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On a Free Boundary Problem Modelling Thermal Oxidation of Silicon

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Das Modellproblem der Thermaloxidation von Silikon als einphasiges Nicht-Gleichgewichtsproblem betrachtend, benutzen wir das Schaudersche Fixpunktprinzip zum Nachweis der Existenz und Eindeutigkeit der klassischen Lösung.

Рассматривая проблему моделирующую термальное окисление кремния как однофазовую неравновесную, мы используем теорему Шаудера о неподвижной точке для доказательства существования и единственности классического решения.

Considering the problem modelling thermal oxidation of silicon as one-phase non-equilibrium problem, we use Schauder's fixed point theorem to prove the existence and uniqueness of the classical solution.

1. Introduction. A. B. CROWLEY [1] presented many physical situations that can be reduced to non-equilibrium two-phase Stefan problems, that is, the standard equilibrium condition $v = 0$ at the free boundary $x = s(t)$ is replaced by the kinetic law $\dot{s}(t) = \beta\big(v(s(t)), t\big)$. In [5], it has been shown for this problem that if $|\beta(\xi)| \leqq C_1 |\xi| + C_2$ for all $\xi \in \mathbb{R}$, a solution exists, but the uniqueness of the solution is an open question. In [3], the authors considered the non-equilibrium one-phase problem which arises in groundwater mass transport and non-equilibrium chemistry and showed that if $\beta(\xi) = \xi^n + a_{n-1}\xi^{n-1} + \cdots + a_1\xi$ for some $n \in \mathbb{N}$, under some conditions, the unique solution exists. In [2], the authors considered a problem that is somewhat similar to the one in [3], modelling thermal oxidation of silicon and using results on evolution equations in Hilbert spaces. They proved the existence and uniqueness of weak solutions and got estimates for growth of thickness of the oxide layer. But the conclusion $u \geqq 0$ in Lemma 1 there could not be obtained, because the coefficient au_1 of the term $(\overline{u}, (x\overline{u})_x)_H$ in the equation above [2:(4.1)] may be negative. In this paper, we use Schauder's fixed point theorem to prove the existence and uniqueness of classical solutions to this problem.

Let $b(t) > 0$, $\Omega_t = \big(0, b(t)\big)$, $Q = \{(x, t) : x \in \Omega_t, \quad t \in (0, T)\}$, where $T \in (0, +\infty)$, then as in [2], we consider the model problem

$$
\text{(P)} \qquad
\begin{aligned}
&(v_t - Dv_{xx})(x, t) = 0 && \text{in } Q,\\
&v(x, 0) = v^0(x) && \text{in } (0, b^0),\\
&-Dv_x(0, t) + h\big(v(0, t) - v^*\big) = 0 && \text{in } (0, T),\\
&Dv_x\big(b(t), t\big) + \big(\dot{b}(t) + k\big)\, v\big(b(t), t\big) = 0 && \text{in } (0, T),\\
&b(0) = b^0, \quad \dot{b}(t) = mv\big(b(t), t\big) && \text{in } (0, T),\\
&v \in C^{2,1}(Q) \cap C(\overline{Q}), \qquad v_x \in C\big(\overline{\Omega}_t \times (0, T)\big), && b \in C^1[0, T],
\end{aligned}
$$

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where v is a non-negative function and the constants D, h, k, m, v^*, b^0 are positive as in [2]. In the following sections, without loss of generality, we can assume $D = h = k = m = v^* = b^0 = 1$. We shall prove the existence and uniqueness of the classical solution to problem (P), in consequence, and obtain the same results as in [2].

2. Existence theorem. Let the closed convex subset $E = \{b \in C^1[0, T]: b(0) = 1, 0 \leq \dot{b}(t) \leq K\}$ in the Banach space $C^1[0, T]$, where $K > 0$ is a constant, be to be determined. At first, for a given $b \in E$, we consider the auxiliary problem

$$\text{(AP1)} \quad (v_t - v_{xx})(x, t) = 0 \qquad \text{in } Q, \tag{2.1}$$

$$\begin{aligned} &v(x, 0) = v^0(x) && \text{in } (0, 1),\\ &-v_x(0, t) + v(0, t) - 1 = 0 && \text{in } (0, T),\\ &v_x(b(t), t) + \big(v(b(t), t) + 1\big)\, v(b(t), t) = 0 && \text{in } (0, T), \end{aligned} \tag{2.2}$$

$$v \in C^{2,1}(Q) \cap C^0(\bar{Q}), \qquad v_x \in C(\bar{\Omega}_t \times (0, T]), \qquad b \in C^1[0, T].$$

Then we have

Lemma 1: *If $v = v(x,t)$ is a smooth solution to problem* (AP1), *then $|v_x| \leq C_1$ and $|v_t|, |v_{xx}| \leq C_2$ in $\bar{Q}$, $\|v_x\|_{C^{1,1/2}(\bar{Q})} \leq C_2$, where C_1 and C_2 are positive constants depending only on $\|v^0\|_{C^1[0,1]}$ and $|v|_\infty = \max_{\bar{Q}} |v|$, $\|v^0\|_{C^2[0,1]}$, $\delta_1 = \min b(t)$, $\delta_2 = \max b(t)$ and $K = \max |\dot{b}(t)|$, respectively.*

Proof: Setting $v_x = z$, we see that z satisfies (2.1). By the maximum principle, we get the first estimate. In order to prove the second one, we consider the function $w = \exp\big(-\lambda_1 t - \lambda_2(\delta_1 - x)^2\big)\, v_t(x, t)$ satisfying the following problem:

$$\begin{aligned} &w_t - w_{xx} + 4\lambda_2(\delta_1 - x)\, w_x + \big(\lambda_1 - 2\lambda_2 - 4\lambda_2^2(\delta_1 - x)^2\big)\, w = 0,\\ &-w_x(0, t) + (1 + 2\lambda_2\delta_1)\, w(0, t) = 0,\\ &w_x + \big(2\lambda_2(x - \delta_1) + 2v + 1 + \dot{b}(t)\big)\, w = -\big(2v(b(t), t) + 1\big)\, \dot{b}(t)\, v_x(b(t), t),\\ &w(x, 0) = \exp\big(-\lambda_2(\delta_1 - x)^2\big)\, d^2v^0/dx^2. \end{aligned}$$

Choosing λ_1 and λ_2 such that $2\lambda_2\delta_1 - 2\,|v|_\infty + 1 - K > 0$ and $\lambda_1 - 2\lambda_2 - 4\lambda_2^2 \times (\delta_2 - \delta_1)^2 > 0$, by the maximum principle, we conclude the second estimate, and the third one analogously by (2.1). The last one is obtained by [4: Lemma 3.1] ∎

Introducing new independent variables ξ and τ by $\xi = x/b(t)$ and $\tau = \int_0^t d\sigma/b^2(\sigma)$, we get the following problem, which is equivalent to problem (AP1):

$$\begin{aligned} \text{(AP2)} \quad &(u_\tau - u_{\xi\xi})(\xi, \tau) - \xi\dot{a}(\tau)\, u_\xi(\xi, \tau)/a(\tau) = 0 && \text{in } (0, 1) \times (0, T^*),\\ &-u_\xi(0, \tau) + a(\tau)\big(u(0, \tau) - 1\big) = 0 && \text{in } (0, T^*),\\ &u_\xi(1, \tau) + a(\tau)\, u(1, \tau)\big(u(1, \tau) + 1\big) = 0 && \text{in } (0, T^*),\\ &a(0) = a^0 := 1; \quad u(\xi, 0) = u^0(\xi) := v^0(\xi) && \text{in } (0, 1),\\ &u \in C^{2,1}(\Omega \times \mathring{S}) \cap C(\bar{\Omega} \times S), \quad u_\xi \in C(\bar{\Omega} \times \mathring{S}), \end{aligned}$$

where $a(\tau) = b(t)$, $u(\xi, \tau) = v(x, t)$, $\Omega = (0, 1)$, $S = [0, T^*]$, $\mathring{S} = [0, T^*]$,

$$T^* = \int_0^T d\sigma/b^2(\sigma).$$

Now assume

(A1) $v^0 \in C^2[0, 1]$, $v^0(x) \geqq 0$ for all $x \in [0, 1]$.

(A2) $v_x{}^0(1) + \big(v^0(1) + 1\big)\, v^0(1) = 0$, $-v_x{}^0(0) + v^0(0) - 1 = 0$.

Lemma 2: *Under the assumptions* (A1) *and* (A2), *the problem* (AP1) *is uniquely solvable.*

Proof: We first assume $b \in C^\infty[0, T]$. Then carefully checking the conditions and proof of [4: Theorem 7.4], we conclude that in order to prove that the problem (AP2), and consequently (AP1), has a unique smooth solution, one only needs to prove that the solution u to problem (AP2) has the estimate $|u| \leqq M$ in $\bar{\Omega} \times S$, where M is a generic constant depending only on given data. In the present case, we cannot employ [4: Theorem 7.3], because the last condition in [4: (7.36)] is not satisfied, but the estimate $0 \leqq u \leqq M$ in $\bar{\Omega} \times S$ holds. In fact, using the maximum principle, we easily get $u(\xi, \tau) \leqq \max\,(1, \|v^0\|_{L^\infty[0,1]})$ and the negative minimum value of $u(\xi, \tau)$ in $\bar{\Omega} \times S$ could be only achieved on $\xi = 1$ as $u^0(\xi) \geqq 0$ and $a(\tau) > 0$. If this happens, by virtue of the third equation in (AP2), there exists a $\tau_1 > 0$ such that $u(1, \tau_1) = \min u(\xi, \tau) \leqq -1 < 0$. Therefore, there exists a $\tau_0 \in (0, \tau_1]$ such that

$$u(1, \tau_0) = -1, \tag{2.3}$$

$u(1, \tau) > -1$, $0 \leqq \tau \leqq \tau_0 \leqq \tau_1$. Then observing the problem (AP2) in $\Omega \times (0, \tau_0)$ and again using the maximum principle, we have $u(\xi, \tau) > -1$ in $\Omega \times (0, \tau_0)$. Noting (2.3) and employing the strong maximum principle, we obtain

$$u_\xi(1, \tau_0) < 0. \tag{2.4}$$

Hence, (2.3) and (2.4) contradict (2.2). This means that $u(\xi, \tau)$ cannot achieve the negative value on $\xi = 1$. So, $u(\xi, \tau) \geqq 0$, and the problem (AP2), and hence (AP1), has a unique smooth solution if $b \in C^\infty[0, T]$. But by means of Lemma 1 we obtain the conclusion of Lemma 2 ∎

Lemma 3: *If $v^0 \in C^1[0, 1]$ and $v^0(x) \geqq 0$, $0 \leqq x \leqq 1$, then the problem* (AP1) *has a unique and bounded solution $v \in V^{1,0}(Q) \cap C^{1/2,1/4}(\bar{Q})$ with $|v_x(x, t)| \leqq M$ a.e. in Q and, for all $\varphi \in W^{1,1}(Q)$,*

$$\begin{aligned}
&\int_0^{b(T)} v(x, T)\, \varphi(x, T)\, dx + \int_0^1 v^0(x)\, \varphi(x, 0)\, dx \\
&- \int_0^T v\big(b(t), t\big)\, \varphi\big(b(t), t\big)\, \dot{b}(t)\, dt + \int_0^T \big(v(0, t) - 1\big)\, \varphi(0, t)\, dt \\
&+ \int_0^T \varphi\big(b(t), t\big)\, \big(v(b(t), t) + 1\big)\, v\big(b(t), t\big)\, dt \\
&- \iint_Q \big(v(x, t)\, \varphi_t(x, t) - v_x(x, t)\, \varphi_x(x, t)\big)\, dx\, dt = 0.
\end{aligned} \tag{2.5}$$

Proof: Taking approximations $v_n{}^0$ of v^0 satisfying conditions (A1), (A2) and $v_n{}^0 \to v^0$ in $C^1(0, 1)$, we get the solutions corresponding $v_n(x, 0) = v_n{}^0(x)$ by Lemmas 1 and 2 with the estimates

$$|v_n| \leqq M, \quad |v_{nx}| \leqq C_1 \ \text{in } \bar{Q}. \tag{2.6}$$

Then, from (2.1), we have

$$0 = \iint_Q v_{nt}^2 - \iint_Q v_{nxx} v_{nt} = \iint_Q v_{nt}^2 - \oint_{\partial Q} (v_{nx} v_{nt}\, dt + v_{nx}^2/2\, dx)$$

$$= \iint_Q v_{nt}^2 + 2^{-1} \int_0^{b(t)} v_{nx}^2(x, t)\, dx - 2^{-1} \int_0^1 \left(v_{nx}^0(x)\right)^2 dx$$

$$- 2^{-1} \int_0^t v_{nx}\big(b(t), t\big)\, \dot{b}(t)\, dt + \left[3^{-1} v_n^3\big(b(t), t\big) + 2^{-1} v_n^2\big(b(t), t\big)\right]\Big|_t^0$$

$$- \int_0^t [(v_n + 1)\, v_{nx}]|_{x=b(t)}\, \dot{b}(t)\, dt + 2^{-1}(v_n - 1)^2\,(0, t)|_0^t.$$

Using (2.6), we obtain $\|v_{nt}\|_{L^2(Q)} \leqq C$. Therefore, there exists a subsequence of $\{v_n\}$ (still denoged by $\{v_n\}$) such that $v_n \to v$ in $C^{1/2-\varepsilon, 1/4-\varepsilon}(\bar{Q})$ $(0 < \varepsilon < 1/4)$, $v \in C^{1/2, 1/4}(\bar{Q})$, $v_{nx} \to v_x$, $v_{nxx} \to v_{xx}$, $v_{nt} \to v_t$ weakly in $L^2(Q)$. Hence these yield (2.5). ∎

Remark 4: From this lemma, we can follow the way in [2] and thus obtain the results of [2].

Next we consider the operator F as follows: For any $b \in E$, by Lemma 2, we get the solution v of (AP1), then we set $F\big(b(t)\big) = \dot{S}(t)$, where $S(t) = \int_0^t v\big(b(t), t\big)\, dt + 1$. By virtue of Lemma 1 and taking an appropriate constant K, we see that $F: E \to E$ and F is pre-compact and continuous. In fact, by $0 \leqq u \leqq M$, choosing $K \geqq M$, we have $0 \leqq \dot{S}(t) = v\big(b(t), t\big) \leqq M$, so, $F: E \to E$. Moreover, for any t_1, t_2, we observe

$$|\dot{S}(t_1) - \dot{S}(t_2)| = \left|v\big(b(t_1), t_1\big) - v\big(b(t_2), t_2\big)\right|$$

$$\leqq C_1 |b(t_1) - b(t_2)| + C_2\, |t_1 - t_2| \leqq (C_1 K + C_2)\, |t_1 - t_2|.$$

By the Arzelë-Ascoli Theorem, F is pre-compact. In order to prove the continuity of F, we consider $b_1, b_2 \in E$; their corresponding solutions to problem (AP1) are v_1 and v_2. Suppose $b_1 \leqq b_2$ in $[0, t_1]$, and let $w = v_1 - v_2$. Then setting $Q_1 = \{(x, t): 0 < x < b_1(t),\ 0 < t < t_1\}$ w satisfies the system

$$\begin{aligned} &(w_t - w_{xx})\,(x, t) = 0 \quad \text{in } Q_1, \\ &w(x, 0) = 0, \quad -w_x(0, t) + w(0, t) = 0, \\ &w_x\big(b_1(t), t\big) = [-(v_1 + 1)\, v_1 - v_{2x}]|_{x=b_1(t)}. \end{aligned} \tag{3.1}$$

In order to estimate the right-hand side of (3.1), we observe the following:

$$\begin{aligned} I &:= [-(v_1 + 1)\, v_1 - v_{2x}]\,\big(b_1(t), t\big) \\ &= [-(v_1 - v_2)\,(v_1 + v_2 + 1)]\,\big(b_1(t), t\big) \\ &\quad + [-(v_2 + 1)\, v_2 + v_{2x}]\,\big(b_1(t), t\big) + [(v_2 + 1)\, v_2 + v_{2x}]\,\big(b_2(t), t\big) \\ &= [(v_2 - v_1)\,(v_1 + v_2 + 1)]\,\big(b_1(t), t\big) \\ &\quad + \left\{[(2v_2 + 1)\, v_{2x}]\,\big(b^*(t), t\big) = v_{2xx}\big(\bar{b}(t), t\big)\right\}\big(b_1(t) - b_2(t)\big), \end{aligned}$$

where

$$b^*(t) = b_1(t) + \theta^*(b_2(t) - b_1(t)), \quad (0 \leqq \theta^*, \bar{\theta} \leqq 1).$$
$$\bar{b}(t) = b_1(t) + \bar{\theta}(b_2(t) - b_1(t))$$

From Lemma 1, we have $|I| \leqq C_2 |w| + C_2 |b_1(t) - b_2(t)|$. As in the proof of Lemma 1, we get

$$|w| \leqq C_2 |b_1(t) - b_2(t)|_{L^\infty[0,t_1]} \quad \text{in } \bar{\theta}_1. \tag{3.2}$$

Therefore

$$\begin{aligned} |\dot{S}_1(t) - \dot{S}_2(t)| &= \left|v_1(b_1(t), t) - v_2(b_2(t), t)\right| \\ &\leqq \left|v_1(b_1(t), t) - v_2(b_1(t), t)\right| + \left|v_2(b_1(t), t) - v_2(b_2(t), t)\right| \\ &\leqq C_2 |b_1(t) - b_2(t)|_{L^\infty[0,t_1]}. \end{aligned} \tag{3.3}$$

Here we have used the estimate of Lemma 1 and (3.2). From the above proof, we see that (3.3) still holds as $t_1 = T$, which shows that F is continuous. Employing Schauder's fixed point theorem, we conclude that F has a fixed point. Thus we proved

Theorem 1: *Under the assumptions* (A1) *and* (A2) *the problem* (P) *has at least one solution with the estimates of Lemma* 1.

3. Uniqueness theorem. Concerning the uniqueness theorem, we have

Theorem 2: *Under the assumptions* (A1) *and* (A2), *the problem* (P) *has at most one solution with the estimates of Lemma* 1.

Proof: Suppose that there are two solutions (v_1, b_1) and (v_2, b_2) to problem (P). Let $w = v_1 - v_2$. We assume that $b_1 \leqq b_2$ in $(0, t_1)$ $(t_1 \leqq T)$. Then as in Section 2, we get (3.2). But, by Lemma 1 and (3.2), we have

$$\begin{aligned} |b_1(t) - b_2(t)| &\leqq \int_0^t \left|v_1(b_1(y), y) - v_2(b_2(y), y)\right| dy \\ &\leqq \int_0^t \left|v_1(b_1(y), y) - v_2(b_1(y), y)\right| dy \\ &\quad + \int_0^t \left|v_2(b_1(y), y) - v_2(b_2(y), y)\right| dy \\ &\leqq \int_0^t \left|w(b_1(y), y)\right| dy + C_1 t \, |b_1(t) - b_2(t)|_{L^\infty[0,t_1]} \\ &\leqq (C_1 + C_2)\, t \, |b_1(t) - b_2(t)|_{L^\infty[0,t]}. \end{aligned}$$

Hence we obtain $b_1(t) = b_2(t)$ if $t \leqq \max\left(1/(C_1 + C_2), t_1\right)$. It is easy to see that the above procedure can be continued to T ∎

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