A non linear diffusion problem arising in semiconductor process modelling with a singularity

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ABSTRACT

This paper deals with a nonlinear diffusion problem arising in semiconductor physics and having a singularity : the (two-dimensional) impurity diffusion and segregation phenomenon. We describe the technical problem, which leads to a system of nonlinear parabolic equations coupled by transmission conditions and depending on a parameter $\varepsilon > 0$. We prove uniqueness results for both the nonstationary and the related stationary problems and we study the asymptotic behaviour of the solution of the former. As a consequence, the steady solutions can be viewed as asymptotic impurity distributions. Finally, we analyze the limit case of the solution as ε approaches zero. This allows to justify the introduction of idealized models in the numerical simulation of this kind of problems.

RESUME

Ce papier est consacré à l'étude d'un problème de diffusion non linéaire intervenant en Physique des Semiconducteurs et possédant une singularité : le phénomène de diffusion et ségrégation d'impuretés dans du silicium. Nous décrivons d'abord le problème technique, qui conduit à un système d'équations paraboliques non linéaires couplées par des conditions de trnasmission et dépendant d'un paramètre $\varepsilon > 0$. Nous démontrons des résultats d'existence et d'unicité pour le problème non stationnaire et pour le problème stationnaire associé, et nous étudions le comportement asymptotique de la solution. Finalement, nous analysons le cas limite, pour lequel $\varepsilon=0$. Ceci permet de justifier l'introduction des modèles simplifiés dans la simulation numérique de ce type de problèmes.

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CONTENTS

1. - INTRODUCTION. THE PHYSICAL PROBLEM.

The two-dimensional impurity diffusion phenomenon in silicon is a relatively well-known problem. One of the main advantages of silicon in Semiconductor Process Modelling is the possibility of using the planar technology : The oxide is practically a perfect mask for impurity diffusion. Thus, localized diffusions can be made available, and the chemical potential continuity leads to an interface condition which can be written in terms of the impurity concentrations in both silicon and oxide regions (the *segregation* phenomenon). This correction provides the definition of a physical model which takes into account the doping profiles in a very realistic way (see e.g. [2,4,7]).

The aim of this paper is to present some existence and uniqueness results for this type of problems, as well as to justify rigorously the idealized model, for which no diffusion is assumed to occur in the oxide mask (see D.D. WARNER & C.L. WILSON [13]). By the way, the asymptotic behaviour of the impurity distribution is determined, and an iterative method for the numerical solution is found.

The methods combine with finite element techniques and can be adapted to the numerical simulation of most part of silicon semiconductors, such as MOS transistors, charge transfer (CCD) semiconductors, etc... (see [2,12,13]).

In all the sequel we will be concerned with the two-dimensional diffusion of one impurity in silicon, provided an "old" impurity atoms distribution has already been implanted. To extend the results to the three-dimensional case, only technical arguments are required. The geometry of an idealized structure is displayed in Fig. 1, where Ω_1 is filled by silicon and Ω_2 represents the oxide mask. Let us describe the equations that model the diffusion of a "new" impurity concentration. The transport of the impurity atoms in Ω_i (i=1,2) is given by the continuity equation

(1.1) $$\frac{\partial C_i}{\partial t} = -\nabla\cdot\vec{J}_i \ \textit{in } \Omega_i,$$

where C_i is the concentration and $\vec{J}_i$ is the density (or impurity flux). The latter is determined by diffusion and drift terms of the form (see [6]) :

(1.2) $$\vec{J}_i = -D_i\cdot\nabla C_i + z\ \mu_i C_i \vec{E}_i,$$

where D_i is the diffusion coefficient, μ_i is the mobility, $\vec{E}_i$ is the electric field, and z is the charge ($z = +1$ for donnors such as arsenic, while $z=-1$ for acceptors such as boron). In Ω_1, this gives :

(1.3) $$\vec{J}_1 = -D_1(\vec{\nabla}C_1 + \frac{qz}{kT} C_1 \nabla\psi),$$

where q is the electron charge, k is the BOLTZMANN's constant, T is the absolute temperature (300°K at 27°C) and ψ is the electrostatic potential. In Ω_2, we can further assume that $E_2 = 0$ and D_2 is a constant. Thus the continuity equation (1.2) in Ω_2 becomes linear. For physical reasons (cf. [6]), we will assume that

(i) the global charge density is zero, and
(ii) the electron and hole populations in Ω_1 are in thermodynamical equilibrium, and satisfy the BOLTZMANN's statistics.

If C_1' is an "old" impurity concentration in Ω_1, we obtain from (i) :

(1.4) $$zC_1 + zC_1' + p-n = 0,$$

where n (resp. p) is the *electron* (resp. *hole*) concentration and z' is the "old" impurity charge. Assumption (ii) gives :

(1.5) $$pn = n_i^2 \equiv \text{constant},$$

and

(1.6) $$n = n_i \cdot \exp(\frac{q\psi}{kT}).$$

Here, the constant n_i is the intrinsic carrier concentration. From (1.4)-(1.6) we obtain :

(1.7) $$\begin{cases} \psi = \dfrac{kT}{q} \cdot \text{Log}\, \dfrac{n}{n_i}, \\ \textit{where } n = \dfrac{1}{2}\{zC_1 + z'C_1' + \sqrt{(zC_1+z'C_1')^2 + 4n_i^2}\} . \end{cases}$$

We incorporate the following formulation of D_1, which was derived by S.M. HU [6] to account for the charged vacancy reaction :

(1.8) $$D_1 = D_{01} \frac{1+\beta f}{1+\beta} .$$

In (1.8), D_{01} is an intrinsic diffusion coefficient corresponding to a weak concentration ($C_i \ll n_i$), f is the ratio of the electron or hole concentration at the diffusion temperature ($f = n/n_i$ for donnors and $f = p/n_i$ for acceptors) and β is a phenomenological coefficient discussed in detail in [6]. From (1.3), (1.7) and (1.8) one has :

$$(1.9) \qquad \vec{J}_1 = -D_{01} \frac{1+\beta f}{1+\beta} \left(1+ \frac{C_1}{\sqrt{(zC_1+z'C_1')^2+4n_i^2}}\right) \vec{\nabla} C_1 .$$

Setting

$$D_1^{tot}(C_1) = D_{01} \frac{1+\beta f}{1+\beta} \left(1+ \frac{C_1}{\sqrt{(zC_1+z'C_1')^2+4n_i^2}}\right),$$

the continuity equation in silicon reads

$$(1.10) \qquad \frac{\partial C_1}{\partial t} = \vec{\nabla}\cdot(D_1^{tot}(C_1)\vec{\nabla} C_1) \ \textit{in}\ \Omega_1 .$$

At strong impurity concentration (and in particular for the arsenic) the limit of solubility in silicon can be attained. As a consequence, a "clustering" phenomenon appears (see e.g. [6]) which leads to an effective concentration N_1, given by

$$(1.11) \qquad N_1 = C_1/(1+ (\frac{C_1}{N_m})^{\alpha})^{1/\alpha},$$

where α and N_m are positive constants. The conservation law (1.10) becomes now

$$\frac{\partial C_1}{\partial t} = \nabla\cdot(D_1^{tot}(N_1)\vec{\nabla} N_1),$$

i.e.,

$$(1.12) \qquad \frac{\partial C_1}{\partial t} = \vec{\nabla}\cdot(D_1^{clust}(C_1)\vec{\nabla} C_1) \ \textit{in}\ \Omega_1,$$

where

$$(1.13) \qquad D_1^{clust}(C_1) = D_1^{tot}(N_1(C_1)) \frac{dN_1}{dC_1}(C_1).$$

On the other hand, the diffusion coefficient in the oxide mask D_2 is typically set equal to $10^{-5} \cdot D_1^{tot}(0)$. Thus, the diffusion equation in Ω_2 can be rewritten as follows

$$(1.14) \qquad \frac{\partial C_2}{\partial t} = \varepsilon \, D_2^{tot} \, \Delta C_2,$$

where ε is a small positive parameter and D_2^{tot} is a formal diffusion coefficient of the same order of magnitude than D_1^{tot} for weak impurity concentration.

We finally complete (1.10) (or (1.12)) and (1.14) with boundary and initial conditions. The impurity concentrations are held at a constant value C_o on the window Γ_1^h and on Γ_2^h (see Fig. 1). Along the side Γ_1^f the concentration is equal to zero. The outward normal component $\vec{J}_1 \cdot \vec{n}_1$ (resp. $\vec{J}_2 \cdot \vec{n}_2$) of impurity flux is required to vanish on Γ_1^ℓ (resp. Γ_2^ℓ). At the initial time t=0, we set $C_1 = C_2 = 0$; on the interface S the concentrations are required to verify (see [7]) :

$$(1.15) \qquad C_1 = mC_2$$

with m being a positive constant, and the flux continuity condition

$$(1.16) \qquad \vec{J}_1 \cdot \vec{n}_1 = -\vec{J}_2 \cdot \vec{n}_2 .$$

This model is appropriate for the numerical simulation of many technological cases arising in the configuration of integrated circuits. However, for impurities such as phosphorous, leading to multiple vacancy reactions, the model is inadequate. In simplified models, (cf. e.g. [1,6,12,13]), the concentration C_2 in the oxide mask is neglected, so that the flux across S is zero. The use of these models in the simulation of "Very Large Scale Integration" (V.L.S.I.) processes will be justified below (see Section 4).

2. - EXISTENCE AND UNIQUENESS RESULTS FOR THE NONSTATIONARY AND STATIONARY PROBLEMS.

In this Section, some existence and uniqueness results are derived for the nonlinear impurity diffusion problem described in Section 1. We will also prove the existence and uniqueness of solution for the associated stationary problem. For simplicity, only a domain as in Fig. 1 is considered, but the methods also apply for more general data (see E. CAQUOT, E. FERNANDEZ CARA & A. MARROCCO [2] for other related problems).

Let T be a positive constant. We consider the following

Problem (P_ε) *: Find a couple* (u,v) *satisfying :*

(2.1) $$\frac{\partial u}{\partial t} - \nabla\cdot(D_1(u)\nabla u) = 0 \text{ in } \Omega_1 \times (0,T),$$

(2.2) $$\frac{\partial v}{\partial t} - \varepsilon D_2\,\Delta v = 0 \text{ in } \Omega_2 \times (0,T),$$

with the boundary conditions

$(BC)_1$ $$\begin{cases} u = C_o \text{ on } \Gamma_1^h,\ u=0 \text{ on } \Gamma_1^f, \\ v = C_o \text{ on } \Gamma_2^h, \end{cases}$$

$(BC)_2$ $$\begin{cases} \dfrac{\partial u}{\partial n_1} = 0 \text{ on } \Gamma_1^\ell, \\ \dfrac{\partial v}{\partial n_2} = 0 \text{ on } \Gamma_2^\ell, \end{cases}$$

the interface (or transmission) conditions :

(IC) $$u = mv\ ,\ D_1(u)\frac{\partial u}{\partial n_1} = -\varepsilon D_2 \frac{\partial v}{\partial n_2} \text{ on } S,$$

and the initial-value conditions :

(IVC) $$u|_{t=0} = u_o \text{ in } \Omega_1,\ v|_{t=0} = v_o \text{ in } \Omega_2.$$

Here, ε is a positive parameter (which is small with respect to the other orders of magnitude arising in the problem), C_o and m are positive constant, and the functions u_o and v_o are assumed to satisfy :

(2.3) $$\begin{cases} u_o \in L^2(\Omega_1),\ v_o \in L^2(\Omega_2), \\ 0 \le u_o \le C_o \text{ a.e. in } \Omega_1,\ 0 \le v_o \le C_o \text{ a.e. in } \Omega_2. \end{cases}$$

The given constant D_2 is also positive and in all the sequel we require the function $s \to D_1(s)$ to verify :

(2.4) $$\begin{cases} s \to D_1(s) \text{ is locally Lipschitz continuous, and} \\ D_1(s) \ge \alpha > 0, \text{ with } \alpha \text{ being a constant.} \end{cases}$$

In practice $D_2 = D_1(0)$, so ε gives directly the ratio of order of magnitude of the diffusion coefficients in both media at weak impurity concentration ($\varepsilon \simeq 10^{-5}$).

We will also be concerned with the stationary problem associated to (P_ε), which reads :

Problem $(P_\varepsilon)^*$ *:* Find a couple (u,v) satisfying :

(2.6) $\nabla \cdot (D_1(u)\nabla u) = 0$ *in* Ω_1,

(2.7) $\Delta v = 0$ *in* Ω_2,

together with the boundary conditions $(BC)_1$ and $(BC)_2$ and conditions (IC) on S. ∎

For small values of ε, problem (P_ε) models satisfactorily the segregation phenomenon in Semiconductor Process Modelling. The solutions of $(P_\varepsilon)^*$ correspond to steady impurity concentrations, and it will be proved below (cf. Section 3) that they also provide the asymptotic distribution.

In the sequel, for a couple $(u,v) \in H^1(\Omega_1) \times H^1(\Omega_2)$, we denote by $U = \{u,v\}$ the function (a.e. defined in Ω) given by :

$$U = \begin{cases} u \text{ in } \Omega_1, \\ v \text{ in } \Omega_2. \end{cases}$$

In this Section, our main results are the following

Theorem 1 : For every $\varepsilon > 0$, *problem* $(P_\varepsilon)^*$ *possesses exactly one solution* $(\bar{u}_\varepsilon, \bar{v}_\varepsilon)$ *which also satisfies*

(2.8) $\{\bar{u}_\varepsilon, m\bar{v}_\varepsilon\} \in H^1(\Omega)$,

(2.9) $0 \le \{\bar{u}_\varepsilon, m\bar{v}_\varepsilon\} \le \tilde{C}_o \equiv C_o \max(1,m)$ *a.e. in* Ω.

Theorem 2 : For every $\varepsilon > 0$, *problem* (P_ε) *possesses exactly one solution* $(u_\varepsilon, v_\varepsilon)$ *which also satisfies :*

$$(2.10)\qquad \begin{cases} \{u_\varepsilon, mv_\varepsilon\} \in L^2(0,T;H^1(\Omega)) \cap L^\infty(0,T;L^2(\Omega)), \\ \{\frac{\partial u_\varepsilon}{\partial t}, m\frac{\partial v_\varepsilon}{\partial t}\} \in L^2(0,T;W'), \end{cases}$$

with W *being*

$$W = \{\Phi | \Phi = \{\phi,\psi\} \in H^1(\Omega) \ ; \ \Phi=0 \ on \ \Gamma_1^h \cup \Gamma_2^h \cup \Gamma_1^f\}$$

and where W' *designes its dual space. Furthermore, one has :*

$$(2.11)\qquad 0 \le \{u_\varepsilon(x,t), mv_\varepsilon(x,t)\} \le \tilde{C}_o \ a.e. \ in \ \Omega \ for \ all \ t.$$

Remark 2.1 : From standard regularity theory for second order elliptic problems, the solution $(\bar{u}_\varepsilon,\bar{v}_\varepsilon)$ of $(P_\varepsilon)^*$ must also satisfy :

$$\bar{u}_\varepsilon \in C^{2,\gamma}(\Omega_1) \ , \ \bar{v}_\varepsilon \in C^\infty(\Omega_2),$$

provided D_1 is (say) twice continuously differentiable. ∎

For the proofs of Theorems 1 and 2 we need some preliminary results. In the remainder of this Section, and up to the end of Section 3, the subscript ε will be omitted. Given a (small) positive parameter δ, we introduce the auxiliary function :

$$(2.12)\qquad m_\delta(x) = \begin{cases} 1 + \frac{m-1}{\delta}|x-x_c| \ \text{for} \ |x-x_c| \le \delta, \ x \in \bar{\Omega}_2, \\ m \ \text{for} \ |x-x_c| > \delta. \end{cases}$$

Obviously, $m_\delta \in H^1(\Omega_2)$ and the following properties hold as $\delta \to 0$:

$$(2.13)\qquad m_\delta \to m, \ \frac{1}{m_\delta} \to \frac{1}{m} \ \textit{weakly in} \ H^1(\Omega_2) \ \textit{and strongly in} \ L^q(\Omega_2) \quad \forall q > 1.$$

Thus, it seems quite natural to approach problems (P) and $(P)^*$ by the following :

Problem (Q_δ) *: Find a couple* (u_1,u_2) *satisfying*

$$(2.14)\qquad \frac{\partial u_1}{\partial t} - \nabla\cdot(D_1(u_1)\nabla u_1) = 0 \ in \ \Omega_1 \times (0,T),$$

$$(2.15)\qquad \frac{\partial u_2}{\partial t} - \varepsilon D_2 m_\delta(x)\nabla\cdot(\frac{1}{m_\delta(x)}\nabla u_2) = 0 \ in \ \Omega_2 \times (0,T),$$

together with the boundary conditions

$$(BC_\delta)_1 \quad \begin{cases} u_1 = C_o \text{ on } \Gamma_1^h , \; u_1 = 0 \text{ on } \Gamma_1^f, \\ u_2 = m_\delta C_o \text{ on } \Gamma_2^h \end{cases}$$

and $(BC)_2$, the interface conditions

$$(IC_\delta) \qquad u_1 = u_2, \; D_1(u_1) \frac{\partial u_1}{\partial n_1} = - \frac{\varepsilon D_2}{m_\delta} \frac{\partial u_2}{\partial n_2} \text{ on } S,$$

and the initial-value conditions

$$(IVC\ ) \qquad u_1|_{t=0} = u_o \text{ in } \Omega_1, \; u_2|_{t=0} = mv_o \text{ in } \Omega_2.$$

Problem $(Q_\delta)^*$ *: Find a couple* (u_1,u_2) *satisfying :*

$$(2.16) \quad \begin{cases} \nabla\cdot(D_1(u_1)\nabla u_1) = 0 \text{ in } \Omega_1, \\ \nabla\cdot(\frac{1}{m_\delta(x)} \nabla u_1) = 0 \text{ in } \Omega_2, \end{cases}$$

together with the boundary conditions $(BC_\delta)_1$ and $(BC)_2$ and conditions (IC_δ) on S. ∎

The solution (u_1^δ,v_1^δ) of (say) problem (Q_δ) is intended to provide an approximation (u^δ,v^δ) of the solution of (P) by means of the change

$$u^\delta = u_1^\delta, \; v^\delta = \frac{1}{m_\delta} v_1^\delta .$$

Concerning the existence and uniqueness of solution in (Q_δ) and $(Q_\delta)^*$, we have the following results :

<u>Proposition 2.1</u> : Let $\varepsilon > 0$ *and* $\delta > 0$ *be given. Then problem* $(Q_\delta)^*$ *possesses exactly one solution* $(\bar{u}_1,\bar{u}_2)$ *which also satisfies*

$$(2.17) \qquad \bar{U} = \{\bar{u}_1,\bar{u}_2\} \in H^1(\Omega) \cap C^{o,\gamma}(\bar{\Omega})$$

for a $\gamma \in (0,1)$, *and*

$$(2.18) \qquad 0 \le \bar{U} \le \tilde{C}_o \text{ a.e. in } \Omega.$$

Proposition 2.2 : Let $\varepsilon > 0$ *and* $\delta > 0$ *be given. Then problem* (Q_δ) *possesses exactly one solution* (u_1, u_2) *which also satisfies :*

$$\text{(2.19)} \qquad \begin{array}{l} \{u_1,u_2\} \in L^2(0,T;H^1(\Omega)) \cap L^\infty(0,T;L^2(\Omega)), \\ \{\frac{\partial u_1}{\partial t}, \frac{\partial u_2}{\partial t}\} \in L^2(0,T;W'). \end{array}$$

Furthermore, one has :

$$\text{(2.20)} \qquad 0 \le \{u_1,u_2\} \le \tilde{C}_o \text{ a.e. in } \Omega \text{ for all } t \in [0,T].$$

The proofs of these results are rather classical and rely on simple applications of the maximum principle for second order elliptic and parabolic equations. Thus, we only give a sketch of them (for a related result see [5]).

Sketch of the proof of Proposition 2.1 :

1st Part : Existence of solutions.

Let $U_\Gamma = \{u_{1\Gamma}, u_{2\Gamma}\}$ be a function in $H^1(\Omega)$ satisfying $(BC_\delta)_1$, and set

$$\tilde{W} = \{u_{1\Gamma}, u_{2\Gamma}\} + W.$$

Let $\tilde{D}_1(\cdot)$ be the truncated diffusion coefficient given by

$$\tilde{D}_1(s) = \begin{cases} D_1(0) \text{ if } s < 0, \\ D_1(s) \text{ if } 0 \le s \le C_o, \\ D_1(C_o) \text{ if } s > C_o. \end{cases}$$

The function $s \to \tilde{D}_1(s)$ is locally Lipschitz, satisfies (2.4) and also :

$$\tilde{D}_1(s) \le \max_{s \in [0,\tilde{C}_o]} \tilde{D}_1(s) \equiv \tilde{\beta} < +\infty.$$

As a consequence, the compactness method of J.L. LIONS [8] applies to the variational equality

$$\text{(2.21)} \qquad \begin{cases} \int_{\Omega_1} D_1(u_1)\nabla u_1 \cdot \nabla\phi + \varepsilon D_2 \int_{\Omega_2} \frac{1}{m_\delta} \nabla u_2 \cdot \nabla\psi = 0 \\ \forall \{\phi,\psi\} \in W, \ \{u_1,u_2\} \in \tilde{W}, \end{cases}$$

and shows the existence of a solution $\{\bar{u}_1,\bar{u}_2\}$. From the maximum principle (see [10]),

$$0 \leq \bar{U} = \{\bar{u}_1,\bar{u}_2\} \leq \tilde{C}_o \ \textit{in}\ \Omega,$$

whence $\tilde{D}_1(\bar{u}_1) \equiv D_1(\bar{u}_1)$ and (classically) $(\bar{u}_1,\bar{u}_2)$ is a solution of problem $(Q_\delta)^*$. ∎

Remark 2.3 : Another proof of the existence of solutions reads as follows. Let B be the closed convex set in $C^o(\bar{\Omega}_1)$:

$$B = \{\phi | \phi \in C^o(\bar{\Omega}_1)\ ;\ 0 \leq \phi \leq \tilde{C}_o \ \textit{in}\ \bar{\Omega}_1\}.$$

For $\phi \in B$, we say that (u_1,u_2) solves problem $(Q_{\delta,\phi})^*$ if it satisfies :

$$\nabla\cdot(D_1(\phi)\nabla u_1) = 0 \ \textit{in}\ \Omega_1,$$

$$\nabla\cdot(\frac{1}{m_\delta}\ \nabla u_2) = 0 \ \textit{in}\ \Omega_2,$$

together with the boundary conditions $(BC_\delta)_1$ and $(BC)_2$ and conditions (IC_δ) on S. Evidently, for each $\phi \in B$, problem $(Q_{\delta,\phi})^*$ possesses exactly one solution (u_1,u_2), furthermore satisfying

$$U = \{u_1,u_2\} \in H^1(\Omega) \cap C^{o,\gamma}(\bar{\Omega})$$

for a $\gamma = \gamma(\Omega,\alpha,C^o,\varepsilon,\delta) \in (0,1)$. Let us define the mapping $T : B \to B$ as follows :

> *For $\phi \in B$, we set $u_1 = T\phi$ if (and only if) (u_1,v_1) is the (unique) solution of $(Q_{\delta,\phi})^*$.*

Then T is a completely continuous operator from B into itself, and from Schauder's Theorem, the equation

$$(2.22) \qquad u_1 = Tu_1,\ u_1 \in B$$

possesses at least one solution $\bar{u}_1 \in B$. To conclude, remark that $\bar{u}_1$ is a solution of (2.22) if and only if there exists a function $\bar{u}_2$ such that $(\bar{u}_1,\bar{u}_2)$ solves $(Q_\delta)^*$. ∎

Remark 2.4 : The fixed-point argument above also suggests an iterative procedure for the solution of problem $(Q_\delta)^*$:

a) For n=0, choose $u_1^o \in B$.

b) Then, for given $n \geq 0$ and $u_1^n \in B$, compute

$$u_1^{n+1} = Tu_1^n .$$

This algorithm has been adapted to a finite element approximation of $(P)^*$ in [5], and the numerical results it provides are highly satisfactory. The reader is also referred to [2] for other iterative methods concerning the numerical solution of $(P)^*$ (and (P)). ∎

3rd Part : Uniqueness of solution.

We adapt an argument due to P.L. LIONS [9]. Let (u_1,u_2) and $(\bar{u}_1,\bar{u}_2)$ be two solutions of problem $(Q_\delta)^*$, and set

$$\text{(2.23)} \qquad \{\phi,\psi\} = \{\frac{u_1-\bar{u}_1}{\rho+|u_1-\bar{u}_1|} , \frac{u_2-\bar{u}_2}{\rho+|u_2-\bar{u}_2|}\} ,$$

for $\rho > 0$. Then $\{\phi,\psi\} \in W$ and

$$\nabla\phi = \rho \frac{\nabla(u_1-\bar{u}_1)}{(\rho+|u_1-\bar{u}_1|)^2} , \quad \nabla\psi = \rho \frac{\nabla(u_2-\bar{u}_2)}{(\rho+|u_2-\bar{u}_2|)^2} .$$

As a consequence, we have

$$\left\{\begin{aligned} 0 &= \int_{\Omega_1} (D_1(u_1)\nabla u_1 - D_1(\bar{u}_1)\nabla\bar{u}_1)\cdot\nabla\phi + \varepsilon D_2 \int_{\Omega_2} \frac{1}{m_\delta} \nabla(u_2-\bar{u}_2)\cdot\nabla\psi \\ &= \rho\int_{\Omega_1} D_1(u_1)\left(\frac{|\nabla(u_1-\bar{u}_1)|}{\rho+|u_1-\bar{u}_1|}\right)^2 + \rho\int_{\Omega_1} (D_1(u_1)-D_1(\bar{u}_1)) \frac{\nabla\bar{u}_1\cdot\nabla(u_1-\bar{u}_1)}{(\rho+|u_1-\bar{u}_1|)^2} \\ &+ \rho\varepsilon D_2 \int_{\Omega_2} \frac{1}{m_\delta} \left(\frac{|\nabla(u_2-\bar{u}_2)|}{\rho+|u_2-\bar{u}_2|}\right)^2 \\ &\geq \alpha\rho \int_{\Omega_1} \left(\frac{|\nabla(u_1-\bar{u}_1)|}{\rho+|u_1-\bar{u}_1|}\right)^2 - C_1\rho \int_{\Omega_1} \frac{|\nabla u_1|\cdot|\nabla(u_1-\bar{u}_1)|}{\rho+|u_1-\bar{u}_1|} , \end{aligned}\right.$$

where C_1 depends on $D_1(\cdot)$, m and C_o, but is independent from ρ.

Thus, for a new constant $C_2 > 0$, one obtains the estimate

$$(2.24) \qquad \int_{\Omega_1} \left(\frac{|\nabla(u_1-\bar{u}_1)}{\rho+|u_1-\bar{u}_1|}\right)^2 \leq C_2,$$

and this uniformly in ρ. Notice that (2.24) also reads

$$\int_{\Omega_1} |\nabla(\log \frac{\rho+W}{\rho})|^2 \leq C_2,$$

where $W = |u_1-\bar{u}_1|$. Since the $H^1(\Omega_1)$ function

$$h_\rho = \log \frac{\rho+W}{\rho}$$

vanishes on Γ_1^h, there exists a constant C_3 such that

$$\int_{\Omega_1} |h_\rho|^2 \leq C_3 \quad \forall\, \rho > 0.$$

From Fatou's Lemma we deduce that the function (a.e. defined in Ω_1)

$$\chi(x) = \overline{\lim_{\rho\to 0}}\, |h_\rho(x)|^2$$

belongs to $L^1(\Omega_1)$. But this is only possible if $W=0$ a.e., that is to say :

$$u_1 = \bar{u}_1 \textit{ a.e. in } \Omega_1.$$

From the identity

$$\int_{\Omega_1} (D_1(\bar{u}_1)\nabla u_1 - D_1(\bar{u}_1)\nabla\bar{u}_1)\cdot\nabla\phi + \varepsilon\rho\mathcal{D}_2\int_{\Omega_2} \left(\frac{|\nabla(u_2-\bar{u}_2)|}{\rho+|u_2-\bar{u}_2|}\right)^2 = 0,$$

one also has $u_2 = \bar{u}_2$. ∎

<u>Sketch of the proof of Proposition 2.2</u> :

<u>1st Part</u> : <u>Existence of solutions.</u>

We argue as previously. Notice that the compactness method in [8] applies again in the case of the time-dependent variational equality

$$(2.25)\quad \begin{cases} \displaystyle\int_{\Omega_1} \frac{du_1}{dt}\cdot\phi + \int_{\Omega_2} \frac{1}{m\delta}\frac{du_2}{dt}\cdot\psi + \int_{\Omega_1} \tilde{D}_1(u_1(t))\nabla u_1(t)\cdot\nabla\phi \\ \displaystyle\qquad + \varepsilon\int_{\Omega_2} \frac{1}{m_\delta}\nabla u_2(t)\cdot\nabla\psi = 0 \quad \forall\ \{\phi,\psi\}\in W, \\ \{u_1,u_2\}\in L^2(0,T;H^1(\Omega)),\ \frac{d}{dt}\{u_1,u_2\}\in L^2(0,T;W'), \\ \{u_1(t),u_2(t)\}\in\tilde{W}\ ,\quad u_1|_{t=0} = u_o,\ u_2|_{t=0} = mv_o. \end{cases}$$

From the maximum principle, we also have

$$0 \le U(t) \le \tilde{C}_o \ \textit{a.e. in}\ \Omega\ ,\ t\in(0,T),$$

for a solution $U = \{u_1,u_2\}$ of (2.25). Thus, $\tilde{D}_1(u_1) = D_1(u_1)$ and (u_1,u_2) is a solution of (Q_δ). ∎

Remark 2.5 : Although a fixed-point formulation of (Q_δ) does not lead (at least easily) to any existence result, we can introduce as in Remark 2.4 an iterative method of solution :

a) For n=0, choose $u_1^o \in \mathcal{B}$, with

$$\mathcal{B} = \{\phi \,|\, \phi\in L^\infty(\Omega_1\times(0,T))\ ;\ 0\le\phi\le\tilde{C}_o\ \textit{a.e.}\}\ .$$

b) Then, for given $n \ge 0$ and $u_1^n \in \mathcal{B}$, compute the solution $U = \{u_1,u_2\}$ of

$$\begin{cases} \dfrac{\partial u_1}{\partial t} - \nabla\cdot(D_1(u_1^n)\nabla u_1) = 0 \ \textit{in}\ \Omega_1\times(0,T), \\ \dfrac{\partial u_2}{\partial t} - \varepsilon D_2\, m_\delta(x)\nabla\cdot\left(\dfrac{1}{m_\delta(x)}\nabla u_2\right) = 0 \ \textit{in}\ \Omega_2\times(0,T), \end{cases}$$

together with the boundary conditions $(BC_\delta)_1$ and $(BC)_2$, conditions (IC_δ) on S and the initial-value conditions (IVC_δ) ; next take $u_1^{n+1} = u_1$. ∎

2nd Part : Uniqueness of solution.

Let (u_1,u_2) and $(\hat{u}_1,\hat{u}_2)$ be two solutions of (Q_δ), and set

$$(2.26)\qquad \{\phi(t),\psi(t)\} = \left\{ \frac{u_1(t)-\hat{u}_1(t)}{\rho+|u_1(t)-\hat{u}_1(t)|}\ ,\ \frac{u_2(t)-\hat{u}_2(t)}{\rho+|u_2(t)-\hat{u}_2(t)|} \right\}$$

for t a.e. in $[0,T]$ and $\rho > 0$. Then $\{\phi(t),\psi(t)\} \in W$, while

$$\left\{\begin{aligned} R(t) &\equiv \int_{\Omega_1} \{\frac{d}{dt}(u_1(t)-\hat{u}_1(t))\cdot\phi(t)+(D_1(u_1(t))\nabla u_1(t)-D_1(\hat{u}_1(t))\nabla\hat{u}_1(t))\cdot\nabla\phi(t)\} \\ &= -\int_{\Omega_2} \frac{1}{m_\delta(x)}\{\frac{d}{dt}(u_2(t)-\hat{u}_2(t))\cdot\psi(t) + \varepsilon D_1\rho(\frac{|\nabla(u_2(t)-\hat{u}_2(t))|}{\rho+|u_2(t)-\hat{u}_2(t)|})^2\} \end{aligned}\right.$$

Notice that

$$\left\{\begin{aligned} &\int_{\Omega_i} \frac{d}{dt}(u_i(t)-\hat{u}_i(t))\,\frac{u_i(t)-\hat{u}_i(t)}{\rho+|u_i(t)-\hat{u}_i(t)|} \\ &\qquad = \int_{\Omega_i} \frac{d}{dt}\{|u_i(t)-\hat{u}_i(t)| - \rho\log\frac{\rho+|u_i(t)-\hat{u}_i(t)|}{\rho}\} \end{aligned}\right.$$

for $i=1,2$. Thus, for $q = |u_2-\hat{u}_2|$, one has :

$$\int_0^t R(s)ds \le -\int_{\Omega_2} \{q(t) - \rho\cdot\log\frac{\rho+q(t)}{\rho}\} \le 0,$$

and the following inequalities hold for all $t \in [0,T]$:

$$\left\{\begin{aligned} 0 \ge &\int_0^t \{\int_{\Omega_1} ((D_1(u_1)-D_1(\hat{u}_1))\nabla\hat{u}_1 + D_1(u_1)\nabla(u_1-\hat{u}_1))\cdot\nabla\phi\}\,ds \\ &\quad + \int_{\Omega_1} \{|u_1(t)-u_1(t)| - \rho\cdot\log\frac{\rho+|u_1(t)-\hat{u}_1(t)|}{\rho}\} \\ \ge &\int_0^t \{\rho\int_{\Omega_1} (\frac{|\nabla(u_1-\hat{u}_1)|}{\rho+|u_1-\hat{u}_1|})^2 - C_2\rho\}\,ds, \end{aligned}\right.$$

where C_2 can be chosen as in the proof of Proposition 2.1.

As a consequence, there exists $C_3 > 0$ such that

$$\int_0^t \{\int_{\Omega_1} (\log\frac{\rho+|u_1-\hat{u}_1|}{\rho})^2\}dx \le C_3 \quad \forall\ \rho > 0.$$

From Fatou's Lemma we deduce that

$$u_1(x,t) = \hat{u}_1(x,t) \ \textit{a.e. in}\ \Omega_1 \times (0,T).$$

But u_1 and $\hat{u}_1$ can be viewed as continuous functions from [0,T] into $L^2(\Omega_1)$. Thus, $u_1 = \hat{u}_1$. From the identity

$$\int_{\Omega_2} \frac{d}{dt}(u_2-\hat{u}_2)\frac{u_2-\hat{u}_2}{\rho+|u_2-\hat{u}_2|} + \varepsilon\rho D_2 \int_{\Omega_2} \left(\frac{|\nabla(u_2-\hat{u}_2)|}{\rho+|u_2-\hat{u}_2|}\right)^2 = 0,$$

we finally obtain $u_2 = \hat{u}_2$. ■

For the proof of Theorems 1 and 2, we also prepare the following

Lemma 2.1 : *There exists some functions* $U_\delta^\Gamma = \{u_{1\delta}^\Gamma, u_{2\delta}^\Gamma\}$ *with the following properties :*

(2.27) $\qquad U_\delta^\Gamma \in H^1(\Omega) \quad \forall\ \delta > 0,$

(2.28)
$$\begin{cases} u_{1\delta}^\Gamma = C_o \text{ on } \Gamma_1^h, \quad u_{1\delta}^\Gamma = 0 \text{ on } \Gamma_1^f, \\ u_{2\delta}^\Gamma = m_\delta C_o \text{ on } \Gamma_2^h, \\ u_{1\delta}^\Gamma = u_{2\delta}^\Gamma \text{ on } S, \end{cases}$$

(2.29) $\qquad U_\delta^\Gamma$ *is uniformly bounded in* $H^1(\Omega)$ *(independently from* δ*)*

Proof : Let $\delta > 0$ be given, and define g_δ on $\partial\Omega_2$ as follows (cf. Fig. 1) :

$$g_\delta(x) = \begin{cases} 1+\frac{m-1}{\delta}|x-x_c| \text{ for } x \in \Gamma_2^h, \ |x-x_c| \le \delta, \\ m \text{ for } x \in \Gamma_2^h, \ |x-x_c| > \delta, \\ 1+\frac{m-1}{|x_N-x_C|}|x-x_D| \text{ for } x \in \Gamma_2^\ell, \\ 1 \text{ for } x \in S. \end{cases}$$

Obviously, g_δ $W^{1,1}(\partial\Omega_2)$ for every $\delta > 0$ and there exists a constant $C_4 > 0$, only depending on Ω_2 and m, such that

(2.30) $$\|g_\delta\|_{W^{1,1}(\partial\Omega_2)} \le C_4.$$

Thus, g_δ is also uniformly bounded in $H^{1/2}(\partial\Omega_2)$.

For each $\delta > 0$, let $u^{\Gamma}_{2\delta}$ be the solution of the Dirichlet problem

(2.31) $$\begin{cases} -\Delta v = 0 \textit{ in } \Omega_2, \\ v = g_\delta \textit{ on } \partial\Omega_2, \end{cases}$$

and set $u^{\Gamma}_{1\delta} \equiv C_o$. Then it is readily seen that (2.27)-(2.29) hold. ∎

Proof of Theorem 1

Step 1 : "A priori" estimates.

For each $\delta > 0$, let $(u^{\delta}_1, u^{\delta}_2)$ be the solution of problem $(Q_\delta)^*$, and set

$$u^{\delta}_1 = u^{\Gamma}_{1\delta} + z_\delta, \quad u^{\delta}_2 = u^{\Gamma}_{2\delta} + y_\delta,$$

with $\{u^{\Gamma}_{1\delta}, u^{\Gamma}_{2\delta}\}$ as in Lemma 2.1. Then one has :

$$\begin{cases} \int_{\Omega_1} D_1(u^{\delta}_1)|\nabla z_\delta|^2 + \varepsilon D_2 \int_{\Omega_2} \frac{1}{m_\delta} |\nabla y_\delta|^2 \\ \qquad = - \int_{\Omega_1} D_1(u^{\delta}_1)\nabla u^{\Gamma}_{1\delta}\cdot\nabla z_\delta - \varepsilon D_2 \int_{\Omega_2} \frac{1}{m_\delta} \nabla u^{\Gamma}_{2\delta}\cdot\nabla y \end{cases}$$

Since $\{u^{\Gamma}_{1\delta}, u^{\Gamma}_{2\delta}\}$ is uniformly bounded in $H^1(\Omega)$, there exists a constant $C_5 > 0$ depending on $\Omega, m, D_1(\cdot)$, C_o, ε and D_2, but independent from δ such that

(2.32) $$\|\{u^{\delta}_1, u^{\delta}_2\}\|_{H^1} \le C_5 \quad \forall\, \delta > 0. ∎$$

Step 2 : Extraction of a subsequence

From (2.32), there exist $u^*_1 \in H^1(\Omega_1)$ and $u^*_2 \in H^1(\Omega_2)$ such that, at least for a subsequence again indexed by δ,

(2.33a) $$u^{\delta}_1 \to u^*_1 \textit{ weakly in } H^1(\Omega_1),$$

(2.33b) $$u^{\delta}_2 \to u^*_2 \textit{ weakly in } H^1(\Omega_2).$$

It is clear that the functions

$$u^* = u^*_1, \quad v^* = \frac{1}{m} u^*_2,$$

satisfy :

$$\int_{\Omega_1} D_1(u^*)\nabla u^*\cdot\nabla\phi + \varepsilon D_2 \int_{\Omega_2} \nabla v^*\cdot\nabla\psi = 0 \quad \forall\ \{\phi,\psi\}\in W.$$

On the other hand, $u^* = C_o$ on Γ_1^h and $u^* = 0$ on Γ_1^f. Taking limits as $\delta \to 0$ in the identities

$$\begin{cases} u_2^\delta = m_\delta C_o \ \ on\ \Gamma_2^h, \\ u_1^\delta = u_2^\delta \ \ on\ S, \end{cases}$$

we also obtain :

$$\begin{cases} v^* = C_o \ \ on\ \Gamma_2^h, \\ u^* = mv^* \ \ on\ S. \end{cases}$$

This proves that (u^*,v^*) is a solution of $(P)^*$.

Step 3 : Uniqueness of solution.

We argue as in the proof of Proposition 2.1, choosing as test functions

$$\{\phi,\psi\} = \left\{ \frac{u_1-\bar{u}_1}{\rho+|u_1-\bar{u}_1|}, \frac{m(u_2-\bar{u}_2)}{\rho+|u_2-\bar{u}_2|} \right\}$$

for $\rho > 0$. This yields again uniform estimates for the norm in $L^2(\Omega_1)$ of the functions

$$\log \frac{\rho+|u_1-\bar{u}_1|}{\rho}, \quad \rho > 0,$$

which, together with Fatou's Lemma, imply

$$u_1 = \bar{u}_1 \ \ a.e.\ in\ \Omega_1.$$

From the identity

$$\int_{\Omega_1} (D_1(u_1)\nabla u_1 - D(\bar{u}_1)\nabla\bar{u}_1)\cdot\nabla\phi + \varepsilon\rho D_2 m \int_{\Omega_2} \left(\frac{|\nabla(u_2-u_2)|^2}{\rho+|u_2-u_2|}\right) = 0$$

we also have $u_2 = \bar{u}_2$. ■

Proof of Theorem 2 : It is analogous to the proof of Theorem 1. Only the "a priori" estimates are derived in a essentially different manner, and they read as follows. From the identity

$$\begin{cases} \int_{\Omega_1} \frac{dz_\delta}{dt} \cdot z_\delta + \int_{\Omega_1} D_1(u_1^\delta)|\nabla z_\delta|^2 + \int_{\Omega_2} \frac{1}{m_\delta}\frac{dy_\delta}{dt} \cdot y_\delta + \varepsilon D_2 \int_{\Omega_2} \frac{1}{m_\delta} \ |\nabla y_\delta| \\ \quad = -\int_{\Omega_1} D_1(u_1^\delta)\nabla u_{1\delta} \cdot \nabla z_\delta - \varepsilon D_2 \int_{\Omega_2} \frac{1}{m_\delta} \nabla u_{2\delta}^\Gamma \cdot \nabla y_\delta \end{cases}$$

we deduce :

$$\int_{\Omega_1} |z_\delta(t)|^2 + \int_{\Omega_2} |y_\delta(t)|^2 + \int_0^t \int_{\Omega_1} |\nabla z_\delta(s)|^2 \, ds + \int_0^t \int_{\Omega_2} |\nabla y_\delta(s)|^2 ds \leq C_6,$$

where the positive constant C_6 depends on $\Omega, m, D_1(\cdot)$, C_o, ε, D_2 and T, but is independent from δ. Thus, $\{u_1^\delta, u_2^\delta\}$ is uniformly bounded in $L^2(0,T;H^1(\Omega)) \cap L^\infty(\Omega\times(0,T))$. Now it is easy to prove that $\{u_1^\delta, u_2^\delta\}$ is also uniformly bounded in $L^2(0,T;W')$. ∎

3. - THE ASYMPTOTIC BEHAVIOUR OF THE NONSTATIONARY SOLUTION.

The aim of this Section is to prove the convergence of the nonstationary solution of problem (P) to the solution of $(P)^*$ as $t \uparrow +\infty$. It will be shown (Lemma 3.2) that this convergence is monotonic in $L^2(\Omega)$, so we can write

$$\{\bar{u}, \bar{v}\} = \sup_{t \in [0,+\infty)} \{u(t), v(t)\},$$

for the solution $(\bar{u}, \bar{v})$ of problem (P) .

We start with some preliminary results.

Lemma 3.1 : Let $U = \{u,v\}$ *, with* (u,v) *being the solution of problem* (P). *Assume that* $u_o \leq \bar{u}$ *and* $v_o \leq \bar{v}$ *a.e., where* $(\bar{u},\bar{v})$ *is the solution of* $(P)^*$. *Then* $U = \{u,v\}$ *is defined for all* $t \in [0,+\infty)$, *and*

(3.1) $$U(t) = \{u(t), v(t)\} \leq \{\bar{u}, \bar{v}\} \qquad \forall t \geq 0,$$

for the natural partial ordering in $L^2(\Omega)$.

Proof : Clearly, only (3.1) has to be proved. Let us put

$$u(t) = \bar{u} + z(t),\ v(t) = \bar{v} + y(t),$$

and choose

$$\{\phi(t),\psi(t)\} = \{\frac{z^+(t)}{\rho+z^+(t)}, \frac{my^+(t)}{\rho+y^+(t)}\},\quad \rho > 0.$$

Evidently, $\{\phi(t),\psi(t)\} \in W$ and a simple computation leads to

$$\begin{cases} \int_{\Omega_1} \frac{d}{dt}[z^+(t) - \rho \operatorname{Log} \frac{\rho+z^+(t)}{\rho}] + m\int_{\Omega_2} \frac{d}{dt}[y^+(t) - \rho \operatorname{Log} \frac{\rho+y^+(t)}{\rho}] \\ \quad + \frac{\alpha\rho}{2}\int_{\Omega_1} (\frac{|\nabla z^+(t)|}{\rho+z^+(t)})^2 + \varepsilon D_2\rho m\int_{\Omega_2} (\frac{|\nabla y^+(t)|}{\rho+y^+(t)})^2 \\ \quad \leq C_7\rho \int_{\Omega_1} |\nabla u(t)|^2, \end{cases}$$

for a constant C_7 only depending on $D_1(\cdot)$. Thus, integrating in time,

$$\int_0^t \{\frac{\alpha}{2}\int_{\Omega_1} (\operatorname{Log} \frac{\rho+z^+(s)}{\rho})^2 + \varepsilon D_2 m \int_{\Omega_2} (\operatorname{Log} \frac{\rho+y^+(s)}{\rho})^2\}ds \leq C_8 \int_0^t \{\int_{\Omega_1} |\nabla u(s)|^2\}ds \quad ,$$

where C_8 only depends on $D_1(\cdot)$ and the domain Ω. We conclude as in the proof of Proposition 2.2 that

$$z^+(t) = 0,\ y^+(t) = 0,$$

and the Lemma holds. ■

For the sake of simplicity, in the remainder of this Section it will be assumed that the initial data vanish :

$$u_o = 0 \textit{ in } \Omega_1,\ v_o = 0 \textit{ in } \Omega_2.$$

Lemma 3.2 : *The function*

$$t \to U(t) = \{u(t),v(t)\},$$

where (u,v) *is the solution of* (P), *is nondecreasing for the standard partial ordering in* $L^2(\Omega)$.

Proof : It is analogous to the proof of Lemma 3.1. It suffices to set (for arbitrary h > 0)

$$z(t) = u(t+h)-u(t), \quad y(t) = v(t+h)-v(t)$$

for t a.e. in $[0,+\infty)$, and to choose the test functions in W as follows :

$$\{\phi(t),\psi(t)\} = \{\frac{z^-(t)}{\rho+z^-(t)} \ , \ \frac{my^-(t)}{\rho+y^-(t)}\} . \blacksquare$$

From these two Lemmas we derive the main result in this Section :

Theorem 3 : Let $U = \{u,v\}$ *(resp.* $\bar{U} = \{\bar{u},\bar{v}\}$*) with* $(\bar{u},\bar{v})$ *being the solution of problem* (P) *(resp.* $(\bar{u},\bar{v})$ *is the solution of* $(P)^*$*). Then one has*

$$U(t) \uparrow \bar{U} \text{ in } L^2(\Omega) \text{ as } t \uparrow +\infty .$$

Proof : From Lemmas 3.1 and 3.2 and Lebesgue's Monotonic Convergence Theorem, a function $\tilde{U} = \{\tilde{u},\tilde{v}\} \in L^2(\Omega)$ exists with the following properties :

$$u(t) \uparrow \tilde{u} \text{ in } L^2(\Omega_1) \text{ and } v(t) \uparrow \tilde{v} \text{ in } L^2(\Omega_2) \text{ as } t \uparrow +\infty .$$

Evidently, $\tilde{U} \le \{\bar{u},\bar{v}\}$. Thus, we only have to prove that there exists a sequence $\{t_n\}_{n\ge 0}$ with $t_n \uparrow +\infty$, such that

(3.2) $\qquad u(t_n) \to \bar{u} \ , \ v(t_n) \to \bar{v}$ a.e.

Let us consider the following test functions

$$\phi_\rho(t) = \frac{\bar{u}-u(t)}{\rho+(\bar{u}-u(t))} \ , \ \psi_\rho = \frac{m(\bar{v}-v(t))}{\rho+(\bar{v}-v(t))} .$$

As in the proofs of Lemmas 3.1 and 3.2, one has :

$$\{\phi_\rho(t),\psi_\rho(t)\} \in W, \text{ for } t \text{ a.e. in } [0,+\infty), \ \rho > 0.$$

Hence,

$$\left\{\begin{aligned}&\int_{\Omega_1}\frac{d}{dt}(\bar{u}-u)\phi_\rho+\int_{\Omega_2}\frac{d}{dt}(\bar{v}-v)\psi_\rho\\&+\int_{\Omega_1}(D_1(\bar{u})\nabla\bar{u}-D_1(u)\nabla u)\cdot\nabla\phi_\rho+\varepsilon D_2\int_{\Omega_2}\nabla(\bar{v}-v)\cdot\nabla\psi_\rho=0,\end{aligned}\right.$$

and we obtain :

$$\left\{\begin{aligned}&\int_{\Omega_1}\frac{d}{dt}[(\bar{u}-u)-\rho\,\mathrm{Log}\,\frac{\rho+(\bar{u}-u)}{\rho}]+m\int_{\Omega_2}\frac{d}{dt}[(\bar{v}-v)-\rho\,\mathrm{Log}\,\frac{\rho+(\bar{v}-v)}{\rho}]\\&+\rho\int_{\Omega_1}D_1(\bar{u})\left(\frac{|\nabla(\bar{u}-u)|}{\rho+(\bar{u}-u)}\right)^2+\varepsilon D_2\rho m\int_{\Omega_2}\left(\frac{|\nabla(\bar{v}-v)|}{\rho+(\bar{v}-v)}\right)^2\\&+\rho\int_{\Omega_1}(D_1(u)-D_1(\bar{u}))\frac{\nabla u\cdot\nabla(\bar{u}-u)}{(\rho+(\bar{u}-u))^2}=0.\end{aligned}\right.$$

An integration in the variable t, and the same type of estimates that were used in the proof of Lemma 3.1 lead to the following inequalities :

$$\left\{\begin{aligned}&\int_{\Omega_1}[(\bar{u}-u(t))-\rho\,\mathrm{Log}\,\frac{\rho+(\bar{u}-u(t))}{\rho}]+m\int_{\Omega_2}[(\bar{v}-v(t))-\rho\,\mathrm{Log}\,\frac{\rho+(\bar{v}-v(t))}{\rho}]\\&+\int_0^t\{\frac{\alpha\rho}{2}\int_{\Omega_1}\left(\frac{|\nabla(\bar{u}-u(s))|}{\rho+(\bar{u}-u(s))}\right)^2+\varepsilon D_2\rho m\int_{\Omega_2}\left(\frac{|\nabla(\bar{v}-v(s))|}{\rho+(\bar{v}-v(s))}\right)^2\}\,ds\\&\le\rho t+\int_{\Omega_1}[(\bar{u}-u_o)-\rho\,\mathrm{Log}\,\frac{\rho+(\bar{u}-u_o)}{\rho}]+m\int_{\Omega_2}[(\bar{v}-v_o)-\rho\,\mathrm{Log}\,\frac{\rho+(\bar{v}-v_o)}{\rho}],\end{aligned}\right.$$

where C_9 is independent from ρ and t. Now Poincaré-Fiedrichs' inequality yields :

$$(3.4)\qquad\int_0^t\{\int_{\Omega_1}\left(\mathrm{Log}\,\frac{\rho+(\bar{u}-u(s))}{\rho}\right)^2+\int_{\Omega_2}\left(\mathrm{Log}\,\frac{\rho+(\bar{v}-v(s))}{\rho}\right)^2\}\,ds\le C_{10}(1+\rho t)$$

for a new constant C_{10}.

We require the following Lemma, whose proof is given at the end of this Section.

Lemma 3.3 : With the previous notation, the function

$$t \to \{\text{Log}\,\frac{t^{-1}+(\bar{u}-u(t))}{t^{-1}}\ ,\ \text{Log}\,\frac{t^{-1}+(\bar{v}-v(t))}{t^{-1}}\ \}$$

is continuous from $[0,+\infty)$ *into* $L^2(\Omega)$. ∎

Let us set $\rho = t^{-1}$ in (3.4) and let t increase to $+\infty$. From Lemma 3.3 and the Mean Value Theorem, we deduce the existence of some $t_n > 0$ satisfying $t_n \uparrow +\infty$ and

$$\int_{\Omega_1} (\text{Log}\,\frac{t_n^{-1}+(\bar{u}-u(t_n))}{t_n^{-1}})^2 + \int_{\Omega_2} (\text{Log}\,\frac{t_n^{-1}+(\bar{v}-v(t_n))}{t_n^{-1}})^2 \le 2C_{10}.$$

As in the proof of Theorem 1, Fatou's Lemma applies, and (3.3) holds. ∎

<u>Proof of Lemma 3.3</u> : For instance, let us prove that the function

$$t \to W(t) \equiv \text{Log}\,\frac{t^{-1}+(\bar{u}-u(t))}{t^{-1}}$$

satisfies

$$W \in L^2(0,T;H^1(\Omega_1)),\quad \frac{\partial W}{\partial t} \in L^2(0,T;H^1(\Omega_1)')$$

for all $T > 0$. But this is a trivial consequence of (2.8),(2.10) (see Section 2), and the fact that $(\bar{u},\bar{v})$ is the solution of problem $(P)^*$. ∎

4. - <u>THE LIMIT ANALYSIS AS</u> $\varepsilon \downarrow 0$.

This Section is concerned with the behaviour of the solutions $U_\varepsilon = \{u_\varepsilon, v_\varepsilon\}$ of problems (P_ε) as ε approaches zero. It will be proved that u_ε converges (in an appropriate sense) towards the solution of a limit problem (corresponding to an idealized model in Semiconductor Process Modelling) which reads :

Problem $(\hat{P})$ *: Find a function* $\hat{u}$ *satisfying :*

(4.1) $$\frac{\partial \hat{u}}{\partial t} - \nabla\cdot(D_1(\hat{u})\nabla\hat{u}) = 0 \text{ in } \Omega_1 \times (0,T),$$

together with the boundary conditions

(BC)$_3$ $$\begin{cases} \hat{u} = C_o \text{ on } \Gamma_1^h,\ \hat{u} = 0 \text{ on } \Gamma_1^f, \\ \dfrac{\partial \hat{u}}{\partial n_1} = 0 \text{ on } \Gamma_1^\ell \cup S, \end{cases}$$

and the initial-value condition

$$\hat{u}|_{t=0} = u_o \textit{ in } \Omega_1. \blacksquare$$

Obviously, problem $(\hat{P})$ possesses exactly one solution $\hat{u}$ furthermore satisfying

$$\begin{cases} \hat{u} \in L^2(0,T;H^1(\Omega_1)) \cap L^\infty(0,T;L^2(\Omega_1)), \\ \dfrac{\partial \hat{u}}{\partial t} \in L^2(0,T;V'), \end{cases}$$

where V is given by :

$$V = \{\phi | \phi \in H^1(\Omega_1) \ ; \ \phi = 0 \textit{ on } \Gamma_1^h \cup \Gamma_1^f\}$$

Theorem 4 : For each $\varepsilon > 0$, *let* $U_\varepsilon = \{u_\varepsilon, v_\varepsilon\}$ *be the solution of problem* (P_ε). *Then one has :*

$$(4.2) \quad \begin{cases} u_\varepsilon \to \hat{u} \textit{ weakly in } L^2(0,T;H^1(\Omega_1)) \cap L^\infty(0,T;L^2(\Omega_1)) \\ u_\varepsilon \to \hat{u} \textit{ strongly in } L^2(\Omega_1 \times (0,T)) \textit{ and a.e.,} \\ \dfrac{\partial u_\varepsilon}{\partial t} \to \dfrac{\partial \hat{u}}{\partial t} \textit{ weakly in } L^2(0,T;V'), \end{cases}$$

where $\hat{u}$ *is the (unique) solution of* $(\hat{P})$.

Proof :

Step 1 : "A priori" estimates.

Let us put

$$u_\varepsilon = u_\Gamma + z_\varepsilon, \ v_\varepsilon = v_\Gamma + y_\varepsilon \ ,$$

with $\{u_\Gamma, v_\Gamma\}$ being a function in $L^2(\Omega)$ satisfying :

$$\begin{cases} \{u_\Gamma, mv_\Gamma\} \in H^1(\Omega), \\ u_\Gamma = u_\varepsilon \textit{ on } \Gamma_1^h \cup \Gamma_1^f \ , \\ v_\Gamma = v_\varepsilon \textit{ on } \Gamma_2^h \ . \end{cases}$$

Then one has

$$\left\{\begin{aligned} &\int_{\Omega_1} \frac{dz_\varepsilon}{dt} \cdot z_\varepsilon + m\int_{\Omega_2} \frac{dy_\varepsilon}{dt} \cdot y_\varepsilon + \int_{\Omega_1} D_1(u_\varepsilon)|\nabla z_\varepsilon|^2 + \varepsilon D_2 m\int_{\Omega_2} |\nabla y_\varepsilon|^2 \\ &\qquad = -\int_{\Omega_1} D_1(u_\varepsilon)\nabla u_\Gamma \cdot \nabla z_\varepsilon - \varepsilon D_2 m\int_{\Omega_2} \nabla v_\Gamma \cdot \nabla y_\varepsilon \\ &\qquad \leq C_{11} + \frac{\alpha}{2}\int_{\Omega_1} |\nabla z_\varepsilon|^2 + \frac{\varepsilon D_2 m}{2}\int_{\Omega_2} |\nabla y_\varepsilon|^2 , \end{aligned}\right.$$

with C_{11} being a positive constant not depending on ε. Hence,

$$\int_{\Omega_1} |z_\varepsilon(t)|^2 + m\int_{\Omega_2} |y_\varepsilon(t)|^2 + \int_0^t \{\int_{\Omega_1} |\nabla z_\varepsilon(s)|^2 + \varepsilon\int_{\Omega_2} |\nabla y_\varepsilon(s)|^2\} \leq C_{12}$$

for a new $C_{12} > 0$, so that :

(4.3a) u_ε *is uniformly bounded in* $L^2(0,T;H^1(\Omega_1)) \cap L^\infty(\Omega_1 \times (0,T))$,

(4.3b) v_ε *is uniformly bounded in* $L^\infty(\Omega_2 \times (0,T))$,

(4.3c) $\sqrt{\varepsilon}\, v_\varepsilon$ *is uniformly bounded in* $L^2(0,T;H^1(\Omega_2))$. ∎

Step 2 : Extraction of a subsequence

Notice that for a function $\psi \in \mathcal{D}(\overline{\Omega}_2)$ whose trace vanishes on $\Gamma_2^h \cup S$, we have :

(4.4) $$\int_{\Omega_2} \frac{dv_\varepsilon}{dt} \cdot \psi + \varepsilon D_2 \int_{\Omega_2} \nabla v_\varepsilon \cdot \nabla \psi = 0.$$

From (4.3a)-(4.3c) and (4.4), it is readily seen that

(4.3d) $$\left\{\begin{aligned} &\frac{\partial U_\varepsilon}{\partial t} \textit{ is uniformly bounded in } L^2(0,T;W'), \\ &\frac{\partial v_\varepsilon}{\partial t} \to 0 \textit{ in (say) } \mathcal{D}'(\Omega_2 \times (0,T)) . \end{aligned}\right.$$

Thus, a subsequence $\{u_\mu, v_\mu\}$ exists with the following properties :

$$(4.5)\qquad \begin{cases} u_\mu \to u^* \textit{ weakly in } L^2(0,T;H^1(\Omega_1)) \cap L^\infty(\Omega_1 \times (0,T)), \\ u_\mu \to u^* \textit{ strongly in } L^2(\Omega_1 \times (0,T)) \textit{ and a.e.}, \\ \frac{\partial u_\mu}{\partial t} \to \frac{\partial u^*}{\partial t} \textit{ weakly in } L^2(0,T;V'), \end{cases}$$

and the proof of Theorem 4 will be achieved if we demonstrate that u^* solves problem $(\hat{P})$. ∎

Step 3 : Conclusion

Let ϕ be an arbitrary function in V, and choose ψ such that

$$\{\phi,\psi\} \in W.$$

Then one has :

$$0 = \int_{t_1}^{t_2} \{\int_{\Omega_1} \frac{du_\mu}{dt}\cdot\phi + \int_{\Omega_2} \frac{dv_\mu}{dt}\cdot\psi + \int_{\Omega_1} D_1(u_\mu)\nabla u_\mu\cdot\nabla\phi + \mu D_2 \int_{\Omega_2} \nabla v_\mu\cdot\nabla\psi\}\, ds$$

for all t_1, t_2 satisfying

$$(4.6)\qquad 0 \le t_1 \le t_2 \le T.$$

Using (4.3c) and (4.5) and letting μ decrease to zero, one is led to the following :

$$(4.7)\qquad \int_{t_1}^{t_2} \{\int_{\Omega_1} \frac{du^*}{dt}\cdot\phi + \int_{\Omega_1} D_1(u^*)\nabla u^*\cdot\nabla\phi\} = 0.$$

Since (4.7) holds all arbitrary t_1, t_2 verifying (4.6), a classical argument in measure theory proves that u^* is the solution of problem $(\hat{P})$. ∎

Thus, this result justifies rigorously the introduction of problem $(\hat{P})$ in the simulation of impurity diffusion phenomena in silicon (see e.g. [6,12,13]).

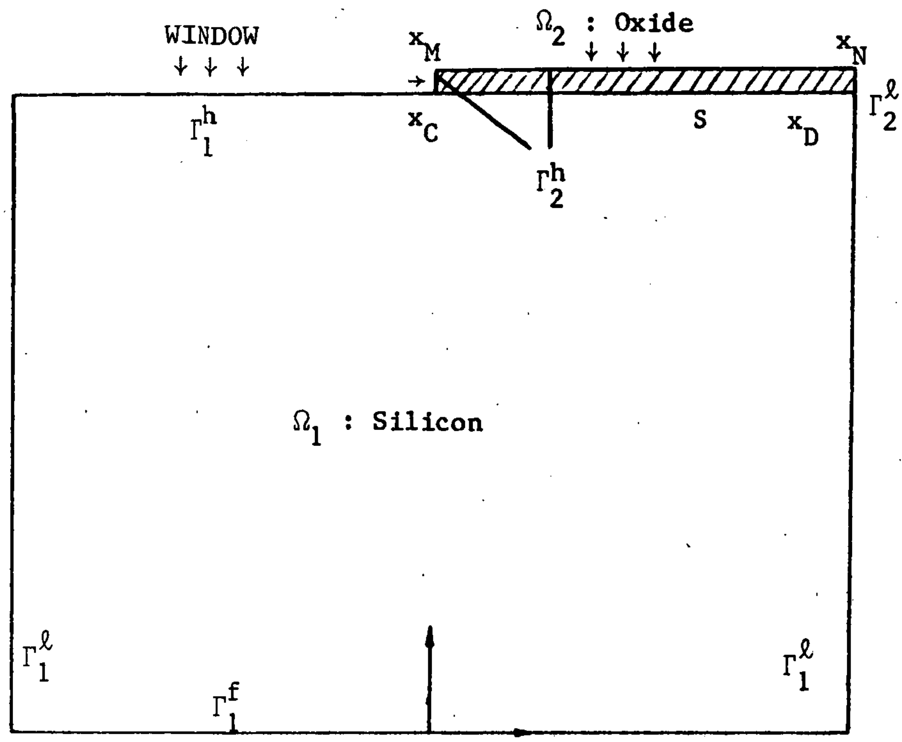

Fig. 1 : The idealized structure

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