in the solid bulk we get:

(4.2) $\varrho_s(R + z^-) = \varrho^+$ or $\varrho_s(R) = \varrho^+ + O(\delta)$

which confirms the result of the "singular surface approach" $(3.1)_1$ and the surface density ϱ^S in the interfacial layer is given by (4.17) of [1]. Similarly, the temperature solutions θ_l and θ_s in the bulks are (4.19), (4.20) of [1], which have as zero order terms the "singular surface approach" solutions (4.4) and (4.3) from [1]. The surface energy density $\varrho^s e^s$ is represented by (4.18) of [1]. It is evident that the zero order terms of (4.17) and (4.18) of [1] vanish, as it was assumed in the "singular surface approach".

Some additional assumption for the interfacial layer material rheology must be introduced before formulating the mean surface stress $\mathbf{W}^s$, i.e., the assumption:

vii) The stress tensor $\mathbf{T}(l)$ has only non-zero diagonal elements $\tau_{ij} = 0, (i \neq j)$. Then for the stress tensor in the layer we assume the form

$$\mathbf{T}(l) = -p(l)\mathbf{I} + \lambda(l)\mathrm{tr}\,\mathbf{E}(l)\mathbf{I} + 2\mu(l)\mathbf{E}(l) - [3\lambda(l) + 2\mu(l)]\,\alpha(l)\,[\theta(l) - \theta_{\min}]\,\mathbf{I},$$

where the material coefficients λ, μ and α, $p(l)$, the volume deformation $\mathrm{tr}\,\mathbf{E}$ and the radial displacement u_r are regular functions of l. The coefficients of these unknown functions are found by a matching procedure with the corresponding values from both media, and their final form is:

$$\lambda(l) = \frac{\lambda_s}{\delta R_0}\,(z^+ - l)\,, \quad \mu(l) = \frac{\mu_s}{\delta R_0}\,(z^+ - l)\,, \quad \alpha(l) = \frac{\alpha_s}{\delta R_0}\,(z^+ - l)\,,$$

(4.3)
$$p(l) = \left[\frac{p_\infty}{\delta R_0} - \frac{p_2 \delta R_0(c_\nu^- - c_\nu^+)}{(c_\nu^- + c_\nu^+)}\right](l - z^-) + p_2(l^2 - z^{-2}),$$

$$\mathrm{tr}\,\mathbf{E}(l) = \frac{\varepsilon_s}{\delta R_0}(z^+ - l),$$

$$u_r(l) = \frac{D_0}{(R + l)^2} + \frac{\varepsilon_s(R + z^+)}{3\delta R_0}(R + l) - \frac{\varepsilon_s}{4\delta R_0}(R + l)^2,$$

where

$$D_0 = (R + z^-)^2 \left\{ b_0 \left[1 - \frac{\varepsilon^2}{(R + z^-)^2}\right] + b_1'' \left[(R + z^-) - \frac{\varepsilon}{(R + z^-)^2}\right] \right.$$
$$\left. - \frac{\varepsilon_s(R + z^-)}{12\delta R_0}(R + 3\delta R_0 + z^+) \right\},$$

$$\varepsilon_s = \frac{2b_0}{R + z^-} + 3b_1'', \qquad C'' = D_0 + \frac{\varepsilon_s(R + z^+)^4}{12\delta R_0}.$$

With

$$j(l) = 1 + (l/R)^2, \qquad \mathbf{A}_s(l) = (1 + l/R)\mathbf{I}_s\,, \qquad \mathrm{div}_s\mathbf{I}_s = -\frac{2}{R}\mathbf{n},$$

the case of the linear momentum balance in the layer (from (3.2) of [1])

$$\psi = \varrho v = 0, \qquad \psi^s = \varrho^s \mathbf{V} = \mathbf{0}, \qquad \mathbf{w} = -\mathbf{T}, \qquad \mathbf{v} = \mathbf{0}, \qquad \mathbf{W}^s = <-\mathbf{T}(l)\mathbf{A}_s(l)>$$

is:

(4.4) $$\mathrm{div}_s\mathbf{W}^s = \left[1 + \left(\frac{z^+}{R}\right)^2\right]\mathbf{T}_l(R + z^+)\mathbf{n} - \left[1 + \left(\frac{z^-}{R}\right)^2\right]\mathbf{T}_s(R + z^-)\mathbf{n}.$$

The unknown coefficients p_2 and b_1'' will be found after taking into account that

and that $<p(l)> = 0.5\sigma + O(\delta)$ is the classical surface tension:

$$(4.5) \qquad p_2 = \frac{-3\sigma}{(\delta R_0)^3},$$

$$(4.6) \qquad b_1'' = b_1' + \delta B + O(\delta^2);$$

here B can be calculated from (4.3).

Evidently, if we replace b_1 with b_1'' and C with C'' in (3.2)$_2$, (3.3)$_1$ and (3.3)$_2$, the resultant displacements and the stresses will possess zero order terms with respect to δ which will coincide with the respective ones from the "singular surface approach". Here, it is interesting to note that in the layer all the considered functions are regular, i.e., they obey Eq. (4.1), but only the pressure function $p(l)$ contains a term of order $O(\delta^{-1})$ like a "smoothed" Dirac function contributing to the surface tension as a mean interfacial quantity. In the singular surface case the interface is of zero thickness and we can regard the surface tension as a result of some Dirac function similar to the pressure function.

5. Conclusions

An extension of authors' previous paper [1] dealing with the elastic sphere solidification from melt in a quasi-static formulation has been obtained in two approaches: "singular surface approach" and "finite slab approach". Using the results for the temperature and density distribution everywhere in the solid/liquid system from [1], the purely mechanical uncoupled thermoelastic quasi-static problem is treated in both approaches. In the interfacial layer special constitutive relations are posed for the stress tensor, displacements, material coefficients λ, μ and α, the volume deformation and pressure, in order to ensure their continuous change from liquid to solid.

The comparison between the two approaches leads to the conclusion that the solutions for the density, temperature, thermal stresses, displacements and pressure obtained by the "singular surface approach" are the zero order terms in the asymptotic expansion of the corresponding solutions due to the "finite slab approach".

The classical surface tension is due to the pressure function in the interfacial layer. It occurs that the pressure function is singular with respect to the layer thickness and depends only on the thermal parameters of the material.

References

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