Hindawi Publishing Corporation
Journal of Inequalities and Applications
Volume 2008, Article ID 310924, 13 pages
doi:10.1155/2008/310924

Research Article

Nonlinear Boundary Value Problem for Concave Capillary Surfaces Occurring in Single Crystal Rod Growth from the Melt

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Received 6 May 2008; Revised 9 June 2008; Accepted 16 October 2008

Recommended by Michel Chipot

The boundary value problem $z'' = ((\rho\cdot g\cdot z - p)/\gamma)[1+(z')^2]^{3/2} - (1/r)\cdot[1+(z')^2]\cdot z'$, $r \in [r_1, r_0]$, $z'(r_1) = -\tan(\pi/2 - \alpha_g)$, $z'(r_0) = -\tan\alpha_c$, $z(r_0) = 0$, and $z(r)$ is strictly decreasing on $[r_1, r_0]$, is considered. Here, $0 < r_1 < r_0$, ρ, g, γ, p, α_c, α_g are constants having the following properties: ρ, g, γ are strictly positive and $0 < \pi/2 - \alpha_g < \alpha_c < \pi/2$. Necessary or sufficient conditions are given in terms of p for the existence of concave solutions of the above nonlinear boundary value problem (NLBVP). Numerical illustration is given. This kind of results is useful in the experiment planning and technology design of single crystal rod growth from the melt by edge-defined film-fed growth (EFG) method. With this aim, this study was undertaken.

1. Introduction

The free surface of the static meniscus, in single crystal rod growth by EFG method, in hydrostatic approximation is described by the Laplace capillary equation [1, 2]:

$$-\gamma\cdot\left(\frac{1}{R_1}+\frac{1}{R_2}\right)+\rho\cdot g\cdot z = p. \tag{1.1}$$

Here, γ is the melt surface tension; ρ is the melt density; g is the gravity acceleration; R_1, R_2 are the main radii of the free surface curvature at a point M of the free surface of the meniscus; z is the coordinate of M with respect to the Oz axis, directed vertically upward; and p is the pressure difference across the free surface:

$$p = p_m - p_g - \rho\cdot g\cdot H. \tag{1.2}$$

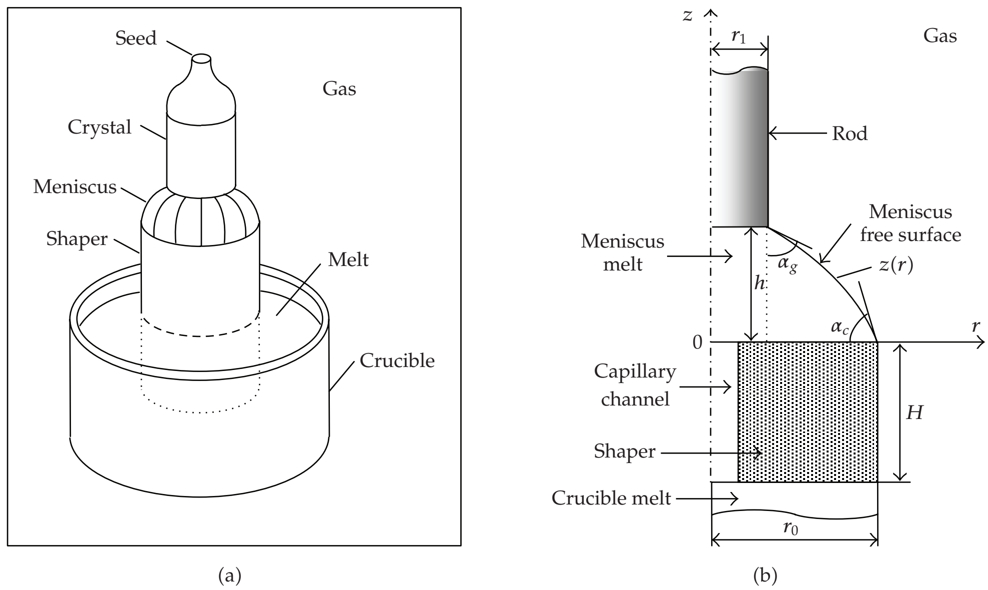

Figure 1: Axisymmetric meniscus geometry in the rod growth by EFG method.

Here, p_m is the pressure in the meniscus melt; p_g is the pressure in the gas; H is the melt column height between the horizontal crucible melt level and the shaper top level (see Figure 1).

To calculate the free surface shape of the meniscus, shape is convenient to employ the Laplace equation (1.1) in its differential form. This form of (1.1) can be obtained as a necessary condition for the minimum of the free energy of the melt column.

For the growth of a single crystal rod of radius r_1; $0 < r_1 < r_0$, the differential equation for axisymmetric meniscus surface is given by the formula

$$z'' = \frac{\rho \cdot g \cdot z - p}{\gamma}\left[1 + (z')^2\right]^{3/2} - \frac{1}{r}\cdot\left[1 + (z')^2\right]\cdot z' \quad \text{for } 0 < r_1 \leq r \leq r_0, \tag{1.3}$$

which is the Euler equation for the free energy functional

$$I(z) = \int_{r_1}^{r_0} \left\{ \gamma \cdot \left[1 + (z')^2\right]^{1/2} + \frac{1}{2}\cdot\rho\cdot g\cdot z^2 - p\cdot z \right\}\cdot r\cdot dr, \qquad z(r_1) = h > 0, \qquad z(r_0) = 0. \tag{1.4}$$

The solution of (1.3) has to satisfy the following boundary conditions, expressing thermodynamic requirements:

$$\begin{aligned} &\text{(a)} \quad z'(r_1) = -\tan\left(\frac{\pi}{2} - \alpha_g\right), \\ &\text{(b)} \quad z'(r_0) = -\tan\alpha_c, \\ &\text{(c)} \quad z(r_0) = 0,\ z(r) \text{ is strictly decreasing on } [r_1, r_0]. \end{aligned} \tag{1.5}$$

However, (a) expresses that at the triple point $(r_1, z(r_1))$, where the growth angle α_g is reached, the tangent to the crystal wall is vertical, (b) expresses that at the triple point $(r_0, 0)$, the contact angle is equal to α_c, and (c) expresses that the lower edge of the free surface is fixed to the outer edge of the shaper.

The growth angle α_g and the contact angle α_c, which appear in the above relations, are material constants and for semiconductors, in nonregular case, they satisfy the following conditions:

$$0 < \frac{\pi}{2} - \alpha_g < \alpha_c < \frac{\pi}{2}. \tag{1.6}$$

An important problem of the crystal growers consists in the location of the range, where p has to be, or can be chosen when $\rho,\ \gamma,\ \alpha_c,\ \alpha_g$ and $r_0,\ r_1$ are given a priori.

The state of the arts at the time 1993-1994, concerning the dependence of the shape and size of the free surface of the meniscus on the pressure difference p across the free surface for small and large Bond numbers, in the regular case of the growth of single crystal rods by EFG technique is summarized in [2]. According to [2], for the general differential equation (1.3), describing the free surface of the meniscus, there is no complete analysis and solution. For the general equation, only numerical integrations were carried out for a number of process parameter values that were of practical interest at the moment.

In [3], the authors investigate the pressure difference influence on the meniscus shape for rods, in the case of middle-range Bond numbers (i.e., $B_0 = 1$) which most frequently occurs in practice and has been left out of the regular study in [2]. They use a numerical approach in this case to solve the meniscus surface equation, written in terms of the arc length of the curve. The stability of the static free surface of the meniscus is analyzed by means of Jacobi equation. The result is that a large number of static menisci having drop-like shapes are unstable.

In [4, 5], automated crystal growth processes, based on weight sensors and computers, are analyzed. An expression for the weight of the meniscus, contacted with crystal and shaper of arbitrary shape, in which there are terms related to the hydrodynamic factor, is given.

In [6], it is shown that he hydrodynamic factor is too small to be considered in the automated crystal growth.

In the present paper, we locate the range where p has to be, or can be chosen in order to obtain the solution of the nonlinear boundary value problem (NLBVP) (1.3), (1.5) which is concave and minimizes the free energy functional.

2. Concave free surface of the meniscus in the case of rod growth

Consider NLBVP:

$$\begin{gathered} z'' = \frac{\rho\cdot g\cdot z - p}{\gamma}\left[1 + (z')^2\right]^{3/2} - \frac{1}{r}\cdot\left[1 + (z')^2\right]\cdot z', \quad r \in [r_1, r_0], \\ z'(r_1) = -\tan\left(\frac{\pi}{2} - \alpha_g\right), \qquad z'(r_0) = -\tan\alpha_c, \qquad z(r_0) = 0, \\ z(r) \text{ is strictly decreasing on } [r_1, r_0], \end{gathered} \tag{2.1}$$

where $r_1,\ r_0,\ g,\ \rho,\ \gamma,\ p,\ \alpha_c,\ \alpha_g$ are real numbers having the following properties:

$$0 < r_1 < r_0,$$
$$g,\ \rho,\ \gamma \text{ are strictly positive},$$
$$0 < \pi/2 - \alpha_g < \alpha_c < \pi/2.$$

Theorem 2.1. *If there exists a concave solution $z = z(r)$ of the NLBVP* (2.1)*, then $n = r_0/r_1$ and p satisfy the following inequalities:*

$$\begin{aligned} &\frac{n}{n-1}\cdot\gamma\cdot\frac{\alpha_c+\alpha_g-\pi/2}{r_0}\cdot\cos\alpha_c+\frac{\gamma}{r_0}\cdot\cos\alpha_g \\ &\quad\le p\le\frac{n}{n-1}\cdot\gamma\cdot\frac{\alpha_c+\alpha_g-\pi/2}{r_0}\cdot\sin\alpha_g+\frac{n-1}{n}\cdot\rho\cdot g\cdot r_0\cdot\tan\alpha_c+\frac{n\cdot\gamma}{r_0}\cdot\sin\alpha_c. \end{aligned} \tag{2.2}$$

Proof. Let $z = z(r)$ be a concave solution of the NLBVP (2.1) and $\alpha(r) = -\arctan z'(r)$. It is easy to see that the function $\alpha(r)$ verifies the equation

$$\alpha'(r)=\frac{p-\rho\cdot g\cdot z(r)}{\gamma}\cdot\frac{1}{\cos\alpha(r)}-\frac{1}{r}\cdot\tan\alpha(r), \tag{2.3}$$

and the boundary conditions

$$\alpha(r_1)=\frac{\pi}{2}-\alpha_g,\qquad \alpha(r_0)=\alpha_c. \tag{2.4}$$

Hence, there exists $r' \in (r_1, r_0)$ such that the following equality holds

$$p=\gamma\cdot\frac{\alpha_c+\alpha_g-\pi/2}{r_0-r_1}\cdot\cos\alpha(r')+\rho\cdot g\cdot z(r')+\frac{\gamma}{r'}\cdot\sin\alpha(r'). \tag{2.5}$$

Since $z''(r) < 0$ on $[r_1, r_0]$, the function $z'(r)$ is strictly decreasing, and $\alpha(r) = -\arctan z'(r)$ is strictly increasing on $[r_1, r_0]$. Therefore, the following inequalities hold:

$$\begin{gathered} \frac{\pi}{2}-\alpha_g\le\alpha(r')\le\alpha_c, \\ \cos\alpha_c\le\cos\alpha(r')\le\sin\alpha_g, \\ \cos\alpha_g\le\sin\alpha(r')\le\sin\alpha_c, \\ \rho\cdot g\cdot(r_0-r')\cdot\tan\left(\frac{\pi}{2}-\alpha_g\right)\le\rho\cdot g\cdot z(r')\le\rho\cdot g\cdot(r_0-r')\cdot\tan\alpha_c. \end{gathered} \tag{2.6}$$

Combining equality (2.5) and inequalities (2.6), we obtain inequality (2.2). □

Corollary 2.2. *If $n \to +\infty$, then $r_1 = r_0/n \to 0$, and*

$$\gamma\cdot\frac{\alpha_c + \alpha_g - \pi/2}{r_0}\cdot\cos\alpha_c + \frac{\gamma}{r_0}\cdot\cos\alpha_g \leq p. \tag{2.7}$$

Corollary 2.3. *If p verifies*

$$p < \gamma\cdot\frac{\alpha_c + \alpha_g - \pi/2}{r_0}\cdot\cos\alpha_c + \frac{\gamma}{r_0}\cdot\cos\alpha_g, \tag{2.8}$$

then there is no $r_1 \in (0, r_0]$ for which the NLBVP (2.1) *has a concave solution.*

Corollary 2.4. *If $n \to 1$, then $r_1 = r_0/n \to r_0$ and $p \to +\infty$.*

Theorem 2.5. *If p verifies*

$$p > \frac{n}{n-1}\cdot\gamma\cdot\frac{\alpha_c + \alpha_g - \pi/2}{r_0}\cdot\sin\alpha_g + \frac{n-1}{n}\cdot g\cdot\rho\cdot r_0\cdot\tan\alpha_c + \frac{n\cdot\gamma}{r_0}\cdot\sin\alpha_c, \tag{2.9}$$

then there exist $r_1 \in [r_0/n, r_0]$ and a concave solution of the NLBVP (2.1).

Proof. Consider the initial value problem (IVP):

$$\begin{gathered} z'' = \frac{\rho\cdot g\cdot z - p}{\gamma}\cdot\left[1 + (z')^2\right]^{3/2} - \frac{1}{r}\cdot\left[1 + (z')^2\right]\cdot z' \quad r \in (0, r_0], \\ z(r_0) = 0, \qquad z'(r_0) = -\tan\alpha_c, \end{gathered} \tag{2.10}$$

the solution $z(r)$ of this problem, the maximal interval I on which the solution exists, and the function $\alpha(r)$ defined on I by

$$\alpha(r) = -\arctan z'(r). \tag{2.11}$$

Remark that $z(r)$ and $\alpha(r)$ verify

$$\begin{aligned} z''(r) &= \frac{1}{\cos^3\alpha(r)}\cdot\left[\frac{\rho\cdot g\cdot z(r) - p}{\gamma} + \frac{\sin\alpha(r)}{r}\right], \\ \alpha'(r) &= \frac{1}{\cos\alpha(r)}\cdot\left[\frac{p - \rho\cdot g\cdot z(r)}{\gamma} - \frac{\sin\alpha(r)}{r}\right], \end{aligned} \qquad r \in I \cap (0, r_0]. \tag{2.12}$$

At r_0, the following inequalities hold

$$
\begin{aligned}
z'(r_0) &= -\tan\alpha_c < 0,\\
z''(r_0) &= \frac{1}{\cos^3\alpha_c}\left[-\frac{p}{\gamma}+\frac{\sin\alpha_c}{r_0}\right]\\
&< -\frac{1}{\cos^3\alpha_c}\left[\frac{n}{n-1}\cdot\frac{\alpha_c+\alpha_g-\pi/2}{r_0}\cdot\sin\alpha_g+\frac{n-1}{n}\cdot\frac{\rho\cdot g}{\gamma}\cdot r_0\cdot\tan\alpha_c+\frac{n-1}{r_0}\cdot\sin\alpha_c\right] < 0.
\end{aligned}
\tag{2.13}
$$

Hence, there exists $r' \in I \cap (0, r_0)$ such that the following inequalities hold

$$
z''(r) < 0, \qquad -\tan\alpha_c \le z'(r), \quad z'(r) \le -\tan\left(\frac{\pi}{2}-\alpha_g\right),
\tag{2.14}
$$

for every $r \in [r', r_0]$.

Now, let r_* be defined by

$$
r_* = \inf\left\{r' \in I \cap (0, r_0)\vdots \text{ such that for any } r \in [r', r_0] \text{ inequalities (2.14) hold}\right\}.
\tag{2.15}
$$

It is clear that $r_* \ge 0$ and for any $r \in (r_*, r_0]$ inequalities (2.14) hold. Remark now that the limits

$$
z'(r_*+0) = \lim_{\substack{r\to r_*\\ r>r_*}} z'(r), \qquad z(r_*+0) = \lim_{\substack{r\to r_*\\ r>r_*}} z(r)
\tag{2.16}
$$

exist and satisfy

$$
\begin{gathered}
-\tan\alpha_c \le z'(r_*+0) \le -\tan\left(\frac{\pi}{2}-\alpha_g\right),\\
(r_0-r_*)\cdot\tan\left(\frac{\pi}{2}-\alpha_g\right) \le z(r_*+0) \le (r_0-r_*)\cdot\tan\alpha_c.
\end{gathered}
\tag{2.17}
$$

The limit $z''(r_*+0) = \lim_{r\to r_*,\, r>r_*} z''(r)$ exists too, and $z''(r_*+0) \le 0$.

Due to the fact that r_* is minimum, one of the inequalities

$$
-\tan\alpha_c \le z'(r_*+0), \qquad z'(r_*+0) \le -\tan\left(\frac{\pi}{2}-\alpha_g\right), \qquad z''(r_*+0) \le 0
\tag{2.18}
$$

has to be equality.

The equality $-\tan\alpha_c = z'(r_*+0)$ is impossible because $z'(r_*+0) \ge z'(r) > -\tan\alpha_c$ for $r \in (r_*, r_0)$.

We show in what follows that $r_* \ge r_0/n$ and $z'(r_*+0) = -\tan(\pi/2-\alpha_g)$.

If $r_* \geq r_0/n$, then we have to show only the equality $z'(r_* + 0) = -\tan(\pi/2 - \alpha_g)$. This can be made showing that the equality $z''(r_* + 0) = 0$ is impossible. Assuming the contrary, that is, $z''(r_* + 0) = 0$, using $(2.12)_1$, we obtain

$$\begin{aligned} z(r_* + 0) &= \frac{p}{g \cdot \rho} - \frac{\gamma}{g \cdot \rho \cdot r_*} \cdot \sin\alpha(r_* + 0) \\ &> \frac{n}{n-1} \cdot \frac{\gamma}{g \cdot \rho} \cdot \frac{\alpha_c + \alpha_g - \pi/2}{r_0} \cdot \sin\alpha_g \\ &\quad + \frac{n-1}{n} \cdot r_0 \cdot \tan\alpha_c + \frac{n \cdot \gamma}{g \cdot \rho \cdot r_0} \cdot \sin\alpha_c - \frac{n \cdot \gamma}{g \cdot \rho \cdot r_0} \cdot \sin\alpha_c \\ &> \left(r_0 - \frac{1}{n} \cdot r_0\right) \cdot \tan\alpha_c \\ &> z\left(\frac{r_0}{n}\right) \\ &> z(r_* + 0), \end{aligned} \tag{2.19}$$

which is impossible.

Assume now that $r_* < r_0/n$ and consider the difference $\alpha(r_0) - \alpha(r_0/n)$,

$$\begin{aligned} \alpha(r_0) - \alpha\left(\frac{r_0}{n}\right) &= \alpha'(\zeta) \cdot \left[r_0 - \frac{r_0}{n}\right] \\ &= \left[\frac{p - g \cdot \rho \cdot z(\zeta)}{\gamma} - \frac{\sin\alpha(\zeta)}{\zeta}\right] \cdot \frac{1}{\cos\alpha(\zeta)} \cdot \frac{n-1}{n} \cdot r_0 \\ &> \left[\frac{n}{n-1} \cdot \frac{\alpha_c + \alpha_g - \pi/2}{r_0} \cdot \sin\alpha_g + \frac{n-1}{n} \cdot \frac{g \cdot \rho}{\gamma} \cdot r_0 \cdot \tan\alpha_c \right. \\ &\quad \left. + \frac{n}{r_0} \cdot \sin\alpha_c - \frac{g \cdot \rho}{\gamma} \cdot \frac{n-1}{n} \cdot r_0 \cdot \tan\alpha_c - \frac{n}{r_0} \cdot \sin\alpha_c\right] \cdot \frac{1}{\sin\alpha_g} \cdot \frac{n-1}{n} \cdot r_0 \\ &= \frac{n}{n-1} \cdot \frac{\alpha_c + \alpha_g - \pi/2}{r_0} \cdot \frac{\sin\alpha_g}{\sin\alpha_g} \cdot \frac{n-1}{n} \cdot r_0 \\ &= \alpha_c + \alpha_g - \frac{\pi}{2}. \end{aligned} \tag{2.20}$$

Hence, $\alpha(r_0/n) < \pi/2 - \alpha_g$, which is impossible.

In this way, it was shown that $r_* \geq r_0/n$ and $z'(r_* + 0) = -\tan(\pi/2 - \alpha_g)$. □

Theorem 2.6. *If for $1 < n' < n$ and p, the inequalities hold*

$$\begin{aligned} &\frac{n}{n-1} \cdot \gamma \cdot \frac{\alpha_c + \alpha_g - \pi/2}{r_0} \cdot \sin\alpha_g + \frac{n-1}{n} \cdot g \cdot \rho \cdot r_0 \cdot \tan\alpha_c + \frac{n \cdot \gamma}{r_0} \cdot \sin\alpha_c \\ &\quad < p < \frac{n'}{n'-1} \cdot \gamma \cdot \frac{\alpha_c + \alpha_g - \pi/2}{r_0} \cdot \cos\alpha_c + \frac{\gamma}{r_0} \cdot \cos\alpha_g, \end{aligned} \tag{2.21}$$

then there exist r_1 in the closed interval $[r_0/n, r_0/n']$ and a concave solution of the NLBVP (2.1).

Proof. The existence of r_1 and the inequality $r_1 \geq r_0/n$ follow from Theorem 2.5. The inequality $r_1 \leq r_0/n'$ follows from Theorem 2.1. □

Theorem 2.7. *A concave solution $z_1(r)$ of the NLBVP* (2.1) *is a weak minimum of the free energy functional of the melt column*

$$I(z) = \int_{r_1}^{r_0} \left\{ \gamma \cdot \left[1 + (z')^2\right]^{1/2} + \frac{1}{2} \cdot g \cdot \rho \cdot z^2 - p \cdot z \right\} r \cdot dr, \qquad z(r_1) = z_1(r_1), \qquad z(r_0) = z_1(r_0) = 0. \tag{2.22}$$

Proof. Since (2.1) is the Euler equation for (2.22), it is sufficient to prove that the Legendre and Jacobi conditions are satisfied in this case.

Denote by $F(r, z, z')$, the function defined as

$$F(r, z, z') = r \cdot \left\{ \frac{1}{2} \cdot \rho \cdot g \cdot z^2 - p \cdot z + \gamma \cdot \left[1 + (z')^2\right]^{1/2} \right\}. \tag{2.23}$$

It is easy to verify that we have

$$\frac{\partial^2 F}{\partial z'^2} = \frac{r \cdot \gamma}{\left[1 + (z')^2\right]^{3/2}} > 0. \tag{2.24}$$

Hence, the Legendre condition is satisfied.

The Jacobi equation

$$\left[\frac{\partial^2 F}{\partial z^2} - \frac{d}{dr} \left(\frac{\partial^2 F}{\partial z \partial z'} \right) \right] \cdot \eta - \frac{d}{dr} \left[\frac{\partial^2 F}{\partial z'^2} \cdot \eta' \right] = 0 \tag{2.25}$$

in this case is given by

$$\frac{d}{dr} \left(\frac{r \cdot \gamma}{\left[1 + (z')^2\right]^{3/2}} \cdot \eta' \right) - g \cdot \rho \cdot r \cdot \eta = 0. \tag{2.26}$$

For (2.26), the following inequalities hold

$$\frac{r \cdot \gamma}{\left[1 + (z')^2\right]^{3/2}} \geq r_1 \cdot \gamma \cdot \cos^3 \alpha_c, \qquad -\rho \cdot g \cdot r \leq 0. \tag{2.27}$$

Hence,

$$\left(\eta' \cdot r_1 \cdot \gamma \cdot \cos^3 \alpha_c\right)' = 0 \tag{2.28}$$

is a Sturm-type upper bound for (2.26) [7].

Since every nonzero solution of (2.28) vanishes at most once on the interval $[r_1, r_0]$, the solution $\eta(r)$ of the initial value problem,

$$\frac{d}{dr}\left(\frac{r\cdot\gamma}{[1+(z')^2]^{3/2}}\cdot\eta'\right) - g\cdot\rho\cdot r\cdot\eta' = 0, \qquad \eta(r_1) = 0, \qquad \eta'(r_1) = 1, \tag{2.29}$$

has only one zero on the interval $[r_1, r_0]$ [7]. Hence, the Jacobi condition is satisfied. □

Theorem 2.8. *If the solution $z(r)$ of the IVP* (2.10) *is convex (i.e., $z''(r) > 0$) on the interval $[r_1, r_0]$, then it is not a solution of the NLBVP* (2.1).

Proof. $z''(r) > 0$ on $[r_1, r_0]$ implies that $z'(r)$ is strictly increasing on $[r_1, r_0]$. Hence, $z'(r_1) < z'(r_0) < -\tan\alpha_c < -\tan(\pi/2 - \alpha_g)$. □

Theorem 2.9. *The solution $z(r)$ of the IVP* (2.10) *is convex at r_0 (i.e., $z''(r_0) > 0$) if and only if*

$$p < \frac{\gamma}{r_0}\cdot\sin\alpha_c. \tag{2.30}$$

Moreover, if (2.30) *holds, then the solution $z(r)$ of the IVP* (2.10) *is convex on $I \cap (0, r_0)$.*

Proof. That is because the change of convexity implies the existence of $r' \in I \cap [0, r_0]$ such that $\alpha(r') > \alpha_c$, $z(r') > 0$, and $p = g\cdot\rho\cdot z(r') + (\gamma/r')\cdot\sin\alpha(r') > (\gamma/r_0)\cdot\sin\alpha_c$ which is impossible. □

Theorem 2.10. *If $p > (\gamma/r_0)\cdot\sin\alpha_c$ and $z(r)$ is a nonconcave solution of the NLBVP* (2.1), *then for p, the following inequality holds*

$$\frac{\gamma}{r_0}\cdot\sin\alpha_c < p < g\cdot\rho\cdot r_0\cdot\tan\alpha_c + \frac{\gamma}{r_1}\cdot\sin\alpha_c. \tag{2.31}$$

Proof. Denote by $z(r)$ the solution of the NLBVP (2.1) which is assumed to be nonconcave. Let $\alpha(r) = -\arctan z'(r)$ for $r \in [r, r_0]$. There exists $r' \in (r_1, r_0)$ such that $\alpha'(r') = 0$. Hence, $p = g\cdot\rho\cdot z(r') + (\gamma/r')\cdot\sin\alpha(r')$. Since $\alpha'(r') < \alpha_c$ and $r' > r_1$, the following inequalities hold $(\gamma/r')\cdot\sin\alpha(r') \le (\gamma/r_1)\cdot\sin\alpha_c$ and $z(r') \le r_0\cdot\tan\alpha_c$. Using these inequalities, we obtain (2.31). □

3. Numerical illustration

Numerical computations were performed for InSb rod for the following numerical data [8]:

$$\begin{gathered} r_0 = 7\cdot10^{-4}\,[\mathrm{m}], \qquad r_1 = 3.5\cdot10^{-4}\,[\mathrm{m}], \\ \alpha_c = 63.8^o = 1.1135\,[\mathrm{rad}], \qquad \alpha_g = 28.9^0 = 0.5044\,[\mathrm{rad}], \\ \rho = 6582\,[\mathrm{kg/m^3}], \qquad \gamma = 4.2\cdot10^{-1}\,[\mathrm{N/m}], \\ g = 9.81\,[\mathrm{m/s^2}], \qquad n = 2, \qquad n' = 1.02. \end{gathered} \tag{3.1}$$

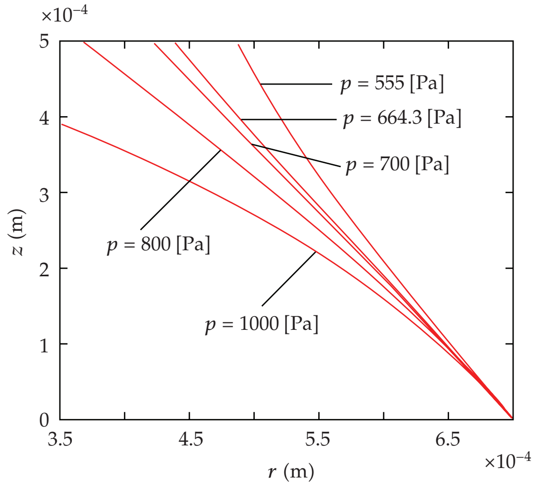

Figure 2: z versus r for $p = 555, 664.3, 700, 900, 1000$ [Pa].

The objective was to verify if the necessary conditions are also sufficient or if the sufficient conditions are also necessary. Moreover, the above data are realistic, and the computed results can be tested against the experiments in order to evaluate the accuracy of the theoretical predictions. This test is not the subject of this paper.

Inequality (2.2) is a necessary condition for the existence of a concave solution of the NLBVP (2.1) on the closed interval $[r_0/n, r_0]$ $(n > 1)$. Is this condition also sufficient? Computation shows that for the considered numerical data, the inequality (2.2) becomes $550.24\,[\text{Pa}] \le p \le 1149.96\,[\text{Pa}]$.

Numerical integration of the IVP (2.10) shows that for $p = 664.3, 700, 900, 1000$, [Pa], there exists $r' \in (3.5 \times 10^{-4}; 7 \times 10^{-4})$ [m] such that the NLBVP has a concave solution on $[r', r_0]$, but for $p = 555$ [Pa], there is no $r' \in (3.5 \times 10^{-4}; 7 \times 10^{-4})$ [m] such that the NLBVP has a concave solution on $[r', r_0]$ (Figures 2 and 3). Moreover, there is no p in the ranges [550.24, 1149.96] [Pa]for which $\alpha = \pi/2 - \alpha_g = 1.06639$ [rad] is reached at $r' = 3.5 \times 10^{-4}$ m.

Consequently, the inequality (2.2) is not a sufficient condition.

Inequality (2.8) is a sufficient condition for the inexistence of a point $r' \in [0, r_0]$ such that the NLBVP (2.1) has a concave solution on the interval $[r', r_0]$. Is it this condition also necessary? Computation made for the same numerical data shows that inequality (2.8) becomes $p < 537.76$ [Pa]. We have already obtained by numerical integration that for $p = 555$ [Pa], there exists no $r' \in (0; 7 \times 10^{-4})$ [m] such that the NLBVP has a concave solution on the interval $[r', 7 \times 10^{-4}]$ [m] (see Figures 2 and 3). Consequently, the inequality (2.7) is not a necessary condition.

Inequality (2.9) is a sufficient condition for the existence of a point r' in the interval $(0, r_0]$ such that the NLBVP (2.1) has a concave the solution on the interval $[r', r_0]$. Is this condition also necessary?

Computation made for the same numerical data shows that inequality (2.9) becomes $p > 1149.96$ [Pa]. Numerical integration of the IVP (2.10) shows that for $p = 1000$ [Pa], there exists $r' \in (0, 7 \times 10^{-4}]$ [m] such that the IVP (2.10) has a concave solution on $[r', 7 \times 10^{-4}]$ [m] (Figures 2 and 3). Consequently, the inequality (2.9) is not a necessary condition.

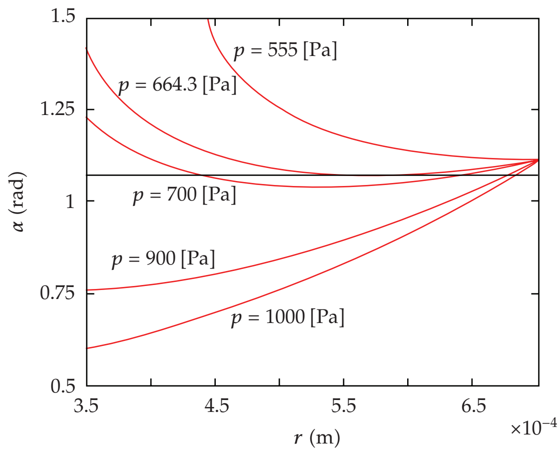

Figure 3: α versus r for $p = 555, 664.3, 700, 900, 1000$ [Pa].

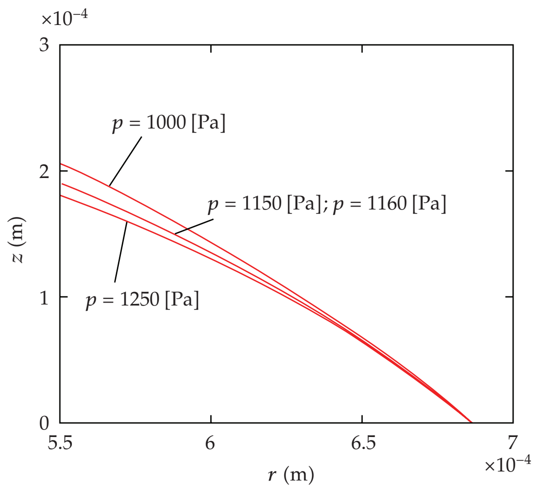

Figure 4: z versus r for $p = 1000, 11500, 1160, 1250$ [Pa].

Inequality (2.21) is a sufficient condition for the existence of a point r' in the interval $[r_0/n, r_0/n']$ such that the NLBVP (2.1) on the interval $[r', r_0]$ has a concave solution. Computation made for the same numerical data shows that $[r_0/n, r_0/n'] = [3.5 \times 10^{-4},\ 6.86 \times 10^{-4}]$ [m] and inequality (2.21) becomes $1149.966 < p < 1161.92$ [Pa]. Numerical integration of the IVP (2.10) illustrates the above phenomenon for $p = 1150, 1160$ [Pa] and also the fact that the condition is not necessary (see $p = 1000, 1250$ [Pa]) (Figures 4 and 5).

Inequality (2.30) is a necessary and sufficient condition for the convexity of the solution of the IVP (2.10). For the considered numerical data, the inequality (2.30) becomes $p < 538.35$ [Pa]. Figures 6 and 7 illustrate this phenomenon for $p = 538, 250$ [Pa].

Inequality (2.31) is a necessary condition for a concave-convex solution of the NLBVP (2.1). Is this condition also sufficient?

For the considered numerical data, computation shows that inequality (2.31) becomes 538.35 [Pa] $< p <$ 1168.65 [Pa]. Numerical integration of the IVP (2.10) for $p = 664.3, 700$ [Pa]

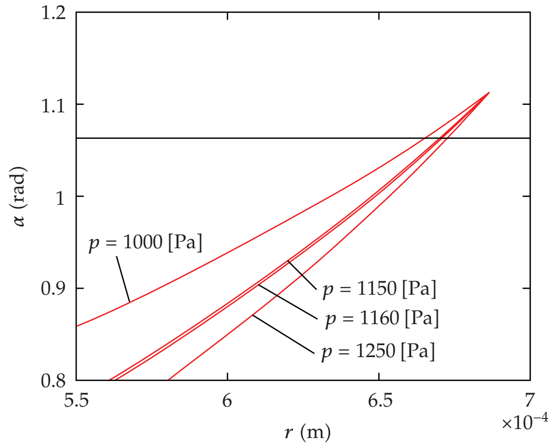

Figure 5: α versus r for $p = 1000, 11500, 1160, 1250$ [Pa].

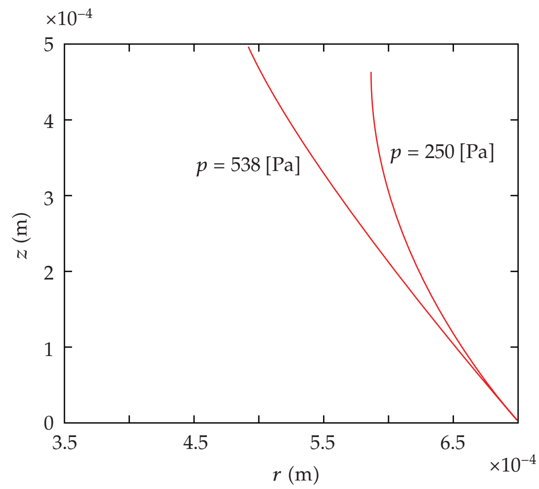

Figure 6: z versus r for $p = 538, 250$ [Pa].

shows that the solution is a concave-convex solution of the NLBVP (2.1), but for $p = 555$ [Pa], it is not anymore solution of the NLBVP (2.1) (Figures 2 and 3).

Consequently, condition (2.31) is not necessary.

4. Conclusion

(1) Theorems localize the pressure difference axis values for which the considered NLBVP (2.1) possesses solution and values for which it has no solution. In particular, theoretical results reveal that for the growth of a single crystal rod of radius r_1 in the range $[r_0/n, r_0/n']$ $(n > n' > 1)$, it is sufficient to choose the pressure difference p such that the inequality (2.21) holds.

(2) By computation, these values are found in a real case, and the accuracy of the computed results is discussed theoretically.

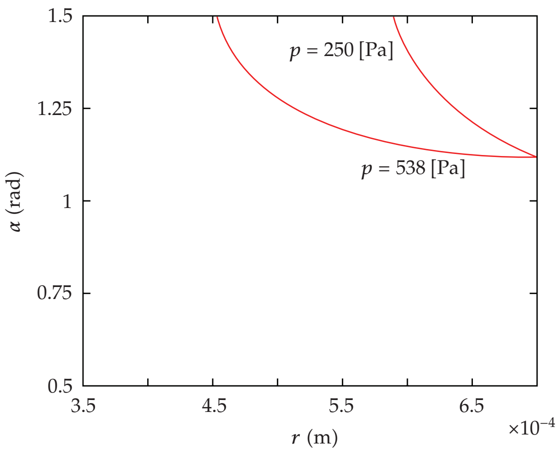

Figure 7: α versus r for $p = 538, 250$ [Pa].

Acknowledgments

The authors would like to thank the anonymous referees for their valuable comments and suggestions which led to an improvement of the manuscript. They are thankful to the Romanian National Authority for Research for supporting the research under the Grant no. 7/2007.

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