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A Free Boundary Value Problem Modeling Thermal Oxidation of Silicon

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Unter Benutzung von Ergebnissen über Evolutionsgleichungen in Hilbert-Räumen wird ein Problem gelöst, welches die Diffusion eines Oxydanten durch eine Oxidschicht und das durch die Oxydation von Silizium verursachte Wachstum dieser Schicht beschreibt. Darüber hinaus werden praktisch interessante Abschätzungen für das Wachstum der Dicke der Oxidschicht angegeben.

Используя результаты об эволюционных уравнениях в Гильбертовых пространствах решается задача, которая описывает диффузию окислителя через слой двуокиси кремния и рост этого слоя в следствии дальнейшего окисления. Кроме того приводятся оценки роста толщины слоя окиси интересные с точки зрения практики.

Using results on evolution equations in Hilbert spaces a problem describing the diffusion of an oxidant through an oxide layer and the growth of this layer caused by the oxidation of silicon is solved. Moreover, estimates for the growth of the thickness of the oxide layer being of practical interest are given.

1. Introduction

This paper deals with a simple spatially one-dimensional model of the thermal oxidation of silicon. It describes the diffusion of an oxidant through an oxide layer and the growth of this layer caused by the oxidation of silicon at the oxide silicon interface.

Denoting by b the *oxide thickness* and by v the *oxidant concentration* we can write the model equations as follows:

$$\begin{aligned}
&(v_\tau - Dv_{\xi\xi})(\tau, \xi) = 0, \qquad 0 < \xi < b(\tau), \qquad \tau > 0,\\
&-Dv_\xi(\tau, 0) + h\big(v(\tau, 0) - v^*\big) = 0, \qquad \tau > 0,\\
&Dv_\xi\big(\tau, b(\tau)\big) + \big(\dot b(\tau) + k\big)\, v\big(\tau, b(\tau)\big) = 0, \qquad \tau > 0,\\
&\dot b(\tau) = mv\big(\tau, b(\tau)\big), \qquad \tau > 0,\\
&v(0, \xi) = v^0(\xi), \qquad 0 < \xi < b^0, \qquad b(0) = b^0.
\end{aligned}$$

The subscripts τ and ξ denote the derivatives with respect to the time τ and the space variable ξ, respectively, and $\dot b$ denotes the derivative of b with respect to its argument. To be precise we require that

b is continuous differentiable and positive,
v is continuous on $\{(\tau, \xi) : \tau \geqq 0, 0 \leqq \xi \leqq b(\tau)\}$,
v_τ, $v_{\xi\xi}$ are continuous on $\{(\tau, \xi) : \tau > 0, 0 \leqq \xi \leqq b(\tau)\}$.

We assume that D, h, k, m, v^*, b^0 are positive constants and that v^0 is a nonnegative function from $L^\infty(0, b^0)$.

The constant D is the diffusivity of the oxidant. The boundary condition at $\xi = 0$ models the interaction of the oxide layer and a gas phase. Similarly, the boundary condition at $\xi = b(\tau)$ represents the oxidant balance at the moving oxide silicon interface. In particular, the term $kv(\tau, b(\tau))$ takes into account the sink caused by the oxidation of silicon. The equation for b means that the speed of the interface is proportional to the oxidation rate. The assumption that the oxidation rate itself is proportional to the oxidant concentration at the interface has been made for the sake of simplicity only. One could treat in a completely analogous way more general equations including the case that the oxidation rate is proportional to the square of the oxidant concentration.

The process of oxidation of silicon has been investigated by several authors (a standard reference is DEAL-GROVE [2]). These authors assumed the diffusion process to be quasi-stationary, i.e., they neglected the term v_τ in the diffusion equation. This is clearly unjustified for an initial transient period and it could be justified rigorously for large times only by results on the problem stated above. This problem is similar to the familiar one-phase Stefan problem which can be reduced to a variational inequality that does not contain explicitly the free boundary (see, e.g., KINDERLEHRER and STAMPACCHIA [5]). For our problem we do not know any such reduction. We shall show, however, that our problem can be transformed to an initial value problem of standard type for a pair of functions (the oxide thickness and the oxidant concentration on a "normalized" domain). To this initial value problem one can apply various results of the theory of evolution equations in Hilbert spaces. We shall prove at first the existence and uniqueness of a weak solution and then derive regularity results which show that any weak solution is a classical solution provided the initial concentration is sufficiently smooth. Moreover, we shall present estimates for the oxide thickness $b(\tau)$ showing that for large times τ this thickness is of the order of $\tau^{1/2}$.

2. Transformation and weak formulation of the problem

Assume that (b, v) is a solution of the problem stated in the introduction. Then one can introduce new (dimensionless) independent variables t and x by

$$t = D \int_0^\tau \frac{d\sigma}{\big(b(\sigma)\big)^2}, \qquad x = \frac{\xi}{b(\tau)}. \tag{2.1}$$

Let $\Omega = (0, 1)$, $\bar{\Omega} = [0, 1]$, $S = [0, T]$, and $\dot{S} = (0, T]$, where $T \in (0, +\infty)$ is arbitrarily fixed. Introducing new unknown functions

$$a(t) = \frac{mv^*}{D}\, b(\tau), \qquad u(t, x) = \frac{v(\tau, \xi)}{v^*} \tag{2.2}$$

and taking into account the regularity assumptions from the introduction we can state

Problem I:

$$\begin{aligned}
&(u_t - u_{xx})\,(t, x) - xa(t)\, u(t, 1)\, u_x(t, x) = 0, \qquad 0 < t \leqq T, \quad 0 < x < 1,\\
&-u_x(t, 0) + a(t)\, p\big(u(t, 0) - 1\big) = 0, \qquad 0 < t \leqq T,\\
&u_x(t, 1) + a(t)\, u(t, 1)\, \big(u(t, 1) + q\big) = 0, \qquad 0 < t \leqq T,\\
&a'(t) = u(t, 1)\, \big(a(t)\big)^2, \qquad 0 < t \leqq T,\\
&u(0, x) = u^0(x) := \frac{v^0(b^0x)}{v^*}, \qquad 0 < x < 1, \qquad a(0) = a^0 := \frac{mv^*}{D}\, b^0,\\
&a \in C^1(S), \qquad u \in C(S \times \bar{\Omega}), \qquad u_t, u_{xx} \in C(\dot{S} \times \bar{\Omega}).
\end{aligned}$$

Here $p := h/(mv^*)$, $q := k/(mv^*)$. Of course the subscripts t and x denote the corresponding derivatives and a' is the derivative of a with respect to its argument.

It would be natural to look for a solution in the interval $[0, T^*)$, where $T^* = D \int_0^\infty (b(\sigma))^{-2} \, d\sigma$. Later we shall see that in fact $T^* = +\infty$. Since this is not known in advance we shall try to solve Problem I for any $T > 0$. If a solution (a, u) of this problem is known, one can determine τ and ξ by

$$\tau = \frac{D}{(mv^*)^2} \int_0^t (a(s))^2 \, ds, \qquad \xi = \frac{D}{mv^*} a(t) \, x. \tag{2.3}$$

From now on we shall assume (without mentioning this everywhere in our results) that

$$p > 0, \qquad q > 0, \qquad a^0 > 0, \qquad u^0 \in L^\infty(\Omega), \qquad u^0 \geqq 0. \tag{2.4}$$

Next we are going to introduce a weak formulation of Problem I. Let $V = H^1(\Omega)$, $H = L^2(\Omega)$, and let V^* be the dual space to V. The norms on V and H will be denoted by $\|\cdot\|$ and $|\cdot|$, respectively. For the scalar product in H we use the notation $(\cdot, \cdot)_H$. If $u \in V$, we write u_0, u_1 instead of $u(0), u(1)$. Similarly, if u is any function defined on S with values in V, then u_0, u_1 denote the functions $t \mapsto u(t, 0)$ and $t \mapsto u(t, 1)$. We define

$$W = \{w \in L^2(S; \mathbf{R} \times V) : w' \in L^2(S; \mathbf{R} \times V^*)\},$$
$$X = L^2(S; \mathbf{R} \times V) \cap L^\infty(S; \mathbf{R} \times L^\infty(\Omega)),$$

where w' denotes the derivative of w in the sense of $(\mathbf{R} \times V^*)$-valued distributions. (Note that $V \subset H \subset V^*$.) The space W is continuously imbedded into $C(S; \mathbf{R} \times H)$. Spaces used here without explanation have their usual meaning and are to be endowed with their standard norms (see, e.g., [3! Ch. IV]). We introduce an operator A: $\mathbf{R} \times V \to \mathbf{R} \times V^*$ as follows:

$$\langle Aw, \overline{w} \rangle = (u_x, \overline{u}_x)_H + a\{u_1(u, (x\overline{u})_x)_H + p(u_0 - 1) \, \overline{u}_0 + u_1(q\overline{u}_1' - a\overline{a})\},$$

where $w = (a, u)$, $\overline{w} = (\overline{a}, \overline{u})$ are arbitrary elements of $\mathbf{R} \times V$ and $x\overline{u}$ denotes the function $x \mapsto x\overline{u}(x)$, $x \in \Omega$. The operator A can also be considered as a mapping from X into $L^2(S; V^*)$. If $w \in X$, then Aw means the function $t \mapsto Aw(t)$, $t \in S$. As usual we shall identify $L^2(S; L^2(\Omega))$ and $L^2(S \times \Omega)$. Accordingly, $u(t)$ and $u(t, \cdot)$ have the same meaning.

Now we are ready to state

Problem II: We are looking for $w \in X$ such that

$$w' + Aw = 0, \qquad w(0) = w^0 := (a^0, u^0).$$

It is easy to check that any solution $w = (a, u)$ of Problem I is a solution of Problem II and that, conversely, any solution $w = (a, u)$ of Problem II with sufficiently smooth u is a solution of Problem I (cf. the proof of Theorem 2 below). Therefore we may call any solution of Problem II a weak solution of Problem I.

3. Results

In this section our results are summarized. The proofs are delayed to the subsequent sections.

Theorem 1: *Problem* II *is uniquely solvable.*

The next two theorems state regularity properties of the weak solution. These results show that for smooth initial data the solution of Problem II is also a solution of Problem I and in particular a classical solution.

Theorem 2: *If* (a, u) *is the solution of Problem* II *the existence and uniqueness of which is guaranteed by Theorem* 1, *then* $u \in C(\mathring{S}; H^3(\Omega))$, $u' \in C(\mathring{S}; V)$, *and* $a \in H^3_{\text{loc}}(\mathring{S})$. *Moreover*

$$-u_{x0} + ap(u_0 - 1) = 0 \quad \text{and} \quad u_{x1} + au_1(u_1 + q) = 0 \quad \text{on } \mathring{S}, \tag{3.1}$$

$$u' - u_{xx} - au_1xu_x = 0 \quad \text{on } \mathring{S} \times \Omega. \tag{3.2}$$

Theorem 3: *Let* (a, u) *be the solution of Problem* II. *If, in addition to our general assumption* (2.4), *we have* $u^0 \in V$, *then*

$$u \in C(S; V), \qquad u' \in L^2(S; H), \qquad a' \in C(S). \tag{3.3}$$

If, moreover, $Aw^0 \in \mathbf{R} \times H$, *i.e.,*

$$u^0 \in H^2(\Omega), \qquad -u^0_{x0} + a^0p(u_0{}^0 - 1) = u^0_{x1} + a^0u_1{}^0(u_1{}^0 + q) = 0, \tag{3.4}$$

then

$$u \in C(S; H^2(\Omega)), \qquad u' \in L^2(S; V) \cap C(S; H), \qquad a \in H^2(S). \tag{3.5}$$

Theorem 4: *Let again* (a, u) *be the solution of Problem* II. *Then, for every* $t \in S$,

$$\left(1 + \frac{q}{p}\right) a(t) + \frac{q}{2} (a(t))^2$$

$$\leqq \int_0^t (a(s))^2 \, ds + c_0 \leqq \left(1 + \frac{q + M}{p}\right) a(t) + \frac{q + M}{p} (a(t))^2,$$

where

$$M = \max \{1, \|u^0\|_{L^\infty(\Omega)}\},$$

$$c_0 = a^0 \left\{\left\| u^0 \left(\frac{1}{p} + a^0x\right)\right\|_{L^1(\Omega)} + 1 + \frac{q}{p} + \frac{a^0q}{2}\right\}.$$

Remark 1: The meaning of Theorem 4 becomes clear if the result is expressed in terms of the variable τ and the unknown $b(\tau)$ of the original problem (cf. (2.1)—(2.3)). Then it reads

$$\left(1 + \frac{q}{p}\right) \frac{b(\tau)}{mv^*} + \frac{q}{2D} (b(\tau))^2 \leqq \tau + \frac{c_0D}{(mv^*)^2} \leqq \left(1 + \frac{q + M}{p}\right) \frac{b(\tau)}{mv^*} + \frac{q + M}{2D} (b(\tau))^2,$$

i.e., for large times τ the oxide thickness $b(\tau)$ is of the order of $\tau^{1/2}$. On the basis of the simplified quasi-stationary model Deal-Grove [2] had obtained that

$$\tau + \tau_0 = \frac{q}{2D} (b(\tau))^2 + \left(1 + \frac{q}{p}\right) \frac{b(\tau)}{mv^*},$$

where τ_0 is a constant depending on the initial thickness. Note that the coefficients of $(b(\tau))^2$ and $b(\tau)$ in this formula are exactly the same as in the lower bound for τ given above. Let us mention that in the case of the one-phase Stefan problem one has also $b(\tau) \leqq \text{const}\,(1 + \tau)^{1/2}$ (see Kinderlehrer and Stampacchia [5]).

Theorem 5: *Let* (a, u) *be the solution of Problem* II *and let* $u^0 \in V$ *be such that* $u_x{}^0 \leqq 0$ *and* $u^0 \leqq 1$. *Then* $u_x(t) \leqq 0$ *for every* $t \in S$.

4. Proofs

In this section all proofs are summarized. For the proof of our first, the Existence-Uniqueness Theorem, we need two Lemmata.

Lemma 1: *Let $w = (a, u)$ be a solution of Problem* II *and let* $M = \max\{1, \|u^0\|_{L^\infty(\Omega)}\}$. *Then, for every $t \in S$,*

(i) $0 \leqq u(t) \leqq M$, (ii) $a^0 \leqq a(t) \leqq a^0 \exp\left(\frac{M}{q}(1 + t)\right)$.

Proof: (i) By v^+, v^- we denote the positive and the negative part of a function v, respectively. Choosing $\overline{w} = (0, u^-)$ as a test function for the equation $w' + Aw = 0$ we find, for every $t \in S$,

$$0 = \int_0^t \langle (w' + Aw)(s), \overline{w}(s)\rangle \, ds$$

$$= -\frac{1}{2}|u^-(t)|^2 - \int_0^t \Big\{|u_x^-|^2 + a\big[u_1\big(u^-, (xu^-)_x\big)_H$$

$$+ p(u_0^- + 1)\, u_0^- + q(u_1^-)^2\big]\Big\}\, ds.$$

(To simplify the notation we have omitted the argument s of the functions of the last integrand. We shall do this also in further calculations.) Since, for every $v \in V$,

$$\big(v, (xv)_x\big)_H = \int_\Omega \big(|v(x)|^2 + xv_x(x)\, v(x)\big)\, dx = \frac{1}{2}|v|^2 + \frac{1}{2} v_1^2 \tag{4.1}$$

this implies that $u^- = 0$, i.e., $u \geqq 0$. Using $\overline{w} = (0, \overline{u})$, where $\overline{u} = (u - M)^+$, as a test function we obtain

$$0 = \frac{1}{2}|\overline{u}(t)|^2 + \int_0^t \Big\{|\overline{u}_x|^2 + a\big[u_1\big(\overline{u} + M, (x\overline{u})_x\big)_H$$

$$+ p(\overline{u}_0 + M - 1)\,\overline{u}_0 + qu_1\overline{u}_1\big]\Big\}\, ds.$$

Consequently, $\overline{u} = 0$, i.e., $u \leqq M$.

(ii) It is easy to see that from $w' + Aw = 0$ it follows that $a' = u_1 a^2$, where $a \in H^1(S)$ and a' is to be understood as the derivative of a in the sense of this Sobolev space. Therefore $a(t) \geqq a^0$, $t \in S$. Moreover, denoting by x and 1 the functions $(t, x) \mapsto x$ and $(t, x) \mapsto 1$, respectively, we obtain

$$0 = \int_0^t \Big\{\langle u', x\rangle + (u_x, 1)_H + au_1\big((u, 2x)_H + q\big)\Big\}\, ds$$

$$= \|xu(t)\|_{L^1(\Omega)} - \|xu^0\|_{L^1(\Omega)} + q \log \frac{a(t)}{a^0} + \int_0^t (u_1 - u_0 + 2au_1\|xu\|_{L^1(\Omega)})\, ds$$

$$\geqq -M(1 + t) + q \log \frac{a(t)}{a^0}.$$

This proves the second assertion ∎

If one wants to solve Problem II, one has to overcome difficulties connected with the growth properties of the nonlinear parts of the operator A. Lemma 1 suggests to introduce besides A a "regularized" operator $\tilde{A}: \mathbf{R} \times V \to \mathbf{R} \times V^*$ by

$$\langle \tilde{A}w, \overline{w} \rangle = (u_x, \overline{u}_x)_H + \tilde{a}\big[\tilde{u}_1\big(\tilde{u}, (x\overline{u})_x\big)_H + p(\tilde{u}_0 - 1)\,\overline{u}_0 + \tilde{u}_1(q\overline{u}_1 - \tilde{a}\overline{a})\big],$$

where $w = (a, u)$, $\overline{w} = (\overline{a}, \overline{u}) \in \mathbf{R} \times V$ and $\tilde{a} = \min\left\{a^+, a^0 \exp\left(\frac{M}{q}(1+T)\right)\right\}$, $\tilde{u} = \min\{u^+, M\}$. Note that $\tilde{A}$ can be regarded as a mapping from $L^2(S; \mathbf{R} \times V)$ to $L^2(S; \mathbf{R} \times V^*)$. Lemma 1 shows that if w is a solution of Problem II, then w is also a solution of

$$w' + \tilde{A}w = 0, \qquad w(0) = w^0, \qquad w \in W. \tag{4.2}$$

Lemma 2: *If $(a, u), (b, v) \in \mathbf{R} \times V$, then*

$$\langle \tilde{A}(a, u) - \tilde{A}(b, v), (a - b, u - v)\rangle \geqq \frac{1}{2}\,\|u - v\|^2 - c\big((a - b)^2 + |u - v|^2\big),$$

where c is independent of $(a, u), (b, v)$.

Proof: Let $\tilde{a}, \tilde{b}$ and $\tilde{u}, \tilde{v}$ be defined as $\tilde{a}$ and $\tilde{u}$ above. Then

$$\begin{aligned}
&\langle \tilde{A}(a, u) - \tilde{A}(b, v), (a - b, u - v)\rangle \\
&= |u_x - v_x|^2 + \big(\tilde{a}\tilde{u}_1(\tilde{u} - \tilde{v}) + \tilde{a}(\tilde{u}_1 - \tilde{v}_1)\,\tilde{v} + (\tilde{a} - \tilde{b})\,\tilde{v}_1\tilde{v}, (xu - xv)_x\big)_H \\
&\quad + \{\tilde{a}(\tilde{u}_0 - \tilde{v}_0) + (\tilde{a} - \tilde{b})\,(\tilde{v}_0 - 1)\}\,p(u_0 - v_0) \\
&\quad + \{\tilde{a}(\tilde{u}_1 - \tilde{v}_1) + (\tilde{a} - \tilde{b})\,\tilde{v}_1\}\,q(u_1 - v_1) - \{\tilde{a}^2(\tilde{u}_1 - \tilde{v}_1) + (\tilde{a}^2 - \tilde{b}^2)\,\tilde{v}_1\} \\
&\quad \times (a - b) \\
&\geqq \|u - v\|^2 - |u - v|^2 - c\big(|u - v|^{1/2}\,\|u - v\|^{3/2} + |a - b|\,\|u - v\| \\
&\quad + (a - b)^2\big) \\
&\geqq \frac{1}{2}\,\|u - v\|^2 - c\big((a - b)^2 + |u - v|^2\big);
\end{aligned}$$

here and later c denotes (possibly different) constants the exact value of which is not important ∎

Proof of Theorem 1 (*weak solvability*): In view of standard results on evolution equations in Hilbert spaces (see, e.g., [3: Ch. VI]) it follows immediately from Lemma 2 that the initial value problem (4.2) has a unique solution (a, u). In the same way as Lemma 1 one can prove that $0 \leqq u(t) \leqq M$ and $a^0 \leqq a(t) \leqq a^0 \exp\left(\frac{M}{q}(1+T)\right)$. Thus, (a, u) is also a solution of Problem II. Since we know already that any solution of Problem II is a solution of (4.2), this completes the proof of the unique solvability of Problem II ∎

Proof of Theorem 2 (*regularity*): Let (a, u) be a solution of Problem II. From results by GRÖGER (see [4: Th. 1 and Rem. 5]) it follows that $u \in C(\dot{S}; V)$ and $u' \in L^2_{\mathrm{loc}}(\dot{S}; V) \cap L^\infty_{\mathrm{loc}}(\dot{S}; H)$. Since $a' = u_1 a^2$ this implies that $a \in H^2_{\mathrm{loc}}(\dot{S})$. We define $A_1, A_2, A_3: V \to V^*$ and $f \in V^*$ by

$$\langle A_1 v, \overline{v}\rangle = (v_x, \overline{v}_x)_H, \qquad \langle A_2 v, \overline{v}\rangle = \big(v, (x\overline{v})_x\big)_H,$$
$$\langle A_3 v, \overline{v}\rangle = p v_0 \overline{v}_0 + q v_1 \overline{v}_1, \qquad \langle f, \overline{v}\rangle = -p\overline{v}_0,$$

where $\bar{v}, v \in V$ are arbitrary. From $w' + Aw = 0$ it follows that

$$u' + A_1 u + a(u_1 A_2 u + A_3 u + f) = 0. \tag{4.3}$$

Differentiating this equation (in the sense of V^*-valued distributions) we get

$$u'' + A_1 u' + a(u_1 A_2 u' + u_1' A_2 u + A_3 u') + a'(u_1 A_2 u + A_3 u + f) = 0. \tag{4.4}$$

On account of the regularity properties of a and u which are already known we conclude that $u'' \in L^2_{\text{loc}}(\mathring{S}; V^*)$. This result along with $u' \in L^2_{\text{loc}}(\mathring{S}; V)$ proves that $u' \in C(\mathring{S}; H)$. The continuity properties of $a, a', u,$ and u' show that $w'(t) + Aw(t) = 0$ must hold for every $t \in \mathring{S}$.

Let $t \in \mathring{S}$. Then, for $\varphi \in C_0^\infty(\Omega)$,

$$-\big(u_x(t), \varphi_x\big)_H = \big(u'(t) - a(t)\, u_1(t)\, x u_x(t), \varphi\big)_H.$$

This means that

$$u_{xx}(t) = u'(t) - a(t)\, u_1(t)\, x u_x(t). \tag{4.5}$$

Since $u \in C(\mathring{S}; V)$, $u' \in C(\mathring{S}; H)$, and $a \in C(S)$ we obtain $u \in C\big(\mathring{S}; H^2(\Omega)\big)$. Further, for every $v \in V$,

$$\begin{aligned}-\big(u_x(t), v_x\big)_H &= \big(u'(t), v\big)_H \\ &\quad + a(t)\big(u_1(t)\big(u(t), (xv)_x\big)_H + p\big(u_0(t) - 1\big) v_0 + q u_1(t)\, v_1\big).\end{aligned}$$

By means of the divergence theorem the applicability of which is guaranteed by the preceding results we get

$$\begin{aligned}&\big(u_{xx}(t), v\big)_H - u_{x1}(t)\, v_1 + u_{x0}(t)\, v_0 \\ &= \big(u'(t) - a(t)\, u_1(t)\, x u_x(t), v\big)_H \\ &\quad + a(t)\big(p\big(u_0(t) - 1\big) v_0 + u_1(t)\big(u_1(t) + q\big) v_1\big).\end{aligned}$$

In view of (4.5) this gives

$$v_0\big(-u_{x0}(t) + a(t)\, p\big(u_0(t) - 1\big)\big) + v_1\big(u_{x1}(t) + a(t)\, u_1(t)\big(u_1(t) + q\big)\big) = 0.$$

Because v_0 and v_1 can be chosen arbitrarily this proves the assertions (3.1).

Since $u' \in L^2_{\text{loc}}(\mathring{S}; V)$ we have, for a.e. $t \in S$,

$$\lim_{\sigma \to 0} \left\| \frac{1}{\sigma}\big(u(t + \sigma) - u(t)\big) - u'(t) \right\| = 0. \tag{4.6}$$

This is a consequence of a result on the differentiability of Bochner integrals. In order to prove $u'' \in L^2_{\text{loc}}(\mathring{S}; H)$ and $u' \in L^\infty_{\text{loc}}(\mathring{S}; V)$ we may assume without loss of generality that $u \in C(S; V)$, $u' \in C(S; H) \cap L^2(S; V)$, and that (4.6) is valid for $t = 0$. Let $t > 0$ and $\sigma > 0$ be such that $t + \sigma \in S$. Then, using the notations $u_\sigma(s) = u(s + \sigma) - u(s)$, $a_\sigma(s) = a(s + \sigma) - a(s)$, $0 \leq s \leq t$, we find (cf. (4.3))

$$\begin{aligned}0 = \int_0^t \Big\langle (u_\sigma' + A_1 u_\sigma)(s) + a(s + \sigma)\big(u_1(s + \sigma)\, A_2 u_\sigma(s) \\ + (u_{\sigma 1} A_2 u + A_3 u_\sigma)(s)\big) + a_\sigma(s)\big((u_1 A_2 u + A_3 u)(s) + f\big), u_\sigma'(s)\Big\rangle\, ds\end{aligned}$$

$$= \int_0^t \Big\{ |u_\sigma'(s)|^2 - a(s+\sigma) \big[u_1(s+\sigma) \big((u_{\sigma x}(s), x u_\sigma'(s))_H - u_{\sigma 1}(s)\, u_{\sigma 1}'(s) \big)$$

$$+ u_{\sigma 1}(s) \big((u_x(s), x u_\sigma'(s))_H - u_1(s)\, u_{\sigma 1}'(s) \big) \big]$$

$$- \frac{1}{2} a'(s+\sigma) \big(p(u_{\sigma 0}(s))^2 + q(u_{\sigma 1}(s))^2 \big)$$

$$- a_\sigma(s) \big[u_1(s) \big((u_x(s), x u_\sigma'(s))_H - u_1(s)\, u_{\sigma 1}'(s) \big)$$

$$- p\big(u_0(s) - 1\big) u_{\sigma 0}'(s) - q u_1(s)\, u_{\sigma 1}'(s) \big] \Big\} \, ds$$

$$+ \frac{1}{2} |u_{\sigma x}(t)|^2 - \frac{1}{2} |u_{\sigma x}(0)|^2 + \frac{1}{2} a(t+\sigma) \big(p(u_{\sigma 0}(t))^2 + q(u_{\sigma 1}(t))^2 \big)$$

$$- \frac{1}{2} a(\sigma) \big(p(u_{\sigma 0}(0))^2 + q(u_{\sigma 1}(0))^2 \big)$$

$$\geqq \int_0^t \Big\{ \frac{1}{2} |u_\sigma'(s)|^2 - c \, \|u_\sigma(s)\|^2 - c(\|u'\|^2_{L^\infty(S;V)} + 1) \, |u_\sigma(s)|^2$$

$$- c\sigma^2 \big(1 + \|u'(s)\|^2\big) - c\big(a_\sigma'(s)\big)^2 \Big\} \, ds + \frac{1}{2} |u_{\sigma x}(t)|^2 - c \, \|u_\sigma(0)\|^2$$

$$+ \frac{a^0}{2} \big(p(u_{\sigma 0}(t))^2 + q(u_{\sigma 1}(t))^2 \big) - c\sigma \big(|u_{\sigma 0}(t)| + |u_{\sigma 1}(t)| \big) - c\sigma^2 .$$

Hence

$$\|u_\sigma(t)\|^2 + \int_0^t |u_\sigma'|^2 \, ds \leqq c \left\{ \sigma^2 + \|u_\sigma(0)\|^2 + \int_0^t (\|u_\sigma\|^2 + |a_\sigma'|^2) \, ds \right\} \leqq c\sigma^2$$

(cf. [4: Lemma 1]). This shows that $u' \in L^\infty(\mathring{S}; V)$ and $u'' \in L^2_{\mathrm{loc}}(\mathring{S}; H)$.

From (4.4) it follows that, for a.e. $t \in S$,

$$u''(t) + B(t)\, u'(t) = g(t), \tag{4.7}$$

where

$$B(t)\, v = A_1 v + a(t) \big(u_1(t) A_2 v + v_1 A_2 u(t) + A_3 v \big), \qquad v \in V,$$

$$g(t) = a'(t) \big(u_1(t) A_2 u(t) + A_3 u(t) + \gamma \big).$$

In view of the regularity properties of a and u proved so far we are allowed to apply Theorem 1 of [4] to the problem (4.7). In particular, we obtain that $u' \in C(\mathring{S}; V)$ and $u'' \in L^2_{\mathrm{loc}}(\mathring{S}; V)$. Because $a' = u_1 a^2$ this implies that $a \in H^3_{\mathrm{loc}}(\mathring{S})$. Finally from (4.5) it follows that $u \in C\big(\mathring{S}; H^3(\Omega)\big)$ and that (3.2) is valid ∎

Proof of Theorem 3 (*regularity*): Let u^0 satisfy the conditions (3.4). Then $u' \in L^2(S; V) \cap C(S; H_w)$, where H_w is the space H equipped with its weak topology (see GRÖGER [4: Th. 3 and Rem. 5]). From Theorem 2 we already know that $u' \in C(\mathring{S}; H)$. Therefore in order to prove $u' \in C(S; H)$ it is sufficient to show that $u' : S \to H$ is continuous from the right at 0. This can be shown by means of Proposition 3.3 in BRÉZIS [1]. We omit the details. From $u' \in L^2(S; V)$ it follows that

$a' = u_1 a^2 \in H^1(S)$. Since $u^0 \in V$ we have also $u \in C(S; V)$. Using once more (4.5) we obtain $u \in C(S; H^2(\Omega))$. This completes the proof of the second part of Theorem 3.

Let again u^0 satisfy the conditions (3.4). Then (cf. (4.3))

$$0 = \int_0^t \left\langle u' + A_1 u + a(u_1 A_2 u + A_3 u + f), \frac{u'}{a} \right\rangle ds$$

$$= \int_0^t \left\{ \frac{|u'|^2}{a} + \frac{1}{a} (u_x, u_x')_H + u_1 \big(u, (xu')_x\big)_H + p(u_0 - 1)\, u_0' + q u_1 u_1' \right\} ds$$

$$\geqq \int_0^t \left\{ \frac{|u'|^2}{a(T)} - M \,\|u\|\, |u'| \right\} ds + \frac{1}{2a(t)} |u_x(t)|^2 - \frac{1}{2a^0} |u_x{}^0|^2$$

$$+ \frac{p}{2} \big((u_0(t) - 1)^2 - (u_0{}^0 - 1)^2\big) + \frac{q}{2} \big((u_1(t))^2 - (u_1{}^0)^2\big)$$

$$+ \frac{1}{3} \big((u_1(t))^3 - (u_1{}^0)^3\big).$$

Now let u^0 be any nonnegative element of V and let $w = (a, u)$ be the solution of Problem II corresponding to the initial value (a^0, u^0). It is easy to see that there exists a sequence $(u_n{}^0)$ of nonnegative functions satisfying (3.4) and converging to u^0 in V. Let w_n be the solution of the initial value problem

$$w_n' + A w_n = 0, \qquad w_n(0) = (a^0, u_n{}^0), \qquad w_n \in X.$$

Standard results on evolution equations can be used to show that the sequence $(w_n) = (a_n, u_n)$ converges to w in W. The estimate derived above is true with a_n, u_n instead of a, u. Passing to the limit as $n \to \infty$ we obtain firstly that $u \in L^\infty(S; V)$ and $u' \in L^2(S; H)$. Since $u \in C(S; H)$ we have also $u \in C(S; V_w)$, where V_w is V with its weak topology. Secondly

$$\frac{1}{2a(t)} |u_x(t)|^2 + \frac{p}{2} \big(u_0(t) - 1\big)^2 + \frac{q}{2} \big(u_1(t)\big)^2 + \frac{1}{3} \big(u_1(t)\big)^3$$

$$\leqq \frac{1}{2a^0} |u_x{}^0|^2 + \frac{p}{2} (u_0{}^0 - 1)^2 + \frac{q}{2} (u_1{}^0)^2 + \frac{1}{3} (u_1{}^0)^3 + C \int_0^t \|u\|^2 \, ds.$$

In view of the properties of a and u which are already established this implies that $\overline{\lim_{t \downarrow 0}} \|u(t)\| \leqq \|u^0\|$. This inequality along with $u \in C(S; V_w) \cap C(\dot{S}; V)$ proves that $u \in C(S; V)$. The assertion $a' \in C(S)$ is an easy consequence of $u \in C(S; V)$ and $a' = u_1 a^2$ ∎

Remark 2: The proofs of the Theorems 2 and 3 indicate that, with somewhat more effort, one could prove even better regularity properties of a and u. We did content ourselves with the results stated in these theorems in order to avoid further tedious calculations.

Proof of Theorem 4: By means of the test function $(0, a + pa^2x)$ it follows from $w' + Aw = 0$ that, for every $t \in S$,

$$0 = a(t)\,\|u(t)\,(1 + pa(t)\,x)\|_{L^1(\Omega)} - a^0\,\|u^0(1 + pa^0x)\|_{L^1(\Omega)}$$
$$+ \int_0^t \{-a'(1 + 2pax, u)_H + a^2[p(u_1 - u_0) + u_1(u, 1 + 2pax)_H$$
$$+ p(u_0 - 1) + qu_1(1 + pa)]\}\,ds$$
$$= a(t)\,\|u(t)\|_{L^1(\Omega)} + p\big(a(t)\big)^2\,\|xu(t)\|_{L^1(\Omega)} - a^0\,\|u^0(1 + pa^0x)\|_{L^1(\Omega)}$$
$$+ (p + q)\,\big(a(t) - a^0\big) + \frac{1}{2}\,pq\,\big((a(t))^2 - (a^0)^2\big) - p\int_0^t a^2\,ds.$$

Here we used that $a' = u_1a^2$ and $(a^2)' = 2u_1a^3$. In view of Lemma 1 the assertion of Theorem 4 is an immediate consequence of the equality just derived ∎

Proof of Theorem 5: Let $z = u_x$. From Theorems 2 and 3 it follows that $z \in C(\mathring{S}; H^2(\Omega)) \cap C(S; H)$, $z' \in C(S; H) \cap L^2(\mathring{S}; H^{-1}(\Omega))$, and

$$z' - z_{xx} - au_1(xz)_x = 0 \quad \text{on } \mathring{S},$$
$$z_0 = ap(u_0 - 1) \quad \text{and} \quad z_1 = -au_1(u_1 + q) \quad \text{on } \mathring{S}, \qquad z(0) = u_x^0.$$

The hypotheses of Theorem 5 imply that $z_0 \leqq 0$, $z_1 \leqq 0$, and $z(0) \leqq 0$. Therefore, using the test function z^+, we obtain (cf. (4.1))

$$0 = \frac{1}{2}\,|z^+(t)|^2 + \int_0^t \big\{|z_x^+|^2 - au_1\big((xz^+)_x, z^+\big)_H\big\}\,ds$$
$$\geqq \frac{1}{2}\,|z^+(t)|^2 + \int_0^t \left\{|z_x^+|^2 - \frac{1}{2}\,au_1\,|z^+|^2\right\} ds \geqq \frac{1}{2}\,|z^+(t)|^2 - c\int_0^t |z^+|^2\,ds.$$

In view of Gronwall's Lemma this yields $z^+ = 0$, i.e. $z = u_x \leqq 0$ ∎

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