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A FREE BOUNDARY PROBLEM ARISING FROM THE PROCESS OF CZOCHRALSKI CRYSTAL GROWTH

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Abstract. A free boundary problem from the process of Czochralski crystal growth is studied. Existence and uniqueness of the solution are established in the cases when the melt is superheated ($\delta > 1$) and the melt is not superheated ($\delta \leq 1$) respectively. The behavior of the free boundary is discussed. The growth rate is bounded in either case and the maximum growth rate can be estimated in terms of given parameters.

1. Introduction. We will study a problem arising from the process of the Czochralski crystal growth, which is one of the most important crystal growth techniques (see [3] and references therein for the detailed descriptions of the process). Under certain assumptions, the following nonlinear boundary value problem (in dimensionless form) is used to model the process of the Czochralski crystal growth (see [3] and references therein).

$$\epsilon(u_t + pu_x) = u_{xx} - 2\alpha u \quad \text{in} \quad Q_T, \tag{1.1}$$

$$u_x + bu = 0 \quad \text{on} \quad x = S(t), \tag{1.2}$$

$$p = S'(t) = -u_x(0,t) - \beta(\delta - 1), \quad t > 0 \tag{1.3}$$

$$u(0,t) = 1, \quad t > 0, \tag{1.4}$$

$$u(x,0) = 1, \quad 0 \leq x \leq r, \tag{1.5}$$

$$S(0) = r, \tag{1.6}$$

where ϵ, α, β, δ, b, and r are positive constants and $Q_T = \{(x,t) \mid 0 < x < S(t), 0 < t \leq T\}$. In the above system (1.1)-(1.6), equation (1.1) is the energy equation. Equation (1.3) is the energy balance at the crystal-melt interface, where u measures dimensionless temperature, α represents the ambient Biot number for convective heat transfer from cylindrical surface and the top surface, β represents the melt Biot number for convective heat transfer from melt and r is initial crystal length.

We will discuss the system (1.1)-(1.6) in the case of $\delta < 1$ (the melt is supercooled), $\delta > 1$ (the melt is superheated), and $\delta = 1$ (the melt is always maintained at the melting temperature of the crystal).

By using coordinate transformations, the system (1.1)-(1.6) can be reduced to

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one with the form

$$\begin{cases} \epsilon u_t = u_{xx} - 2\alpha u \quad \text{in} \quad Q_T, \\ u_x(0,t) - bu(0,t) = 0 \quad t > 0, \\ S'(t) = u_x(S(t),t) - \beta(\delta - 1), \\ u(S(t),t) = 1, \\ u(x,0) = 1, \quad 0 \le x \le r, \\ S(0) = r. \end{cases} \tag{1.7}$$

For the purpose of the following discussion, we will further take constants $b = 1$ and $\epsilon = 1$ since that does not affect the nature of the problem and the results.

2. A priori Estimates. We now investigate the following free boundary problem. That is to find $(S(t), u(x,t))$ satisfying

$$u_t = u_{xx} - 2\alpha u \quad \text{in} \quad Q_T, \tag{2.1}$$
$$u(S(t),t) = 1, \tag{2.2}$$
$$u_x(0,t) - u(0,t) = 0 \quad t > 0, \tag{2.3}$$
$$u(x,0) = 1, \quad 0 \le x \le r, \tag{2.4}$$
$$S'(t) = u_x(S(t),t) - \beta(\delta - 1), \tag{2.5}$$
$$S(0) = r, \tag{2.6}$$

where α, β, δ, and r are positive constants and $Q_T = \{(x,t) \mid 0 < x < S(t), 0 < t \le T\}$. We first establish some estimates which will be used later in this paper.

Lemma 2.1. *Let $u(x,t)$ be a solution of (2.1)-(2.4) with given $S(t) \in C^1$. Then the following estimates hold.*

$$0 \le u(x,t) \le 1, \tag{2.7}$$
$$u_x(S(t),t) \ge 0. \tag{2.8}$$

Proof. Notice that the solution $u(x,t)$ of (2.1)-(2.4) with given $S(t) \in C^1$ satisfies $u(x,t) \in C^{2,1}(\overline{Q_T})$. Estimate (2.7) follows directly from the Maximum principle. Estimate (2.8) follows from the fact that $u(x,t)$ attains maximum value 1 on $x = S(t)$. □

Lemma 2.2. *Let $\{S(t), u(x,t)\}$ be a solution of (2.1)-(2.6) with $\delta \le 1$. Then the following estimates hold.*

$$S'(t) \ge -\beta(\delta - 1) \ge 0, \tag{2.9}$$
$$0 \le u_x(S(t),t) \le \max\{\ 4\sqrt{\alpha}, 2/r\ \}, \tag{2.10}$$
$$|u_x(x,t)| \le \max\{\ 1, 4\sqrt{\alpha}, 2/r\ \}. \tag{2.11}$$

Proof. Estimate (2.9) follows from (2.5) and (2.8). To obtain estimate (2.10), we consider a function

$$w(x,t) = 2\ln(1 + B(S(t) - x)) - 1 + u(x,t)$$

with $B \geq \max\{2\alpha, 1/r\}$ on the domain $D_T = \{(x,t) \mid S(t) - 1/B \leq x \leq S(t), 0 \leq t \leq T\}$. A direct calculation yields

$$\begin{cases} w_t - w_{xx} + 2\alpha w \geq 0 \quad \text{in} \quad D_T, \\ w(S(t), t) = 0, \quad t > 0, \\ w(S(t) - \frac{1}{B}, t) > 0, \quad t > 0, \\ w(x, 0) = 2\ln(1 + B(r - x)), \quad r - \frac{1}{B} \leq x \leq r. \end{cases} \tag{2.12}$$

This means that the function $w(x,t)$ attains minimum value 0 on $x = S(t)$ and so that $w_x(S(t), t) \leq 0$. This yields the estimate (2.10). Lastly, estimate (2.11) follows from maximum principle and the estimates (2.7) and (2.10). □

Lemma 2.3. *Let $\{S(t), u(x,t)\}$ be a solution of (2.1)-(2.6) with $\delta > 1$. Then the following estimates hold.*

$$0 \leq u_x(S(t), t) \leq M_1, \tag{2.13}$$
$$-\beta(\delta - 1) \leq S'(t) \leq M_1, \tag{2.14}$$
$$|u_x(x,t)| \leq M_1, \tag{2.15}$$

where the constant M_1 depends only on α, β and δ.

Proof. By using the method employed in the proof of Lemma 2.2, An upper bound of $u_x(S(t), t)$ can be derived if $S'(t) \geq 0$. Otherwise, an upper bound of $u_x(S(t), t)$ follows from (2.5). This gives the estimate (2.13). The estimates (2.14) and (2.15) follow from (2.13) and the maximum principle. □

3. Existence and uniqueness theorem. In this section, we shall establish the existence and uniqueness theorem for the problem (2.1)-(2.6). We have the following theorem.

Theorem 3.1. *There exists a unique solution for the problem (2.1)-(2.6).*

Proof. We prove the existence theorem by a fixed point argument and consider first the case $\delta \leq 1$. Let $B = C[0,T]$ and $K(M)$ be a closed convex subset in B defined by

$$K(M) \equiv \left\{ S(t) \in B : S(0) = r, 0 \leq \frac{S(t) - S(\tau)}{t - \tau} \leq M \right\}, \tag{3.1}$$

where $M = \max\{ 4\sqrt{\alpha}, 2/r \} + \beta(1 - \delta)$.

For any $h(t) \in K(M)$, there exists a unique solution to the boundary value problem

$$\begin{cases} u_t = u_{xx} - 2\alpha u \quad \text{in} \quad 0 < x < h(t), 0 < t \leq T, \\ u(h(t), t) = 1, \quad 0 < t \leq T \\ u_x(0, t) - u(0, t) = 0, \quad 0 < t \leq T, \\ u(x, 0) = 1, \quad 0 \leq x \leq r, \end{cases} \tag{3.2}$$

with $u(x,t) \in C^{1+1,0+1}$. We denote the solution as $u(x,t;h(t))$. With this $u(x,t)$, we define

$$S(t) = r + \int_0^t \left(\frac{\partial u(h(\tau),\tau;h(t))}{\partial x} - \beta(\delta - 1) \right) d\tau. \tag{3.3}$$

This scheme defines a mapping T such that $S = Th$.

If we can show that T has a fixed point $S(t)$ in $K(M)$, then $(S(t), u(x,t))$ is a solution of (2.1)-(2.6).

We are going to use Schauder fixed point theorem ([2]) to show that T has a fixed point. First, it can be easily verified by Lemma 2.2 that $S(t)$ defined in (3.3) is in $K(M)$. This means that the mapping T maps $K(M)$ into itself.

We next show that T is a continuous mapping. To do this, suppose $h_n(t) \in K(M)$ $(n \geq 1)$ with $h_n(t) \to h(t)$ as $n \to \infty$. Since the solution of (3.2) depends continously on the boundary, we have ([5],[7,8])

$$u_n(h_n(t),t;h_n(t)) \to u(h(t),t;h(t))$$

and

$$\frac{\partial u_n(h_n(t),t;h_n(t))}{\partial x} \to \frac{\partial u(h(t),t;h(t))}{\partial x},$$

where $u_n(x,t;h_n(t))$ is the solution of (3.2) with a right boundary $x = h_n(t)$. The equation (3.3) thus implies that the mapping T is continuous.

Therefore the mapping T has a fixed point in $K(M)$ by Schauder fixed point theorem. This gives a solution for the problem (2.1)-(2.6) when $\delta \leq 1$.

In the case of $\delta > 1$, we define that

$$K(T_1, M_1) \equiv \left\{ S(t) \in C^1[0,T_1] : S(0) = r, S(t) > 0, |S'(t)| \leq M_1 \right\},$$

where M_1 is defined in the lemma 2.3 and T_1 is small enough so that

$$\max(M_1 T_1, \beta(\delta - 1)T_1) < r.$$

By the same method used in the case of $\delta \leq 1$ and a fixed point argument, we can prove that a solution exists on the time interval $[0, T_1]$.

Noting that $S(t) > 0$ and Lemma 2.3, we can continue the process step by step to construct a global solution of (2.1)-(2.6) in $0 < t \leq T$ by the same argument. This completes the proof of the existence.

In order to show the uniqueness of a solution, we consider $(S_i(t), u_i(x,t))$ $i = 1, 2$, where $(S_i(t), u_i(x,t))$ is a solution of (2.1)-(2.6) corresponding $\delta = \delta_i$ in the equation (2.5). We are going to show that if $\delta_1 > \delta_2$ $(0 < \delta_1, \delta_2 \leq 1)$, then $S_1(t) < S_2(t)$ $(t > 0)$. Indeed, we have, from (2.5), $S_1'(0) < S_2'(0)$. Notice that $S_i'(t)$ is continuous for $t \geq 0$, there exists a neighborhood of 0 so that $S_1(t) < S_2(t)$ in that neighborhood. Let

$$t_0 = \sup_t \{t \; : \; S_1(\tau) < S_2(\tau), 0 < \tau < t\}. \tag{3.4}$$

Then $t_0 > 0$ as discussed above. If t_0 is a finite number, then $S_1(t_0) = S_2(t_0)$ and

$$S_1'(t_0) \geq S_2'(t_0). \tag{3.5}$$

On the other hand, $w(x,t) = u_1(x,t) - u_2(x,t)$ satisfies

$$\begin{cases} w_t = w_{xx} - 2\alpha w \quad \text{in} \quad 0 < x < S_1(t), 0 < t \le t_0, \\ w(S_1(t),t) \ge 0, \quad 0 < t \le T \\ w_x(0,t) - w(0,t) = 0, \quad 0 < t \le T, \\ w(x,0) = 0, \quad 0 \le x \le r. \end{cases} \tag{3.6}$$

Thus $w \ge 0$ by maximum principle. Since $w(S_1(t_0),t_0) = 0$, the maximum principle again yields $w_x(S_1(t_0),t_0) < 0$, i.e.

$$\frac{\partial u_1(S_1(t_0),t_0)}{\partial x} < \frac{\partial u_2(S_1(t_0),t_0)}{\partial x}.$$

This means, from (2.5), that $S_1'(t_0)+\beta(\delta_1-1) < S_2'(t_0)+\beta(\delta_2-1)$ or $S_1'(t_0) < S_2'(t_0)$ which contradicts (3.5). Thus $t_0 = \infty$. We thus have proved $S_1(t) < S_2(t)$ $(t > 0)$ when $\delta_1 > \delta_2$ $(0 < \delta_1, \delta_2 \le 1)$. As a corollary, we can obtain that the solution of (2.1)-(2.6) is unique. The case of $\delta > 1$ can be discussed in a similar manner. The proof of the theorem is thus completed. □

4. Properties of the solution to (2.1)-(2.6). We now discuss some properties of the solution to (2.1)-(2.6). In the case of $\delta \le 1$, we see, from (2.5) and (2.8), that $S'(t) \ge 0$. This means that the free boundary is increasing. The upper bound of $S'(t)$ can be obtained by (2.5) and Lemma 2.2.

In the case of $\delta > 1$, however, the free boundary is not monotone at least for some choice of β. It starts with $S'(0) < 0$, so that the free boundary is decreasing initially. Notice that the free boundary $x = S(t)$ can not hit the fixed boundary $x = 0$ because of $u(S(t),t) = 1$ and boundary condition (2.3) and the estimate (2.14) in Lemma 2.3 guarantees that "finite time blow up" will not occur for this problem. Thus if we can show that the free boundary can not be satisfied with $S'(t) \le 0$ and $S(t) \to r_0$ as $t \to \infty$ (see detailed discussion below), then the free boundary will become increasing after some time. Therefore, the free boundary is no longer monotone in this case.

To show that the free boundary is not monotone decreasing, we consider a function $E(t) = \int_0^{S(t)} u(x,t)dx$. A direct calculation of $E'(t)$ and using (2.1)-(2.6) yield

$$E'(t) + 2\alpha E(t) = 2S'(t) + \beta(\delta - 1) - u(0,t). \tag{4.1}$$

The above equation is solvable and the solution can be written as

$$\begin{aligned} E(t) = 2S(t) - re^{-2\alpha t} + \frac{\beta(\delta-1)}{2\alpha}(1 - e^{-2\alpha t}) \\ - e^{-2\alpha t}\int_0^t \Big[4\alpha S(\tau) + u(0,\tau)\Big]e^{2\alpha\tau}d\tau. \end{aligned} \tag{4.2}$$

If $S(t)$ satisfies $S'(t) \le 0$ and $S(t) \to r_0$ as $t \to \infty$, then, as $t \to \infty$, the left hand side of (4.2) is less than r_0 while the right hand side of (4.2) is greater than $\frac{\beta(\delta-1)}{2\alpha} + 2r_0 - 2r - \frac{1}{2\alpha}$. Thus for fixed $\alpha > 0$ and $\delta > 1$, we can find β so that

$\dfrac{\beta(\delta-1)}{2\alpha} + 2r_0 - 2r - \dfrac{1}{2\alpha} > r_0$. Therefore $S'(t) \leq 0$ is not true for all $t > 0$ if $\delta > 1$ and β is big enough.

5. Conclusions. The free boundary problem from the process of Czochralski crystal growth is studied in this paper. Existence and uniqueness of the solution are established in the cases when the melt is superheated ($\delta > 1$) and the melt is not superheated ($\delta \leq 1$) respectively. The free boundary is increasing when $\delta \leq 1$. If $\delta > 1$, the free boundary is decreasing initially but will become increasing after certain time if β "big enough". It would be interesting to know if the free boundary remains to be increasing after certain time. Finite time blow up will not occur for the problem discussed in this paper even if the melt is superheated. The maximum growth rate can be estimated in terms of given parameters.

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