Nonlinear boundary value problem of the meniscus for the dewetted Bridgman crystal growth process

L. Braescu

Abstract—Nonlinear boundary value problem of the Young-Laplace equation which describes the meniscus free surface in semiconductor crystals grown by Dewetted Bridgman technique is considered. The statically stability of the menisci, via the conjugate point criterion of the calculus of variations, is investigated in the cases of the classical semiconductors grown in (i) uncoated crucibles (i.e., the wetting angle θ_c and growth angle α_e satisfy the inequality $\theta_c+\alpha_e<180°$), and (ii) coated crucibles or pollution ($\theta_c+\alpha_e \geq 180°$). Necessary or sufficient conditions for the existence of the statically stable convex (or concave, convex-concave, concave-convex) solutions of the considered BVP are established.

Keywords— Nonlinear boundary value problem, Young-Laplace equation, growth from the melt, dewetted Bridgman crystal growth technique.

I. Introduction

A major problem to which crystal growth researchers have been confronted was the development of techniques capable to monitor and control the external shape of melt-grown crystals, and simultaneously to improve the crystal structures. In the crystal growth processes based on the principle of capillary shaping (Czochralski, Floating zone, Edge-defined film-fed growth, Dewetted Bridgman techniques, etc.), the shape and the dimensions of the crystal are determined by the liquid meniscus and by the heat transfer at the melt-crystal interface.

Historically, the physical origin and the shape of a liquid meniscus have been among the first phenomena studied in capillarity, in particular by Hauksbee (1709) [1], as cited by Maxwell [2] in his introduction to the *Capillary Action* written for the *Encyclopaedia Britannica*: „the first accurate observations of the capillary action of tubes and glass plates were made by Hauksbee. He ascribes the action to an attraction between the glass and the liquid".

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L. Braescu is with the Computer Science Department, West University of Timisoara, Blv. V Parvan 4, Timisoara 300223, ROMANIA (corresponding author phone: +4-025-659-2221; fax: +4-025-659-2316; e-mail: lilianabraescu@ balint1.math.uvt.ro).

The first formal analytical expression was given by Laplace [3], after introduction of the *mean curvature* κ defined as average (arithmetic mean) of the principal curvatures [4]:

$$\kappa = \frac{1}{2}\left(\frac{1}{R_1}+\frac{1}{R_2}\right). \tag{1}$$

Laplace showed that the *mean curvature* of the free surface is proportional to the pressure change across the surface. In crystal growth processes, the proportionality coefficient contains the surface tension γ and the pressure change across the surface (the pressure of the external gas on the melt p_v; the internal pressure applied on the liquid, which can generally be defined at the origin, p_O; the hydrostatic pressure $\rho_l g z$; the pressure determined by the centrifugal force due to a possible liquid rotation $\rho_l \Omega_l^2\left(x^2+y^2\right)/2$ where Ω_l is the angular velocity of the liquid; and when the magnetic fields is used, the Maxwell pressure which is proportional to the square of the magnetic induction $B^2(x,y)/2\mu$) [5]. Thus, the following equality known as Young-Laplace's equation must hold:

$$\frac{1}{R_1}+\frac{1}{R_2}=\frac{p_O-p_v-\rho_l g z+\frac{1}{2}\rho_l\Omega_l^2\left(x^2+y^2\right)-\frac{B^2(x,y)}{2\mu}}{\gamma}. \tag{2}$$

Denoting the meniscus surface by $z(x,y)$, it is known from differential geometry, that the mean curvature is expressed as:

$$\kappa=\frac{E_I G_{II}-2F_I F_{II}+G_I E_{II}}{2\left(E_I G_I-F_I^2\right)} \tag{3}$$

where

$$E_I=1+\left(\frac{\partial z}{\partial x}\right)^2,\quad F_I=\frac{\partial z}{\partial x}\cdot\frac{\partial z}{\partial y},\quad G_I=1+\left(\frac{\partial z}{\partial y}\right)^2$$

represent the coefficients of the first fundamental form of the surface, and

$$E_{II}=\frac{\frac{\partial^2 z}{\partial x^2}}{\sqrt{1+\left(\frac{\partial z}{\partial x}\right)^2+\left(\frac{\partial z}{\partial y}\right)^2}},$$

$$F_{II} = \frac{\dfrac{\partial z}{\partial x} \cdot \dfrac{\partial z}{\partial y}}{\sqrt{1+\left(\dfrac{\partial z}{\partial x}\right)^2+\left(\dfrac{\partial z}{\partial y}\right)^2}},$$

$$G_{II} = \frac{\dfrac{\partial^2 z}{\partial y^2}}{\sqrt{1+\left(\dfrac{\partial z}{\partial x}\right)^2+\left(\dfrac{\partial z}{\partial y}\right)^2}}$$

represent the coefficients of the second fundamental form. Hence, the Young-Laplace equation (2) becomes:

$$\frac{\left[1+\left(\dfrac{\partial z}{\partial y}\right)^2\right]\cdot\dfrac{\partial^2 z}{\partial x^2}-2\cdot\dfrac{\partial z}{\partial x}\cdot\dfrac{\partial z}{\partial y}\cdot\dfrac{\partial^2 z}{\partial x \partial y}+\left[1+\left(\dfrac{\partial z}{\partial x}\right)^2\right]\cdot\dfrac{\partial^2 z}{\partial y^2}}{\left[1+\left(\dfrac{\partial z}{\partial x}\right)^2+\left(\dfrac{\partial z}{\partial y}\right)^2\right]^{\frac{3}{2}}} \tag{4}$$

$$= \frac{p_O - p_v - \rho_l g z + \dfrac{1}{2}\rho_l \Omega_l^2\left(x^2+y^2\right) - \dfrac{B^2(x,y)}{2\mu}}{\gamma}.$$

This equation is a nonlinear partial differential equation of second order, and the unknown function $z(x,y)$ represents the meniscus surface.

In the axi-symmetric case, the Young-Laplace equation (4) can be written using cylindrical polar coordinates $x = r \cdot cos\,\phi,\ y = r \cdot sin\,\phi,\ z = z$ (the meniscus is axi-symmetric). Expressing r and ϕ as functions of x and y, i.e., $r=\sqrt{x^2+y^2}$, $\phi = arctan\,\frac{y}{x}$, the partial derivatives of the function $z(x,y)$ are:

$$\frac{\partial z}{\partial x} = \frac{dz}{dr}\cdot\frac{x}{r},$$

$$\frac{\partial z}{\partial y} = \frac{dz}{dr}\cdot\frac{y}{r},$$

$$\frac{\partial^2 z}{\partial x^2} = \frac{d^2 z}{dr^2}\cdot\frac{x^2}{r^2}+\frac{dz}{dr}\cdot\frac{y^2}{r^3},$$

$$\frac{\partial^2 z}{\partial y^2} = \frac{d^2 z}{dr^2}\cdot\frac{y^2}{r^2}+\frac{dz}{dr}\cdot\frac{x^2}{r^3},$$

$$\frac{\partial^2 z}{\partial x \partial y} = \frac{d^2 z}{dr^2}\cdot\frac{xy}{r^2}-\frac{dz}{dr}\cdot\frac{xy}{r^3}.$$

Replacing these derivatives in (4), *Young-Laplace's equation* written *in cylindrical coordinates is*:

$$\frac{d^2 z}{dr^2}+\frac{1}{r}\cdot\frac{dz}{dr}\cdot\left[1+\left(\frac{dz}{dr}\right)^2\right] \tag{5}$$

$$= \frac{p_O - p_v - \rho_l g z + \dfrac{1}{2}\rho_l \Omega_l^2 \cdot r^2 - \dfrac{B^2(r)}{2\mu}}{\gamma}\cdot\left[1+\left(\frac{dz}{dr}\right)^2\right]^{\frac{3}{2}}$$

for which the solution $z=z(r)$ is searched depending on the radial coordinate $r=\sqrt{x^2+y^2}$. An equivalent formulation of (5) is:

$$\frac{d^2 z}{dr^2} = \frac{p_O - p_v - \rho_l g z + \dfrac{1}{2}\rho_l \Omega_l^2 \cdot r^2 - \dfrac{B^2(r)}{2\mu}}{\gamma}\cdot\left[1+\left(\frac{dz}{dr}\right)^2\right]^{\frac{3}{2}} \tag{6}$$

$$-\frac{1}{r}\cdot\frac{dz}{dr}\cdot\left[1+\left(\frac{dz}{dr}\right)^2\right].$$

For solving the axi-symmetric Young-Laplace equation, initial or/and boundary conditions are determined by the structural features of each specific configuration (Czochralski, Floating zone, Edge-defined film-fed growth, Dewetted Bridgman techniques, etc.).

II. YOUNG –LAPLACE EQUATION FOR THE DEWETTED BRIDGMAN CRYSTAL GROWTH PROCESS

Dewetted Bridgman is a crystal growth technique in which the crystal is detached from the crucible wall by a liquid free surface (liquid meniscus) at the level of the solid-liquid interface which creates a gap between the crystal and the ampoule (see Fig.1).

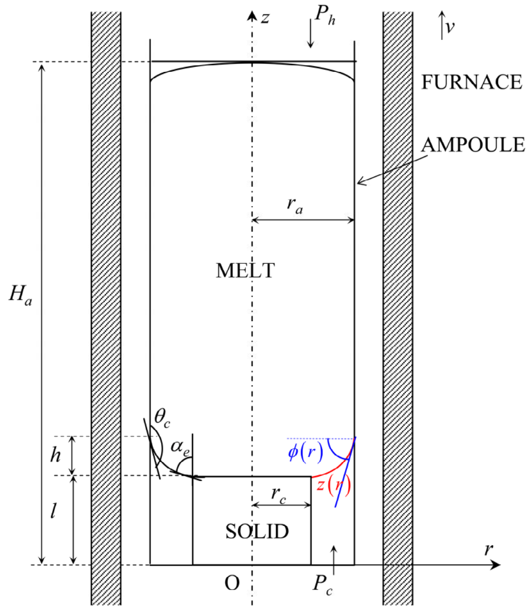

Fig. 1: Schematic dewetted Bridgman crystal growth technique.

The dewetting was first obtained spontaneously in space experiments during InSb Bridgman solidification performed on Skylab-NASA mission-1974 [6], and subsequently in many experiments carried out in orbiting spacecrafts (microgravity) on a wide variety of semiconductors. Since the most important aspect of dewetting is the huge improvement of the crystalline quality (reduction in spurious nucleation, fewer dislocations, lower stresses, etc.), this phenomenon has attracted considerable attention. There have been several studies on the mechanisms which may lead to dewetting.

Duffar et al. focused on the meniscus equilibrium for rough [7] and smooth ampoule surfaces [8]. An analytical formula for gap thickness was reported in zero gravity, through a theoretical model based on Young-Laplace equation in which the principal radii of meniscus curvature were expressed using curvilinear coordinate *s*. They concluded that the gap thickness depends on various parameters: contact angle, growth angle α_e, surface tension, ampoule radius, and gas pressure difference.

Understanding the results obtained in microgravity opened the possibility for the dewetting growth on the earth, that can be obtained by applying a gas pressure difference $\Delta P= P_c-P_h$ between the cold and hot sides of the sample (see Fig.1). In this case, the Young-Laplace equation of a capillary surface (5) written in agreement with the above configuration is:

$$\frac{d^2z}{dr^2}+\frac{1}{r}\cdot\frac{dz}{dr}\cdot\left[1+\left(\frac{dz}{dr}\right)^2\right] = \frac{p_O-p_v-\rho_l gz}{\gamma}\cdot\left[1+\left(\frac{dz}{dr}\right)^2\right]^{\frac{3}{2}} \tag{7}$$

where the external pressure on the melt $p_v = P_c$, and the internal pressure applied on the liquid, p_O is defined as:

$p_O = P_h+\rho_l gH_a+2\gamma/b$.

Here, ρ_l represents density of the melt; g - gravitational acceleration; H_a - ampoule length; γ - surface tension of the melt; $2/b$ - the curvature at the top which in microgravity conditions is $1/b=-(\cos\theta_c)/r_a$; θ_c - contact angle; r_a - ampoule radius; h - the meniscus height; l - level of the liquid-solid interface. Thus Young-Laplace equation can be written as follows:

$$\frac{d^2z}{dr^2}=\left[\frac{\rho_l g\cdot(H_a-z)-\Delta P}{\gamma}+\frac{2}{b}\right] \times\left[1+\left(\frac{dz}{dr}\right)^2\right]^{\frac{3}{2}}-\frac{1}{r}\cdot\frac{dz}{dr}\cdot\left[1+\left(\frac{dz}{dr}\right)^2\right]. \tag{8}$$

The solution of (8) has to verify the following boundary conditions:

$z(r_c)=l$ and $z'(r_c)=\tan\left(\frac{\pi}{2}-\alpha_e\right)$, (8a)

$z(r_a)=l+h$ and $z'(r_a)=\tan\left(\theta_c-\frac{\pi}{2}\right)$, (8b)

$z(r)$ is strictly increasing on $[r_c;\, r_a]$, (8c)

where r_c represent the crystal radius.

Comments:

(i) Condition $z(r_c)=l$ expresses that the coordinate of the crystallization front is equal to $l\geq l_0>0$ (l_0 represents the length of the seed); and the condition $z'(r_c)=\tan(\pi/2-\alpha_e)$ expresses that at the point $(r_c; z(r_c))=(r_c;l)$ where the solidification condition has to be realized (i.e., the left end of the free meniscus surface), the angle between the tangent line to the free surface and the vertical is equal to the growth angle α_e, $\alpha_e\in(0;\pi/2)$.

(ii) Condition $z(r_a)=l+h$ expresses the fact that the meniscus height is equal to h; and the condition $z'(r_a)=\tan(\theta_c-\pi/2)$ expresses that at the point $(r_a; z(r_a))=(r_a;l+h)$ where the free surface touch the ampoule wall (i.e., the right end of the free meniscus surface), the contact (wetting) angle is equal to θ_c, $\theta_c\in(\pi/2;\pi)$.

(iii) Condition (8c) expresses the fact that the meniscus shape is relatively simple.

Equation (8) and boundary conditions (8a)-(8c) represent the nonlinear boundary value problem (NLBVP) of the Young-Laplace equation which describes the equilibrium capillary free surface in semiconductor crystals grown by Dewetted Bridgman. Moreover, equation (8) is the Euler equation of the energy functional of the melt column.

Indeed, the total free energy written for dewetted Bridgman configuration presented in Fig.1, is composed by the surface free energy and the gravity field energy:

$$I(x,y)=\gamma\iint_D\left[1+\left(\frac{\partial z}{\partial x}\right)^2+\left(\frac{\partial z}{\partial x}\right)^2\right]^{1/2}dxdy + \iint_D\left[-\frac{\rho_l gz^2}{2}+\left(\rho_l gH_a-\Delta P+2\frac{\gamma}{b}\right)z\right]dxdy. \tag{9}$$

In cylindrical polar coordinates, the total free energy becomes:

$$I(z)=2\pi\int_{r_c}^{r_a}\left\{\gamma\left[1+\left(\frac{dz}{dr}\right)^2\right]^{\frac{1}{2}}+\left[-\frac{\rho_l gz^2}{2} +\left(\rho_l gH_a-\Delta P+2\frac{\gamma}{b}\right)z\right]\right\}r\,dr \tag{10}$$

or

$$I(z)=2\pi\int_{r_c}^{r_a}F(r,z,z')dr,$$

where

$$F(r,z,z')=\left\{\gamma\left[1+\left(\frac{dz}{dr}\right)^2\right]^{\frac{1}{2}}+\left[-\frac{\rho_l gz^2}{2} +\left(\rho_l gH_a-\Delta P+2\frac{\gamma}{b}\right)z\right]\right\}\cdot r. \tag{11}$$

If there exists a meniscus z_0 such that $I(z_0)$=*minimum*, then the meniscus z_0 is called *statically stable* (i.e., the meniscus is kept in a stable equilibrium for any small variations δz and $\delta z' = \frac{d(\delta z)}{dr}$ [9]).

A solution $z(r)$ is *minimum* for $I(z)$ if and only if the following conditions are satisfied:

(a) existence of the extreme expressed by the Euler equation $\frac{\partial F}{\partial z}-\frac{d}{dr}\left(\frac{\partial F}{\partial z'}\right)=0$;

(b) Legendre condition $\frac{\partial^2 F}{\partial z'^2} > 0$;

(c) Jacobi equation $\frac{d}{dr}\left[\frac{\partial^2 F}{\partial z'^2}\cdot\eta' + \frac{\partial^2 F}{\partial z\,\partial z'}\cdot\eta\right] - \left[\frac{\partial^2 F}{\partial z^2}\cdot\eta + \frac{\partial^2 F}{\partial z\,\partial z'}\cdot\eta'\right] = 0$ satisfying the boundary conditions $\eta(r_a) = 0$, $\eta'(r_a) = 1$, has no conjugate points [9]-[11], i.e. the solution $\eta(r)$ of the Jacobi equation is no null for any r belongs to $(r_c;\, r_a)$.

It is important to underline that the Euler equation only determines extremals, but does not give any information about their stability. In order to be sure that a minimal solution exists, the Legendre and Jacobi conditions should be satisfied.

Using the equality (11), Euler's condition gives the meniscus equation (8). In the case of terrestrial growth, for crucibles with a reasonable practical radius (larger than the melt capillary constant), the curvature of the upper free liquid surface is very small, and hence the term $2/b$ can be neglected [5], [12].

Concerning the conditions (b)-(c), it is easy to observe that Legendre condition is fulfilled: $\frac{\partial^2 F}{\partial z'^2} = \frac{\gamma}{\left[1 + z'^2\right]^{\frac{3}{2}}}\cdot r > 0$.

Replacing the partial derivatives in Jacobi condition, a Sturm-Liouville problem of the form $\frac{d}{dr}\left[p(r)\cdot\eta'\right] + q(r)\cdot\eta = 0$ [11] is obtained:

$$\frac{d}{dr}\left[\frac{r\cdot\gamma}{\left[1+(z')^2\right]^{3/2}}\cdot\eta'\right] + \rho_l g r\cdot\eta = 0 \tag{12}$$

$$\eta(r_a) = 0,\ \eta'(r_a) = 1$$

where

$$p(r) = \frac{r\cdot\gamma}{\left[1+(z')^2\right]^{3/2}},\ q(r) = \rho_l g r.$$

For studying if the non-trivial solution $\eta(r)$ is no null on the interval $(r_c;\, r_a)$, the cases $\theta_c + \alpha_e < 180^\circ$ and $\theta_c + \alpha_e \geq 180^\circ$ should be treated separately because different behaviours of the meniscus shape. However, from sessile drop measurements it is known that semiconductors have the Young contact angles lower than 150° at equilibrium, and the growth angle values are lower than 30° (except InP). This means that the inequality $\alpha_e + \theta_c < 180^\circ$ is generally valid for semiconductors. On the other hand, crystal growth experiments showed that, in some conditions, contact angle may vary from 178° to 152° for the growth angle varying from 0° to 30°, leading to an unexpected inequality between the wetting angle θ_c and growth angle α_e (i.e., $\alpha_e + \theta_c \geq 180^\circ$). This phenomenon was explained on the basis of the thermodynamical analysis [12]-[13], which proved that the chemical contamination modifies the contact angle by increasing it artificially.

III. STATIC STABILITY OF THE MENISCI

A. Case of microgravity

In the case of *microgravity* the meniscus equation (8) becomes [14]-[15]:

$$z'' = \left(-\frac{\Delta P}{\gamma} - \frac{2\cos\theta_c}{r_a}\right)\cdot\left[1 + z'^2\right]^{\frac{3}{2}} - \frac{1}{r}\cdot z'\cdot\left[1 + z'^2\right] \tag{13}$$

and the Jacobi condition is

$$\frac{d}{dr}\left[\frac{r\cdot\gamma}{\left[1+(z')^2\right]^{3/2}}\cdot\eta'\right] = 0 \tag{14}$$

$$\eta(r_a) = 0,\ \eta'(r_a) = 1$$

i.e., $q(r)=0$. Integrating (13), the following analytical expression of the derivative of $z(r)$ is obtained:

$$z'(r) = \pm\frac{\left(-\frac{\cos\theta_c}{r_a} - \frac{\Delta P}{2\gamma}\right)\cdot r^2 + c_1}{\sqrt{r^2 - \left[\left(-\frac{\cos\theta_c}{r_a} - \frac{\Delta P}{2\gamma}\right)\cdot r^2 + c_1\right]^2}}. \tag{15}$$

As the function $z(r)$ is strictly increasing on $[r_c;\, r_a]$, the positive sign is chosen. The constant c_1 is determined from the boundary condition (8b), leading to

$$z'(r) = \frac{r^2\left(-\frac{\Delta P}{2\gamma} - \frac{\cos\theta_c}{r_a}\right) + \frac{\Delta P\cdot r_a^2}{2\gamma}}{\sqrt{r^2 - \left[r^2\left(-\frac{\Delta P}{2\gamma} - \frac{\cos\theta_c}{r_a}\right) + \frac{\Delta P\cdot r_a^2}{2\gamma}\right]^2}}. \tag{16}$$

Replacing $z'(r)$ in the Jacobi's equation, after integration, the derivative of $\eta(r)$ is computed

$$\eta'(r) = \frac{r^2\cdot r_a\cdot\sin^3\theta_c}{\left\{r^2 - \left[r^2\left(-\frac{\Delta P}{2\gamma} - \frac{\cos\theta_c}{r_a}\right) + \frac{\Delta P\cdot r_a^2}{2\gamma}\right]^2\right\}^{\frac{3}{2}}}. \tag{17}$$

It is easy to see that $\eta'(r)>0$, and hence the solution $\eta(r)$ increases. Moreover, due to the boundary condition $\eta(r_a) = 0$, it is obtained that $\eta(r)$ is no null on the interval $(r_c;\, r_a)$, which shows that in the case of zero gravity, *all menisci are statically stable*.

B. Case of terrestrial conditions

In the case of *terrestrial growth conditions* the derivative $z'(r)$ can not be obtained analytically and hence for obtaining information concerning the nonzero solution $\eta(r)$ of the Jacobi equation, Sturm-Picone comparison theorem should be used as follows:

(i) For finding menisci which are *statically stable*, a Sturm majorant equation is searched. Considering the Sturm-Liouville equation (12), new functions satisfying

$$p(r) \geq p_-(r) \quad \text{and} \quad q(r) \leq q^+(r) \tag{18}$$

should be found. Thus, *Sturm's majorant equation*

$$\frac{d}{dr}\left[p_-(r)\cdot\eta'\right] + q^+(r)\cdot\eta = 0 \tag{19}$$

is obtained, and information about its solution can be searched.

Remark: If the solution $\eta(r)$ of the Sturm majorant equation (19) has only the root r_a, then the solution $\eta(r)$ of the Jacobi equation is no null for any r belongs to $(r_c; r_a)$.

(ii) For finding menisci which are *statically unstable*, a Sturm minorant equation is searched. Thus, for the Sturm-Liouville equation new functions satisfying

$$p(r) \leq p^+(r) \quad \text{and} \quad q(r) \geq q_-(r) \tag{20}$$

are built, and the following *Sturm's minorant equation* is obtained:

$$\frac{d}{dr}\left[p^+(r)\cdot\eta'\right] + q_-(r)\cdot\eta = 0 \ . \tag{21}$$

Remark: If the solution $\eta(r)$ of the Sturm minorant equation (21) has minimum two roots, then the solution $\eta(r)$ of the Jacobi equation has at least one zero on the interval $(r_c; r_a)$.

Necessary or sufficient conditions for the existence of the statically stable convex (or concave, convex-concave, concave-convex) menisci are searched in the cases $\theta_c + \alpha_e < 180^\circ$ and $\theta_c + \alpha_e \geq 180^\circ$.

Case $\alpha_e + \theta_c < 180^\circ$

Since the inequality $\theta_c + \alpha_e < 180^\circ$ implies $\theta_c - \frac{\pi}{2} < \frac{\pi}{2} - \alpha_e$, using the function $\phi(r)$ defined by $\frac{dz}{dr} = tan\,\phi$ (see Fig.1) and the corresponding boundary condition $\phi(r_a) = \theta_c - \frac{\pi}{2}$ equivalent to (8b), we obtain that starting from $\theta_c - \frac{\pi}{2}$, the growth angle $\frac{\pi}{2} - \alpha_e$ can be achieved only if $\phi(r)$ decreases from $\frac{\pi}{2} - \alpha_e$ to $\theta_c - \frac{\pi}{2}$, i.e. $\frac{d\phi}{dr} < 0$. On the other hand, $\frac{d^2z}{dr^2} = \frac{1}{cos^2\phi}\cdot\frac{d\phi}{dr}$, and hence $\frac{d^2z}{dr^2} < 0$, i.e., the meniscus should be concave in the neighbourhood of r_a. Due to this reason, in the followings, special attention is paid on the *globally concave* and *convexo-concave* ("S" shape) menisci shapes [16]-[17].

If the meniscus is *globally concave,* then for studying *static stability*, inequalities of the form (18) are found:

$$q(r) = \rho_l g r \leq \rho_l g r_a = q^+(r)$$

and

$$p(r) = \frac{r\cdot\gamma}{\left[1+(z')^2\right]^{3/2}} = \frac{r\cdot\gamma}{\left[1+tan^2\,\phi(r)\right]^{3/2}}$$

$$= \gamma\cdot r\cdot cos^3\,\phi(r) \geq \gamma\cdot(r_a - e)\cdot sin^3\,\alpha_e = p_-(r)\,,$$

here e represents the gap thickness $e = r_a - r_c$.

In the last inequality, the monotony of the function $\phi(r)$ was involved (i.e., decreases for globally concave meniscus). More precisely, starting from $\theta_c - \frac{\pi}{2} \leq \phi(r) \leq \frac{\pi}{2} - \alpha_e$, it is obtained $cos\left(\theta_c - \frac{\pi}{2}\right) \geq cos\left(\phi(r)\right) \geq cos\left(\frac{\pi}{2} - \alpha_e\right)$, and hence $cos^3\left(\phi(r)\right) \geq cos^3\left(\frac{\pi}{2} - \alpha_e\right) = sin^3\,\alpha_e$.

Thus, the corresponding Sturm majorant equation for globally concave menisci is:

$$\frac{d}{dr}\left[\gamma\cdot(r_a - e)\cdot sin^3\,\alpha_e\cdot\eta'\right] + \rho_l g r_a\cdot\eta = 0 \tag{22}$$

which is equivalent to

$$\eta'' + \frac{\rho_l g r_a}{\gamma\cdot(r_a - e)\cdot sin^3\,\alpha_e}\cdot\eta = 0 \ . \tag{23}$$

According to the Hartman inequality [11], roots' number N of the non-trivial solution $\eta(r)$ of (23) satisfies the inequality

$$N < \frac{1}{2}\cdot\left[(r_a - r_c)\cdot\int_{r_c}^{r_a}\frac{\rho_l g r_a}{\gamma\cdot(r_a - e)\cdot sin^3\,\alpha_e}\,dr\right]^{\frac{1}{2}} + 1. \tag{24}$$

Then, imposing for the solution $\eta(r)$ of the Sturm majorant equation to have maximum one root at r_a (i.e. it does not have a root different by r_a), the following limitation of the gap thickness is obtained:

$$\frac{2}{r_a}\cdot\sqrt{\frac{\gamma\cdot sin^3\,\alpha_e}{\rho_l g}} > \frac{e}{\sqrt{r_a\cdot(r_a - e)}}\,. \tag{25}$$

Comment: Numerical simulations made for InSb [18] showed that the globally concave menisci are statically stable for gaps in the range $e \in (0; 0.00123]$m. Since computed gap range for which the meniscus has concave shape is $e \in (0; 0.00143]$m [17], it can be concluded that *globally concave menisci are statically stable*, with possible exception in the case of a larger gap.

For studying *static instability* of the *globally concave* menisci, inequalities of the form (20) are searched. Thus,

$$q(r) = \rho_l g r \leq \rho_l g r_c = \rho_l g\cdot(r_a - e) = q_-(r)$$

and

$$p(r) = \frac{r\cdot\gamma}{\left[1+(z')^2\right]^{3/2}} = \gamma\cdot r\cdot cos^3\,\phi(r)$$

$$\leq \gamma\cdot r_a\cdot cos^3\left(\theta_c - \frac{\pi}{2}\right) = \gamma\cdot r_a\cdot sin^3\,\theta_c = p^+(r)\,.$$

In this case, the corresponding Sturm minorant equation for globally concave menisci is:

$$\frac{d}{dr}\left[\gamma \cdot r_a \cdot sin^3 \theta_c \cdot \eta'\right] + \rho_l g \left(r_a - e\right) \cdot \eta = 0 \tag{26}$$

which is equivalent to

$$\eta'' + \frac{\rho_l g \cdot \left(r_a - e\right)}{\gamma \cdot r_a \cdot sin^3 \theta_c} \cdot \eta = 0 \cdot \tag{27}$$

Imposing for the solution $\eta(r)$ of the Sturm minorant equation to have minimum two roots (see the corresponding Hartman inequality), the following estimation of the gap thickness is found:

$$2 \cdot \sqrt{\frac{\gamma \cdot r_a \cdot sin^3 \theta_c}{\rho_l g}} < e \cdot \sqrt{r_a - e}. \tag{28}$$

Comment: The inequality (28) was evaluated numerically for InSb [18]. It was obtained that there are no gap thickness values satisfying (28), i.e. there are no values of e for which the meniscus is unstable.

Concerning the *convexo-concave* menisci, the problem is more difficult because the function $\phi(r)$, defined by $\frac{dz}{dr} = tan\,\phi$, increases in the first part of the interval $(r_c;\ r_a)$ and after that decreases [16]-[17]. More precisely, using the second derivative $\frac{d^2 z}{dr^2} = \frac{1}{cos^2 \phi} \cdot \frac{d\phi}{dr}$, and the shape convexo-concave, it is obtained that $\frac{d\phi}{dr} > 0$ on the interval $(r_c;\ I)$ and $\frac{d\phi}{dr} < 0$ on the interval $(I;\ r_a)$, where I represents the inflexion point of the meniscus (i.e., $\phi(r)$ is maximum at I).

Thus, for studying *static stability*, the following inequalities of the form (18) are found:

$$q(r) = \rho_l g r \le \rho_l g r_a = q^+(r)$$

and

$$p(r) = \frac{r \cdot \gamma}{\left[1 + (z')^2\right]^{3/2}} = \frac{r \cdot \gamma}{\left[1 + tan^2 \phi(r)\right]^{3/2}}$$

$$= \gamma \cdot r \cdot cos^3 \phi(r) \ge \gamma \cdot \left(r_a - e\right) \cdot cos^3\left(max\,\phi(r)\right) = p_-(r).$$

Sturm majorant equation for convexo-concave menisci is:

$$\frac{d}{dr}\left[\gamma \cdot \left(r_a - e\right) \cdot cos^3\left(max\,\phi(r)\right) \cdot \eta'\right] + \rho_l g r_a \cdot \eta = 0. \tag{29}$$

Comment: Computing $max\,\phi(r)$ for InSb and then imposing for $\eta(r)$ to have maximum one root at r_a, it is obtained that the convexo-concave meniscus is stable for $e \in (0;\ 0.000003]$. Comparing this range with computed gap range $[0.00142;\ 0.00315]$ for ΔP corresponding to the menisci having "*S*" shape [17], it can be concluded that, for the considered parameters, there are no gap thicknesses for which convexo-concave menisci are statically stable.

For obtaining a Sturm minorant equation (static instability), the following inequalities are found:

$$q(r) = \rho_l g r \le \rho_l g r_c = \rho_l g \cdot \left(r_a - e\right) = q_-(r)$$

and

$$p(r) = \frac{r \cdot \gamma}{\left[1 + (z')^2\right]^{3/2}} = \gamma \cdot r \cdot cos^3 \phi(r) \le \gamma \cdot r_a = p^+(r).$$

Hence, the Sturm minorant equation is

$$\eta'' + \frac{\rho_l g \cdot \left(r_a - e\right)}{\gamma \cdot r_a} \cdot \eta = 0, \tag{30}$$

and imposing for $\eta(r)$ to have minimum two roots, the gap thickness inequality is obtained:

$$2 \cdot \sqrt{\frac{\gamma \cdot r_a}{\rho_l g}} < e \cdot \sqrt{r_a - e}. \tag{31}$$

Case $\alpha_e + \theta_c \ge 180^\circ$

Since the inequality $\alpha_e + \theta_c \ge 180^\circ$ implies $\theta_c - \frac{\pi}{2} \ge \frac{\pi}{2} - \alpha_e$, using the function $\phi(r)$ defined by $\frac{dz}{dr} = tan\,\phi$, and the boundary condition $\phi(r_a) = \theta_c - \frac{\pi}{2}$, we obtain that starting from $\theta_c - \frac{\pi}{2}$, the growth angle $\frac{\pi}{2} - \alpha_e$ can be achieved only if $\phi(r)$ increases from $\frac{\pi}{2} - \alpha_e$ to $\theta_c - \frac{\pi}{2}$, i.e. $\frac{d\phi}{dr} > 0$. On the other hand, $\frac{d^2 z}{dr^2} = \frac{1}{cos^2 \phi} \cdot \frac{d\phi}{dr}$, and hence $\frac{d^2 z}{dr^2} > 0$, i.e., the meniscus should be convex in the neighbourhood of r_a (this includes *globally convex* or *concave-convex* menisci [5]). Also, if the meniscus presents convex parts, i.e. the meniscus is *convexo-concave* then the dewetting is feasible [18].

If the meniscus is *globally convex* then for studying *static stability*, the inequalities

$$q(r) = \rho_l g r \le \rho_l g r_a = q^+(r)$$

and

$$p(r) = \frac{r \cdot \gamma}{\left[1 + (z')^2\right]^{3/2}} = \frac{r \cdot \gamma}{\left[1 + tan^2 \phi(r)\right]^{3/2}}$$

$$= \gamma \cdot r \cdot cos^3 \phi(r) \ge \gamma \cdot \left(r_a - e\right) \cdot sin^3 \theta_c = p_-(r),$$

are used. Here the monotony of the function $\phi(r)$ was involved (i.e., increases for globally convex meniscus). More precisely, starting from $\frac{\pi}{2} - \alpha_e \le \phi(r) \le \theta_c - \frac{\pi}{2}$, it is obtained $cos\left(\frac{\pi}{2} - \alpha_e\right) \ge cos\left(\phi(r)\right) \ge cos\left(\theta_c - \frac{\pi}{2}\right)$, and hence $cos^3\left(\phi(r)\right) \ge cos^3\left(\theta_c - \frac{\pi}{2}\right) = sin^3 \theta_c$.

Thus, the following Sturm majorant equation is obtained:

$$\eta'' + \frac{\rho_l g r_a}{\gamma \cdot \left(r_a - e\right) \cdot sin^3 \theta_c} \cdot \eta = 0 \cdot \tag{32}$$

Imposing for the solution $\eta(r)$ of the Sturm majorant equation to have maximum one root at r_a, the following limitation of the gap thickness which assures the statically stable globally convex is obtained:

$$\frac{2}{r_a}\cdot\sqrt{\frac{\gamma\cdot sin^3\theta_c}{\rho_l g}} > \frac{e}{\sqrt{r_a\cdot(r_a-e)}}. \qquad (33)$$

Comment: Numerical simulations made for *Ge* grown in pBN sleeve [18], showed that the globally convex menisci are statically stable for gaps in the range $e\in(0;\ 0.000217]$m. Comparing this range with the computed gap range $[0;0.000186]$ for ΔP corresponding to the convex menisci at r_a [19]-[20], it can be concluded that *convex menisci are statically stable*.

For studying *static instability* of the *globally convex* menisci, the followings inequalities are used

$$q(r)=\rho_l gr\le\rho_l gr_c=\rho_l g\cdot(r_a-e)=q_-(r)$$

and

$$p(r)=\frac{r\cdot\gamma}{\left[1+(z')^2\right]^{3/2}}=\gamma\cdot r\cdot cos^3\phi(r)$$

$$\le\gamma\cdot r_a\cdot cos^3\left(\frac{\pi}{2}-\alpha_e\right)=\gamma\cdot r_a\cdot sin^3\alpha_e=p^+(r).$$

In this case, the corresponding Sturm minorant equation for globally convex menisci is:

$$\frac{d}{dr}\left[\gamma\cdot r_a\cdot sin^3\alpha_e\cdot\eta'\right]+\rho_l g(r_a-e)\cdot\eta=0 \qquad (34)$$

which is equivalent to

$$\eta''+\frac{\rho_l g\cdot(r_a-e)}{\gamma\cdot r_a\cdot sin^3\alpha_e}\cdot\eta=0\cdot \qquad (35)$$

Imposing for $\eta(r)$ to have minimum two roots, the following estimation of the gap thickness is found:

$$2\cdot\sqrt{\frac{\gamma\cdot r_a\cdot sin^3\alpha_e}{\rho_l g}}<e\cdot\sqrt{r_a-e}. \qquad (36)$$

Comment: The inequality (36) was evaluated numerically for *Ge* grown in pBN sleeve. It was obtained that, for the considered parameters, there are no gap thickness values satisfying (36), i.e. there are no values of *e* for which the globally convex meniscus is unstable.

The static stability (instability) of the convexo-concave or concave-convex menisci is investigated in similar way with those presented in the case $\alpha_e+\theta_c<180^\circ$.

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Liliana Braescu was born in Romania in 1967. She received her Ph.D. degree in mathematics from West University of Timisoara, Romania, in 2002.

She has held positions in secondary and high schools, and at the undergraduate and postgraduate levels: Mathematics Teacher at the Secondary School "Avram Iancu," Timisoara, 1991-93; Mathematics Teacher at the High School "Colegiul National Banatean," Timisoara 1993-99; Assistant Professor in the Department of Mathematics, Technical University of Timisoara, 1999-2003; Lecturer in the Department of Mathematics, Technical University of Timisoara, 2003-04; Senior Lecturer in the Faculty of Mathematics and Computer Science, West

University of Timisoara, 2004-06; Associate Professor in the Faculty of Mathematics and Computer Science, West University of Timisoara, 2006-present. Her research has led to 29 papers published in refereed journals, 6 chapters in books (Springer, Cambridge Scientific Publishers, Nova Science Publishers, Wiley & Sons), 1 textbook, 64 communications to scientific meetings (30 published in proceedings), and 9 course materials. Three representative publications are the following: (1) T. F. George, L. Braescu, A. M. Balint, L. Nánai and S. Balint, *Microcomputer Modeling of Growth Processes of Single-Crystal Sheets and Fibers*. Hauppauge, New York: Nova Science Publishers, 2007, 199 pages; (2) S. Balint, L. Braescu and E. Kaslik, "Control procedure in shaped crystal growth using region of attraction," in *Regions of Attraction and Applications to Control Theory,* edited by S. Sivasundaram, Cambridge: Cambridge Scientific Publishers, 2008, 206 pages; and (3) L. Braescu, "Shape of menisci in terrestrial dewetted Bridgman growth," *Journal of Colloid and Interface Science*, vol. 319, pp. 309-315 (2008). Her research interests include control theory, ordinary and partial differential equations, stability and domains of attractions with applicability in modelling of the crystal growth processes, blood coagulation, and dental endosteal implantation.

Associate Professor Braescu has been a member of the following professional societes and organizations: Society of Photo-Optical Instrumentation Engineers, European Materials Research Society, World Scientific and Engineering Academy and Society, Sigma Xi, Ad Astra Association – Romanian Scientific Community, and Romanian Mathematical Society.