

Analytical and numerical studies of the meniscus equation in the case of crystals grown in zero gravity conditions by the Dewetted Bridgman technique

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Abstract—On the physical point of view, the dewetting phenomenon is governed by the Young-Laplace equation of a capillary surface in equilibrium, which is a nonlinear partial differential equation of second order. Starting from this equation, an analytical expression of the meniscus surface in zero gravity condition was established, leading to important information about the meniscus shape, useful for further stability analysis of the growth process. The analytical results were validated by the numerical studies. Therefore, the Young-Laplace equation has been solved numerically, in the axi-symmetric case, using the adaptive 4th order Runge-Kutta method for InSb crystals.

Keywords—Dewetted Bridgman crystal growth technique, Growth from the melt, Nonlinear partial differential equation, Young-Laplace equation.

I. INTRODUCTION

CRYSTALS, used as sensors, as laser radiation source detectors or solar cells, are essential components of many high technology apparatuses produced in the optoelectronic industry. The quality of this kind of apparatus depends, on the quality of the aggregate crystals, which can be obtained by different growth methods. Before its utilization in engineering, the crystals are constrained to some supplementary mechanical processes (cutting, polishing) for bringing them to the desired form. These processes are generating defects and material losses, so the final product has low quality and it is more expensive. For this reason those growth methods are preferred which allow obtaining the crystal directly in the final desired form (without additional machining) and with minimal defects. Techniques of crystal lateral surface shaping without contact with the container walls are preferred: Dewetted Bridgman (DW), Edge-defined

film-fed growth (EFG), Czochralski, Floating-zone; the absence of contact between the crystallizing substance and crucible walls allows one to improve crystal structures and to decrease the mechanical stress level.

Classical Bridgman method involves heating a polycrystalline material above its melting point in a crucible and slowly cooling it from one end where a seed crystal is located (Fig. 1 (a)). Single crystal material is progressively formed along the length of the crucible. The disadvantage of this technique is that the crystal contacts the crucible wall, which generally results in increasing the mechanical stresses, impurity level, and defect density in the grown crystals. The disadvantage can, however, be overcome by the dewetting solidification technique.

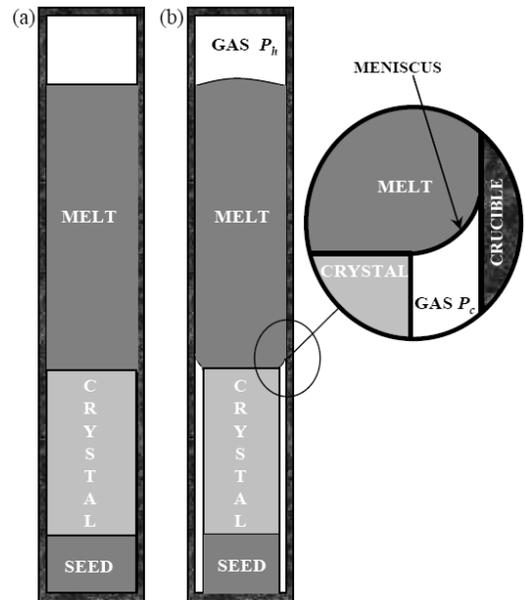


Fig. 1 Schematic Bridgman (a), dewetted Bridgman (b) crystal growth systems and photograph of an ingot showing attached and detached regions (c)

Phenomenon of dewetting is characterized by the classical Bridgman technique, but the crystal is grown without contact with the crucible walls thanks to the stability of a small liquid meniscus (Fig. 1 (b)) creating a gap between the crystal and the crucible wall [1].

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This phenomenon was first obtained spontaneously, in space experiments during the Bridgman solidification of *InSb* performed on the Skylab-NASA mission-1974 [2-3]. Numerous others Bridgman crystal growth experiments in space showed the same behaviour [4].

In dewetting Bridgman technique there are two problems of interest [5]:

- What is the crystal-crucible gap thickness e , therefore the crystal radius, $r_c = r_a - e$?
- What is the shape of the meniscus? This shape is related to the stability of the process.

The main purpose of the present paper is to perform analytical and numerical studies for the meniscus surface in zero gravity conditions, starting from Young-Laplace's equation [6]-[7] of a capillary surface in equilibrium and to establish the properties of the function which describes the meniscus surface, leading to important information for the stability analysis of the growth process [8]-[10].

II. MENISCUS SURFACE'S EQUATION

The equation of a capillary surface in equilibrium in the absence of exterior pressure is given by the function:

$$z = z(x, y) \quad (1)$$

which verifies the Young-Laplace equation with partial derivatives:

$$\left[1 + \left(\frac{\partial z}{\partial y} \right)^2 \right] \cdot \frac{\partial^2 z}{\partial x^2} - 2 \frac{\partial z}{\partial x} \cdot \frac{\partial z}{\partial y} \cdot \frac{\partial^2 z}{\partial x \partial y} + \left[1 + \left(\frac{\partial z}{\partial x} \right)^2 \right] \frac{\partial^2 z}{\partial y^2} \quad (2)$$

$$= \left[\frac{\rho_l g (H_a - z) - \Delta P}{\gamma} + \frac{2}{b} \right] \cdot \left[1 + \left(\frac{\partial z}{\partial x} \right)^2 + \left(\frac{\partial z}{\partial y} \right)^2 \right]^{\frac{3}{2}}$$

where $\Delta P = P_c - P_h$ represents the pressure difference between the cold and hot sides of the sample, θ_c - the contact angle, H_a - the total length of the melt and solid, ρ_l - the density of the liquid, g - the gravitational acceleration, γ - the surface tension of the melt, r_a - the ampoule radius and the term $\frac{2}{b}$ is due to the curvature at the top [11].

When referring to a system of coordinates as in Fig. 2, due to the radial symmetry, and imposing z independent of the polar angle:

$$\begin{cases} x = r \cdot \cos \beta \\ y = r \cdot \sin \beta, & r > 0, \beta \in [0, 2\pi] \\ z = z(r) \end{cases} \quad (3)$$

the meniscus equation is obtained by the rotation around Oz axis of the curve k which satisfies the equation:

$$\frac{z''}{\left[1 + (z')^2 \right]^{\frac{3}{2}}} + \frac{z'}{r \left[1 + (z')^2 \right]^{\frac{1}{2}}} = \frac{\rho_l g (H_a - z) - \Delta P}{\gamma} + \frac{2}{b} \quad (4)$$

In zero gravity conditions, the Young-Laplace equation becomes:

$$\frac{z''}{\left[1 + (z')^2 \right]^{\frac{3}{2}}} + \frac{z'}{r \left[1 + (z')^2 \right]^{\frac{1}{2}}} = \frac{-\Delta P}{\gamma} + \frac{2}{b} \quad (5)$$

where $2/b$ is due to the curvature at the top which depends on the contact angle θ_c and on the ampoule radius, r_a . Under microgravity condition it can be written as: $\frac{1}{b} = -\frac{\cos \theta_c}{r_a}$ [11].

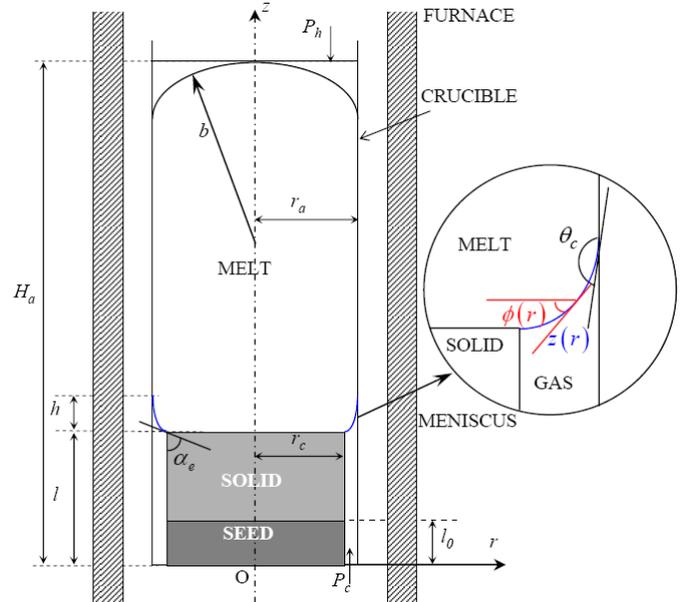


Fig. 2 Dewetting configuration in microgravity conditions

The solution of (5) should satisfy the wetting boundary condition:

$$z(r_a) = l + h, z'(r_a) = \tan \left(\theta_c - \frac{\pi}{2} \right), \theta_c \in \left(\frac{\pi}{2}, \pi \right) \quad (6)$$

and the achievement of the growth angle:

$$z(r_c) = l, z'(r_c) = \tan \left(\frac{\pi}{2} - \alpha_e \right), \alpha_e \in \left(0; \frac{\pi}{2} \right) \quad (7)$$

where l represents the solid-liquid interface coordinate and h is the meniscus height.

Equation (5) can be written as

$$\frac{r \cdot z'' + z' \cdot \left[1 + (z')^2 \right]}{\left[1 + (z')^2 \right]^{\frac{3}{2}}} = \left(-2 \frac{\cos \theta_c}{r_a} - \frac{\Delta P}{\gamma} \right) \cdot r$$

which is equivalent to

$$\left(\frac{r \cdot z'}{\sqrt{1 + (z')^2}} \right)' = \left(-2 \frac{\cos \theta_c}{r_a} - \frac{\Delta P}{\gamma} \right) \cdot r$$

i.e., by integration:

$$\frac{r \cdot z'}{\sqrt{1 + (z')^2}} = -\frac{r^2}{2} \left(\frac{2 \cos \theta_c}{r_a} + \frac{\Delta P}{\gamma} \right) + c_1$$

Squaring the above relation gives:

$$(z')^2 = \frac{\left(-\frac{\cos \theta_c}{r_a} \cdot r^2 - \frac{r^2 \Delta P}{2\gamma} + c_1\right)^2}{r^2 - \left(-\frac{\cos \theta_c}{r_a} \cdot r^2 - \frac{r^2 \Delta P}{2\gamma} + c_1\right)^2}$$

from where is obtained

$$z'(r) = \pm \frac{\left(-\frac{\cos \theta_c}{r_a} - \frac{\Delta P}{2\gamma}\right) \cdot r^2 + c_1}{\sqrt{r^2 - \left[\left(-\frac{\cos \theta_c}{r_a} - \frac{\Delta P}{2\gamma}\right) \cdot r^2 + c_1\right]^2}} \quad (8)$$

As the function $z(r)$ is strictly increasing on $[r_c, r_a]$, where r_c represents the crystal radius, in (8) the positive sign should be chosen.

The constant c_1 is determined from the boundary condition

$$z'(r_a) = \tan\left(\theta_c - \frac{\pi}{2}\right), \text{ leading to:}$$

$$z'(r) = \frac{\left(-\frac{\cos \theta_c}{r_a} - \frac{\Delta P}{2\gamma}\right) \cdot r^2 + \frac{r_a^2 \Delta P}{2\gamma}}{\sqrt{r^2 - \left[\left(-\frac{\cos \theta_c}{r_a} - \frac{\Delta P}{2\gamma}\right) \cdot r^2 + \frac{r_a^2 \Delta P}{2\gamma}\right]^2}} \quad (9)$$

The analytical expression of the meniscus can be obtained integrating relation (9). As the integral can be expressed using elementary functions only in some particular cases, further two different cases will be treated separately: $\Delta P = 0$ and $\Delta P \neq 0$.

Case I: $\Delta P = 0$

On the physical point of view, this means that there is a connection between the cold and hot sides of the sample, so that the pressures P_c and P_h are equal.

In this case (9) becomes

$$z'(r) = \frac{-r \cdot \cos \theta_c}{\sqrt{r_a^2 - (r \cdot \cos \theta_c)^2}} \quad (10)$$

Integrating (10) gives:

$$z(r) = \frac{1}{\cos \theta_c} \cdot \sqrt{r_a^2 - r^2 \cdot \cos^2 \theta_c} + c_2.$$

Using the condition $z(r_a) = l + h$, the analytical expression of the meniscus surface in zero gravity, when $\Delta P = 0$ is obtained:

$$z(r) = \frac{1}{\cos \theta_c} \left(\sqrt{r_a^2 - r^2 \cos^2 \theta_c} - r_a \sin \theta_c \right) + l + h, \quad (11)$$

where $r \in [0, r_a]$.

Thus, by the rotation of the curve k around the vertical coordinate Oz , the meniscus equation is obtained:

$$\begin{cases} x = r \cdot \cos \beta, \beta \in [0, 2\pi] \\ y = r \cdot \sin \beta, r \in [0, r_a] \\ z = \frac{1}{\cos \theta_c} \left(\sqrt{r_a^2 - r^2 \cos^2 \theta_c} - r_a \sin \theta_c \right) + l + h \end{cases}$$

where $\theta_c \in \left(\frac{\pi}{2}, \pi\right)$.

Further, some properties of the function $z(r)$ will be presented.

Proposition 1:

Function $z(r)$ which describes the meniscus surface has the following properties:

- (i) $z(r)$ is strictly increasing for $r \in [0, r_a]$;
- (ii) $z(r)$ is convex for $r \in [0, r_a]$.

Proof:

(i) Deriving the relation (11) gives:

$$\begin{aligned} z'(r) &= \frac{1}{\cos \theta_c} \frac{-2r \cos^2 \theta_c}{2\sqrt{r_a^2 - r^2 \cos^2 \theta_c}} \\ &= \frac{-r \cos \theta_c}{\sqrt{r_a^2 - r^2 \cos^2 \theta_c}} > 0, (\forall) r \in [0, r_a]. \end{aligned}$$

(ii) In order to show the convexity of the function $z(r)$ the sign of the second derivative should be studied for $[0, r_a]$:

$$z''(r) = \left(\frac{-r \cos \theta_c}{\sqrt{r_a^2 - r^2 \cos^2 \theta_c}} \right)' = \frac{-r_a^2 \cos \theta_c}{(r_a^2 - r^2 \cos^2 \theta_c)^{3/2}} > 0, \quad \text{with}$$

$$\theta_c \in \left(\frac{\pi}{2}, \pi\right).$$

Thus, function $z(r)$ is convex. ■

From the above properties it results that in zero gravity condition and null pressure difference the meniscus is always globally convex and this is in agreement with the numerical results obtained in the case of InSb (Fig. 3).

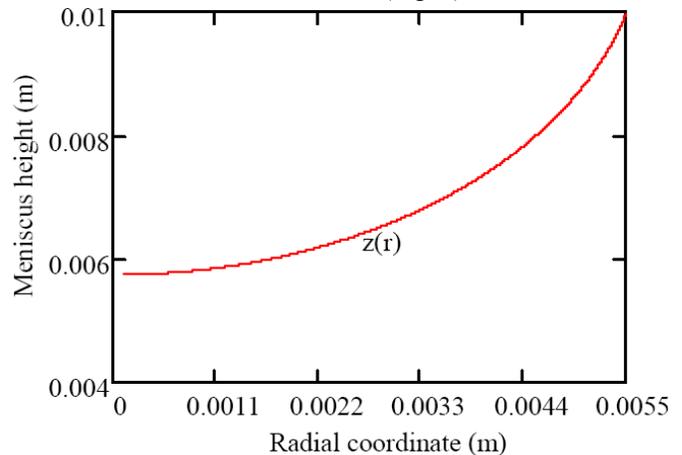


Fig. 3 Meniscus shape $z(r)$ for InSb, $\theta + \alpha = 160^\circ + 25^\circ$, $r_a = 0.0055$ m.

Thickness of the crystal-crucible gap

Dewetting occurs when the growth angle $\alpha_e \in \left(0, \frac{\pi}{2}\right)$ (the angle between the tangent to the meniscus surface and the vertical) is achieved at least at one point on the meniscus surface, i.e. when the equation:

$$\phi(r) = \frac{\pi}{2} - \alpha_e \tag{12}$$

has at least one solution in the range $(0, r_a)$; where ϕ is the angle between the plane $z=0$ and the tangent plane to the meniscus at a point $P(r, \beta)$. For this angle the equality $\tan \phi = z'(r)$ holds and hence information concerning the achievement of the growth angle is given by the equation:

$$\tan \phi = \frac{-r \cos \theta_c}{\sqrt{r_a^2 - r^2 \cos^2 \theta_c}}$$

Rewriting the above relation as:

$$\frac{\sin \phi}{\sqrt{1 - \sin^2 \phi}} = \frac{-r \cos \theta_c}{\sqrt{r_a^2 - r^2 \cos^2 \theta_c}}$$

it comes

$$\sin \phi = -\frac{r \cdot \cos \theta_c}{r_a} \tag{13}$$

which is equivalent to

$$\phi = \arcsin\left(\frac{-r \cdot \cos \theta_c}{r_a}\right), \text{ for } r \in [0, r_a]. \tag{14}$$

Relation (14) gives a condition of dewetting which depends on the growth angle α_e and contact angle θ_c .

The positivity of the derivative

$$\frac{d\phi}{dr} = -\frac{\cos \theta_c}{\sqrt{r_a^2 - r^2 \cos^2 \theta_c}} > 0, \theta_c \in \left(\frac{\pi}{2}, \pi\right)$$

gives that the function $\phi(r)$ is strictly increasing for $r \in [0, r_a]$. Taking into account this monotony and the

boundary condition $z'(r_a) = \tan\left(\theta_c - \frac{\pi}{2}\right)$ which is equivalent

to $\phi(r_a) = \theta_c - \frac{\pi}{2}$, the growth angle is achieved if

$\phi(r)$ decreases from $\theta_c - \frac{\pi}{2}$ to $\frac{\pi}{2} - \alpha_e$, leading to

$\frac{\pi}{2} - \alpha_e < \theta_c - \frac{\pi}{2}$, i.e., $\theta_c + \alpha_e > \pi$. In the opposite case

when $\theta_c + \alpha_e < \pi$, the growth angle can not be achieved due to the monotony of $\phi(r)$.

Under the hypothesis that the growth angle criterion is satisfied, i.e., $\theta_c + \alpha_e > \pi$, the Eqs. (12) and (13) give:

$$\sin\left(\frac{\pi}{2} - \alpha_e\right) = -\frac{(r_a - e) \cdot \cos \theta_c}{r_a} \tag{15}$$

where e represents the crystal-crucible gap thickness and

$r_c = r_a - e$ the crystal radius.

From (15) results the *gap thickness formula* [11]:

$$e = r_a \left(\frac{\cos \theta_c + \cos \alpha_e}{\cos \theta_c} \right) \tag{16}$$

valid under zero gravity condition, $\Delta P = 0$, and $\theta_c + \alpha_e > \pi$.

Theorem:

For a given ampoule radius r_a and $\Delta P = 0$, if $\theta_c \in \left(\frac{\pi}{2}, \pi\right)$

and $\alpha_e \in \left(0, \frac{\pi}{2}\right)$ satisfy the inequality $\theta_c + \alpha_e > \pi$, then the meniscus height in zero gravity is constant and is given by the following relation:

$$h = \frac{r_a}{\cos \theta_c} (\sin \theta_c - \sin \alpha_e). \tag{17}$$

Proof:

Relation (17) is obtained imposing to relation (11) the condition of the growth angle achievement $z(r_c) = l$, which gives:

$$h = \frac{-1}{\cos \theta_c} \left(\sqrt{r_a^2 - r_c^2 \cos^2 \theta_c} - r_a \sin \theta_c \right)$$

and by replacing $r_c = r_a - e$, where e is given by (16). ■

Case II: $\Delta P \neq 0$

The physical meaning of $\Delta P \neq 0$ is that the gases between the cold and hot sides of the sample do not communicate, so that a pressure difference exists.

In order to obtain the meniscus equation, relation (9) should be integrated, but if $\Delta P \neq 0$ the integral can not be expressed using elementary functions. Then, for obtaining information concerning the meniscus shape, achievement of the growth angle, and gap thickness, qualitative studies should be performed.

Introducing $\tan \phi = z'(r)$ in relation (9), gives:

$$\sin \phi = -\frac{r^2 \cos \theta_c}{r_a} - \frac{r^2 \Delta P}{2\gamma} + \frac{r_a^2 \Delta P}{2\gamma} \tag{18}$$

which is equivalent to

$$\phi = \arcsin\left(-\frac{r^2 \cos \theta_c}{r_a} - \frac{r^2 \Delta P}{2\gamma} + \frac{r_a^2 \Delta P}{2\gamma}\right) \tag{19}$$

for any $r \in [0, r_a]$.

In a way similar to previous calculations, the sign of the derivative $\frac{d\phi}{dr}$ will give information about the shape of the meniscus, and about the condition which should be imposed on the sum of the contact and growth angles such that achievement of the growth angle is feasible. Thus, deriving the relation (19) gives:

$$\frac{d\phi}{dr} = \frac{1}{\sqrt{1 - \left(-\frac{\cos \theta_c}{r_a} r - \frac{\Delta P}{2\gamma} r + \frac{r_a^2 \Delta P}{2\gamma} \frac{1}{r} \right)^2}} \cdot \left[\left(-\frac{\cos \theta_c}{r_a} - \frac{\Delta P}{2\gamma} \right) r^2 - \frac{r_a^2 \Delta P}{2\gamma} \right] \frac{1}{r^2} \quad (20)$$

The sign of this derivative depends on the sign of the expression depending on r and ΔP :

$$E(r, \Delta P) = \left(-\frac{\cos \theta_c}{r_a} - \frac{\Delta P}{2\gamma} \right) r^2 - \frac{r_a^2 \Delta P}{2\gamma} \quad (21)$$

and then, the following cases should be considered:

(i) If $\Delta P \in (-\infty; 0]$, then $E(r, \Delta P) > 0$ and hence $\frac{d\phi}{dr} > 0$.

Moreover, $\frac{d^2 z}{dr^2} = \frac{1}{\cos^2 \phi} \cdot \frac{d\phi}{dr} > 0$, i.e., the meniscus is globally convex, and the growth angle can be achieved only if $\theta_c + \alpha_e > \pi$.

(ii) If $\Delta P \in \left(0; -\frac{\gamma \cdot \cos \theta_c}{r_a} \right)$, then the meniscus changes its curvature (concave-convex) at the point $r_l = r_a \cdot \sqrt{\frac{\Delta P \cdot r_a}{-2\gamma \cos \theta_c - \Delta P \cdot r_a}}$, i.e., $E(r_l, \Delta P) = 0$ which is

equivalent to $\frac{d\phi}{dr}(r_l) = \frac{d^2 z}{dr^2}(r_l) = 0$ and the growth angle can be achieved once or twice, depending on its value.

(iii) If $\Delta P \in \left[-\frac{\gamma \cdot \cos \theta_c}{r_a}; +\infty \right)$ then $E(r, \Delta P) < 0$ and hence $\frac{d\phi}{dr} < 0$. In this case the meniscus is globally concave, i.e., $\frac{d^2 z}{dr^2} < 0$, and the growth angle can be achieved only if $\theta_c + \alpha_e < \pi$.

Under the hypothesis that ΔP , θ_c and α_e are chosen such that the growth angle can be achieved, the growth angle criterion (12) is satisfied somewhere along the meniscus. From (18):

$$\sin\left(\frac{\pi}{2} - \alpha_e\right) = -\frac{\cos \theta_c}{r_a} (r_a - e) - \frac{\Delta P}{2\gamma} (r_a - e) + \frac{\Delta P r_a^2}{2\gamma} \frac{1}{(r_a - e)} \quad (22)$$

the following *gap thickness formulas* [11] are obtained:

$$e_1 = r_a \left(\frac{\gamma \cos \alpha_e + 2\gamma \cos \theta_c + \Delta P r_a + \sqrt{\delta}}{\Delta P r_a + 2\gamma \cos \theta_c} \right) \quad (23)$$

$$e_2 = r_a \left(\frac{\gamma \cos \alpha_e + 2\gamma \cos \theta_c + \Delta P r_a - \sqrt{\delta}}{\Delta P r_a + 2\gamma \cos \theta_c} \right) \quad (24)$$

where $\delta = \gamma^2 \cos^2 \alpha_e + \Delta P^2 r_a^2 + 2r_a \gamma \Delta P \cos \theta_c$.

The first gap formula (23) is valid when the growth angle is achieved on the convex part of the meniscus, and the second formula (24) is valid when the achievement of the growth angle occurs on the concave part of the meniscus [12].

III. NUMERICAL RESULTS

The results obtained solving numerically the Young-Laplace equation by Runge-Kutta method for InSb crystals grown in zero gravity by the dewetted Bridgman technique (material parameters used in numerical computations: $\gamma = 0.42 \text{ N/m}$, $\rho_l = 6582 \text{ kg/m}^3$, $r_a = 0.0055 \text{ m}$, $H_a = 0.08 \text{ m}$), confirm the behaviors obtained through the qualitative study:

(i) If $\Delta P \in (-\infty; 0]$, then the meniscus is globally convex

and the growth angle can be achieved once. In the case of achievement of the growth angle the gap thickness is given by e_1 expressed in (23). The numerical results reveal this behaviour for $\Delta P = -50 \in (-\infty; 0]$ and $\theta_c + \alpha_e = 160^\circ + 25^\circ > \pi$, as it can be seen in Fig. 4 showing that the meniscus is globally convex and that the growth angle is achieved. The computed gap thickness $e = r_a - r_{c1} = 0.0055 - 0.00539 = 0.00011 \text{ m}$ is equal to the one given by formula (23), i.e., $e_1 = 0.00011466 \text{ m}$.

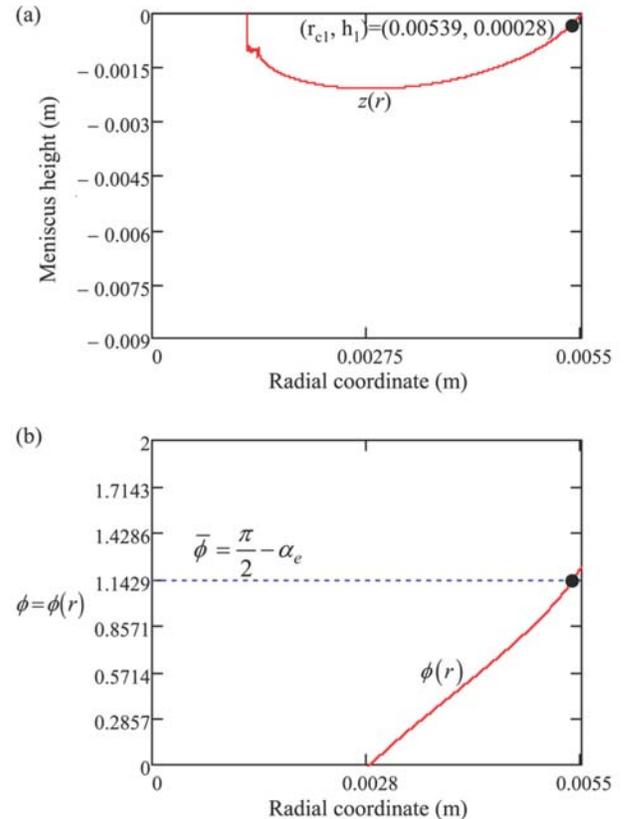


Fig. 4 Meniscus shape $z(r)$ (a) and meniscus angle $\phi(r)$ (b) corresponding to a pressure difference $\Delta P = -50 \text{ Pa}$ and $\theta_c + \alpha_e = 160^\circ + 25^\circ$ for InSb. The place where the growth angle (25°) is achieved is shown by the black dot.

- (ii) If $\Delta P \in \left(0; -\frac{\gamma \cos \theta_c}{r_a}\right)$, then the meniscus is concave-convex (has an inflexion point). When the growth angle is achieved on the concave part, the gap thickness is given by e_2 expressed by (24), and on the convex part, the gap thickness is given by e_1 expressed by (23). The numerical results confirm these behaviours.
- (a) for $\theta_c + \alpha_e = 112^\circ + 25^\circ < \pi$ and $\Delta P = 8 \in \left(0; -\frac{\gamma \cos \theta_c}{r_a}\right) = (0; 28.6)$ the growth angle is not achieved (see Fig. 5), but for $\Delta P = 20 \in (0; 28.6)$ the growth angle is achieved once, as it can be seen on Fig. 6;
- (b) for $\theta_c + \alpha_e = 160^\circ + 25^\circ > \pi$ and $\Delta P = 30 \in \left(0; -\frac{\gamma \cos \theta_c}{r_a}\right) = (0; 71.75)$ the growth angle is achieved twice (see Fig. 7).

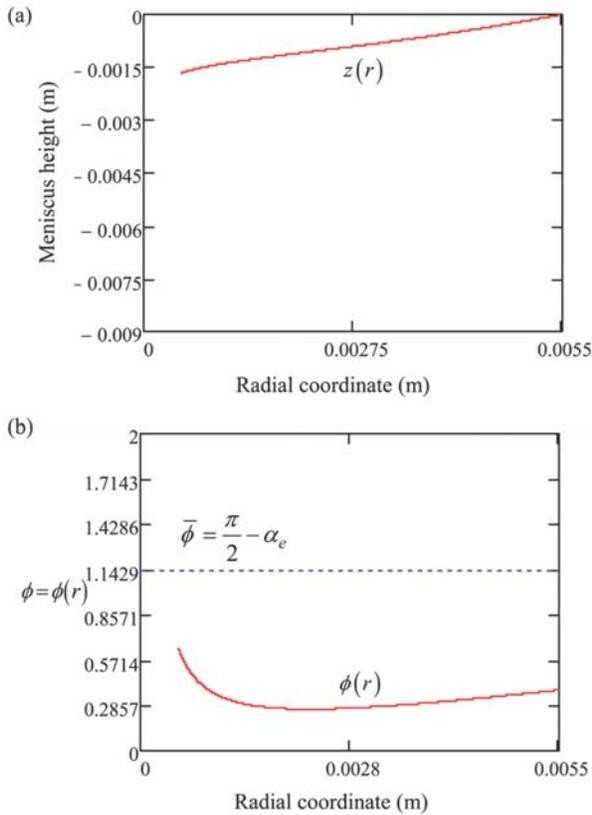


Fig. 5 Meniscus shape $z(r)$ (a) and meniscus angle $\phi(r)$ (b) corresponding to a pressure difference $\Delta P = 8 Pa$ and $\theta_c + \alpha_e = 112^\circ + 25^\circ$ for InSb. The place where the growth angle (25°) is achieved is shown by the black dot.

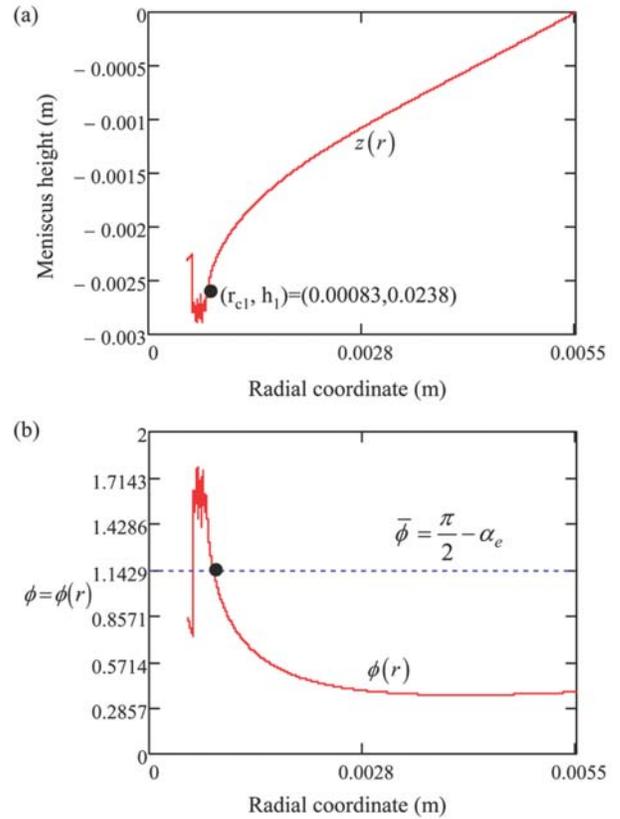


Fig. 6 Meniscus shape $z(r)$ (a) and meniscus angle $\phi(r)$ (b) corresponding to a pressure difference $\Delta P = 20 Pa$ and $\theta_c + \alpha_e = 112^\circ + 25^\circ$ for InSb. The place where the growth angle (25°) is achieved is shown by the black dot.

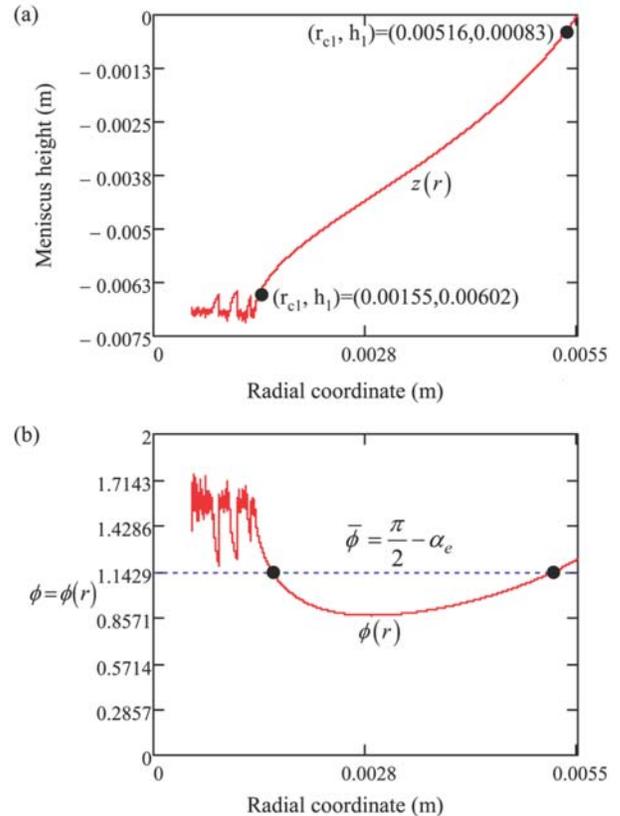


Fig. 7 Meniscus shape $z(r)$ (a) and meniscus angle $\phi(r)$ (b) corresponding to a pressure difference $\Delta P = 30 Pa$ and $\theta_c + \alpha_e = 160^\circ + 25^\circ$ for InSb. The places where the growth angle (25°) is achieved are shown by the black dots.

The above figures show that the menisci are concave-convex, and there are situations where the growth angle is not achieved, or the growth angle is achieved once, or the growth angle is achieved twice. If the growth angle is achieved on the concave part of the meniscus, then the computed gap thickness in Fig. 6 $e = r_a - r_{c1} = 0.0055 - 0.00083 = 0.00467 m$ is equal to $e_2 = 0.00467 m$ given by formula (24) and in Fig. 7, $e = r_a - r_{c1} = 0.0055 - 0.00155 = 0.00395 m$ is equal to $e_2 = 0.00395 m$. If the growth angle is achieved on the convex part of the meniscus, then the computed gap thickness $e = r_a - r_{c2} = 0.0055 - 0.00516 = 0.00035 m$ is equal to $e_1 = 0.00035 m$ given by formula (23), as can be observed in the Fig. 7.

(iii) If $\Delta P \in \left[-\frac{\gamma \cos \theta_c}{r_a}; +\infty \right)$, then the meniscus is

concave and the growth angle can be achieved once. In the case of achievement of the growth angle the gap thickness is given by e_2 expressed in (24). The numerical results show that the meniscus is concave, and that for $\theta + \alpha = 112^\circ + 25^\circ < \pi$,

$\Delta P = 40 \in \left[-\frac{\gamma \cos \theta_c}{r_a}; +\infty \right) = [28.6; +\infty)$ the growth

angle is achieved (Fig. 8). The computed gap thickness $e = r_a - r_{c1} = 0.0055 - 0.00165 = 0.00385 m$ is equal to $e_2 = 0.00385 m$ given by formula (24).

IV. DISCUSSION

Under zero gravity conditions the pressure inside the liquid is imposed by the hot free surface of the liquid and depends only on the crucible radius r_a and on the contact angle θ_c (Fig. 2). Then the curvature of the meniscus at the solid-liquid interface is totally fixed.

The experimental observations under microgravity conditions have shown, that the crystal-crucible gap is remarkably stable [5] which is in agreement with the above analysis: in microgravity, the meniscus is convex (i.e., the second derivative of the function which describes the evolution of the meniscus height is positive) as its curvature is imposed by the melt free surface at the hot side. Only in case of large pressure difference ΔP , the shape of the meniscus at the liquid- solid -gas triple line can be concave.

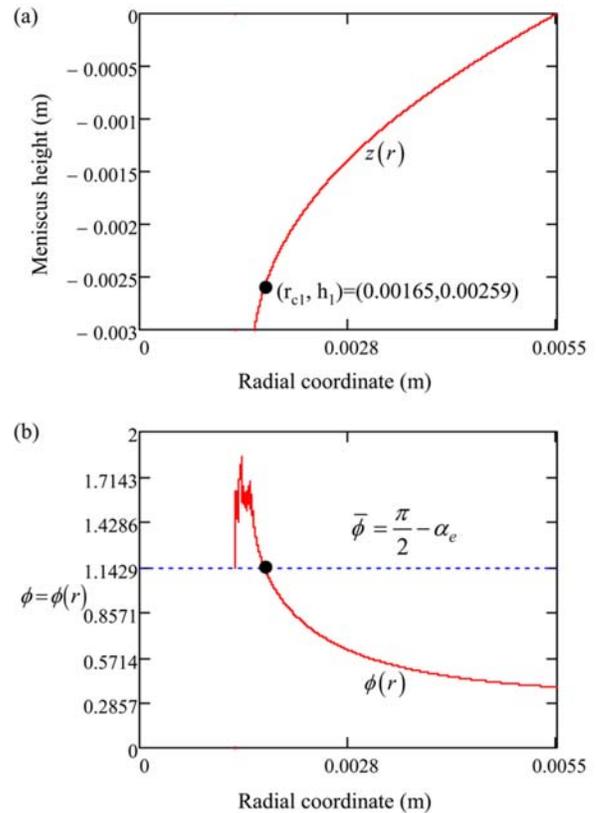


Fig. 8 Meniscus shape $z(r)$ (a) and meniscus angle $\phi(r)$ (b) corresponding to a pressure difference $\Delta P = 40 Pa$ and $\theta_c + \alpha_e = 112^\circ + 25^\circ$ for InSb. The places where the growth angle (25°) is achieved are shown by the black dots.

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REFERENCES

- [1] T. Duffar, I. Paret-Harter, P. Dusserre, Crucible de-wetting during Bridgman growth of semiconductors in microgravity, *Journal of Crystal Growth*, Vol. 100, 1990, pp. 171-184.
- [2] A. F. Witt, H. C. Gatos, *Proc. Space Processing Symp.* MSFC, Alabama, NASA M74-5, Vol. 1, 1974, pp. 425-456.
- [3] H. C. Gatos, A. F. Witt et al., Skylab Science Experiments Proc. Symp. 1974, *Sci. Technol. Series*, Vol. 38, 1975 p.7.
- [4] L. L. Regel, W. R. Wilcox, Detached solidification in microgravity-A review, *Microgravity Sci. Technol.*, Vol. X1/4, 1998, pp. 152-166.
- [5] T. Duffar, L. Sylla, *Vertical Bridgman and dewetting*, In *Crystal growth processes based on capillarity*, Wiley-Blackwell, in press, 2009.
- [6] P. S. Laplace, *Traité de mécanique céleste; suppléments au Livre X*, Euvres Complètes Vol. 4, Gauthier-Villars, Paris, 1806.
- [7] T. Young, An essay on the cohesion of fluids, *Philos. Trans. Roy. Soc. London*, Vol. 95, 1805, pp.65-87.
- [8] L. Braescu, "Nonlinear boundary value problem of the meniscus for the capillarity problems in crystal growth processes", in *Proceedings of 11th WSEAS International Conference on Mathematical and Computational*

Methods in Science and Engineering (Baltimore, USA), pp. 197-202 (2009).

- [9] L. Braescu, "Nonlinear boundary value problem of the meniscus for the dewetted Bridgman crystal growth processes", *International Journal of Mathematical Models and Methods in Applied Sciences*, to be published (2009).
- [10] S. Epure, T. Duffar, L. Braescu, On the capillary stability of the crystal-crucible gap during dewetted Bridgman process, *Journal of Crystal Growth*, to be published (2009) doi:10.1016/j.jcrysgr.2009.11.050.
- [11] T. Duffar, P. Boiton, P. Dusserre, J. Abadie, Crucible de-wetting during Bridgman growth in microgravity, II. Smooth crucibles, *Journal of Crystal Growth*, Vol. 179, 1997, pp. 397-409.
- [12] L. Braescu, S. Epure, T. Duffar, "Mathematical and numerical analysis of capillarity problems and processes," in *Crystal growth processes based on capillarity*, Wiley-Blackwell, 2010, ch.8.



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