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**A NONLINEAR  
DIFFUSION PROBLEM  
ARISING IN SEMICONDUCTOR  
PROCESS MODELLING  
WITH A SINGULARITY**

**Enrique FERNANDEZ CARA**

**Novembre 1982**

A NONLINEAR DIFFUSION PROBLEM ARISING  
IN SEMICONDUCTOR PROCESS MODELLING WITH  
A SINGULARITY

*Enrique FERNANDEZ CARA* \*

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  $\varepsilon$  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 transmission 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.
2. EXISTENCE AND UNIQUENESS RESULTS FOR THE  
NONSTATIONARY AND STATIONARY PROBLEMS.
3. THE ASYMPTOTIC BEHAVIOUR OF THE NON-  
STATIONARY SOLUTION.
4. THE LIMIT ANALYSIS AS  $\epsilon \downarrow 0$ .

References.

## 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  $\Omega_1$  is filled by silicon and  $\Omega_2$  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  $\Omega_i$  ( $i=1,2$ ) is given by the continuity equation

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

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]) :

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

where  $D_i$  is the diffusion coefficient,  $\mu_i$  is the mobility,  $\vec{E}_i$  is the electric

field, and  $z$  is the charge ( $z = +1$  for donors such as arsenic, while  $z = -1$  for acceptors such as boron). In  $\Omega_1$ , this gives :

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

where  $q$  is the electron charge,  $k$  is the BOLTZMANN's constant,  $T$  is the absolute temperature (300°K at 27°C) and  $\psi$  is the electrostatic potential. In  $\Omega_2$ , we can further assume that  $E_2 = 0$  and  $D_2$  is a constant. Thus the continuity equation (1.2) in  $\Omega_2$  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  $\Omega_1$  are in thermodynamical equilibrium, and satisfy the BOLTZMANN's statistics.

If  $C_1'$  is an "old" impurity concentration in  $\Omega_1$ , we obtain from (i) :

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

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

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

and

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

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

$$(1.7) \quad \left\{ \begin{array}{l} \psi = \frac{kT}{q} \cdot \text{Log} \frac{n}{n_i}, \\ \text{where } n = \frac{1}{2} \{ zC_1 + z'C_1' + \sqrt{(zC_1 + z'C_1')^2 + 4n_i^2} \} \dots \end{array} \right.$$

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

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

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 donors and  $f = p/n_i$  for acceptors) and  $\beta$  is a phenomenological coefficient discussed in detail in [6]. From (1.3), (1.7) and (1.8) one has :

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

Setting

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

the continuity equation in silicon reads

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

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

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

where  $\alpha$  and  $N_m$  are positive constants. The conservation law (1.10) becomes now

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

i.e.,

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

where

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

On the other hand, the diffusion coefficient in the oxide mask  $D_2$  is typically set equal to  $10^{-5} \cdot D_1^{\text{tot}}(0)$ . Thus, the diffusion equation in  $\Omega_2$  can be rewritten as follows

$$(1.14) \quad \frac{\partial C_2}{\partial t} = \epsilon D_2^{\text{tot}} \Delta C_2,$$

where  $\epsilon$  is a small positive parameter and  $D_2^{\text{tot}}$  is a formal diffusion coefficient of the same order of magnitude than  $D_1^{\text{tot}}$  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  $C_0$  on the window  $\Gamma_1^h$  and on  $\Gamma_2^h$  (see Fig. 1). Along the side  $\Gamma_1^f$  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  $\Gamma_1^l$  (resp.  $\Gamma_2^l$ ). 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 ] ) :

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

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

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

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

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

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

*with the boundary conditions*

$$(BC)_1 \quad \left\{ \begin{array}{l} u = C_0 \text{ on } \Gamma_1^h, \quad u=0 \text{ on } \Gamma_1^f, \\ v = C_0 \text{ on } \Gamma_2^h, \end{array} \right.$$

$$(BC)_2 \quad \left\{ \begin{array}{l} \frac{\partial u}{\partial n_1} = 0 \text{ on } \Gamma_1^l, \\ \frac{\partial v}{\partial n_2} = 0 \text{ on } \Gamma_2^l, \end{array} \right.$$

*the interface (or transmission) conditions :*

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

*and the initial-value conditions :*

$$(IVC) \quad u|_{t=0} = u_0 \text{ in } \Omega_1, \quad v|_{t=0} = v_0 \text{ in } \Omega_2.$$

Here,  $\varepsilon$  is a positive parameter (which is small with respect to the other orders of magnitude arising in the problem),  $C_0$  and  $m$  are positive constant, and the functions  $u_0$  and  $v_0$  are assumed to satisfy :

$$(2.3) \quad \left\{ \begin{array}{l} u_0 \in L^2(\Omega_1), \quad v_0 \in L^2(\Omega_2), \\ 0 \leq u_0 \leq C_0 \text{ a.e. in } \Omega_1, \quad 0 \leq v_0 \leq C_0 \text{ a.e. in } \Omega_2. \end{array} \right.$$

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

$$(2.4) \quad \left\{ \begin{array}{l} s \rightarrow D_1(s) \text{ is locally Lipschitz continuous, and} \\ D_1(s) \geq \alpha > 0, \text{ with } \alpha \text{ being a constant.} \end{array} \right.$$

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

We will also be concerned with the stationary problem associated to  $(P_\varepsilon)$ , which reads :

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

$$(2.6) \quad \nabla \cdot (D_1(u) \nabla u) = 0 \text{ in } \Omega_1,$$

$$(2.7) \quad \Delta v = 0 \text{ in } \Omega_2,$$

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

For small values of  $\varepsilon$ , problem  $(P_\varepsilon)$  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  $\Omega$ ) 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

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

$$(2.9) \quad 0 \leq \{\bar{u}_\varepsilon, m\bar{v}_\varepsilon\} \leq \tilde{C}_0 \equiv C_0 \max(1, m) \text{ a.e. in } \Omega.$$

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

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

with  $W$  being

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

and where  $W'$  designates its dual space. Furthermore, one has :

$$(2.11) \quad 0 \leq \{u_\varepsilon(x, t), mv_\varepsilon(x, t)\} \leq \tilde{C}_0 \text{ a.e. in } \Omega \text{ for all } t.$$

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 :

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

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  $\varepsilon$  will be omitted. Given a (small) positive parameter  $\delta$ , we introduce the auxiliary function :

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

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

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

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

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

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

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

together with the boundary conditions

$$(BC_\delta)_1 \quad \begin{cases} u_1 = c_0 \text{ on } \Gamma_1^h, u_1 = 0 \text{ on } \Gamma_1^f, \\ u_2 = m_\delta c_0 \text{ on } \Gamma_2^h \end{cases}$$

and  $(BC)_2$ , the interface conditions

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

and the initial-value conditions

$$(IVC) \quad u_1|_{t=0} = u_0 \text{ in } \Omega_1, u_2|_{t=0} = mv_0 \text{ in } \Omega_2.$$

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

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

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

The solution  $(u_1^\delta, v_1^\delta)$  of (say) problem  $(Q_\delta)$  is intended to provide an approximation  $(u^\delta, v^\delta)$  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  $(Q_\delta)$  and  $(Q_\delta)^*$ , we have the following results :

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

$$(2.17) \quad \bar{U} = \{\bar{u}_1, \bar{u}_2\} \in H^1(\Omega) \cap C^0, \gamma(\bar{\Omega})$$

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

$$(2.18) \quad 0 \leq \bar{U} \leq \tilde{C}_0 \text{ a.e. in } \Omega.$$

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

$$(2.19) \quad \begin{aligned} \{u_1, u_2\} &\in L^2(0, T; H^1(\Omega)) \cap L^\infty(0, T; L^2(\Omega)), \\ \left\{ \frac{\partial u_1}{\partial t}, \frac{\partial u_2}{\partial t} \right\} &\in L^2(0, T; W'). \end{aligned}$$

Furthermore, one has :

$$(2.20) \quad 0 \leq \{u_1, u_2\} \leq \tilde{C}_0 \text{ a.e. in } \Omega \text{ for all } t \in [0, T].$$

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 :

1<sup>st</sup> 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

$$\tilde{D}_1(s) = \begin{cases} D_1(0) & \text{if } s < 0, \\ D_1(s) & \text{if } 0 \leq s \leq C_0, \\ D_1(C_0) & \text{if } s > C_0. \end{cases}$$

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

$$\tilde{D}_1(s) \leq \max_{s \in [0, \tilde{C}_0]} \tilde{D}_1(s) \equiv \tilde{\beta} < +\infty.$$

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

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

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

$$0 \leq \bar{U} = \{\bar{u}_1, \bar{u}_2\} \leq \tilde{C}_0 \text{ in } \Omega,$$

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  $C^0(\bar{\Omega}_1)$  :

$$B = \{\phi \mid \phi \in C^0(\bar{\Omega}_1) ; 0 \leq \phi \leq \tilde{C}_0 \text{ in } \bar{\Omega}_1\}.$$

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

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

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

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

$$U = \{u_1, u_2\} \in H^1(\Omega) \cap C^{0, \gamma}(\bar{\Omega})$$

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

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

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  $u_1^0 \in B$ .

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

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

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

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

where  $C_1$  depends on  $D_1(\cdot)$ ,  $m$  and  $C_0$ , but is independent from  $\rho$ .

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

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

and this uniformly in  $\rho$ . 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  $\Gamma_1^h$ , 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  $\Omega_1$ )

$$\chi(x) = \overline{\lim}_{\rho \rightarrow 0} |h_\rho(x)|^2$$

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

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

From the identity

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

one also has  $u_2 = \bar{u}_2$ . ■

Sketch of the proof of Proposition 2.2 :

1st Part : Existence of solutions.

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



$$(2.25) \left\{ \begin{array}{l} \int_{\Omega_1} \frac{du_1}{dt} \cdot \phi + \int_{\Omega_2} \frac{1}{m_\delta} \frac{du_2}{dt} \cdot \psi + \int_{\Omega_1} \tilde{D}_1(u_1(t)) \nabla u_1(t) \cdot \nabla \phi \\ + \varepsilon \int_{\Omega_2} \frac{1}{m_\delta} \nabla u_2(t) \cdot \nabla \psi = 0 \quad \forall \{\phi, \psi\} \in W, \\ \{u_1, u_2\} \in L^2(0, T; H^1(\Omega)), \quad \frac{d}{dt} \{u_1, u_2\} \in L^2(0, T; W'), \\ \{u_1(t), u_2(t)\} \in \tilde{W}, \quad u_1|_{t=0} = u_0, \quad u_2|_{t=0} = mv_0. \end{array} \right.$$

From the maximum principle, we also have

$$0 \leq U(t) \leq \tilde{C}_0 \text{ a.e. in } \Omega, \quad t \in (0, T),$$

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  $(Q_\delta)$ . ■

Remark 2.5 : Although a fixed-point formulation of  $(Q_\delta)$  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  $u_1^0 \in \mathcal{B}$ , with

$$\mathcal{B} = \{\phi \mid \phi \in L^\infty(\Omega_1 \times (0, T)) ; 0 \leq \phi \leq \tilde{C}_0 \text{ a.e.}\}.$$

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

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

together with the boundary conditions  $(BC_\delta)_1$  and  $(BC_\delta)_2$ , conditions  $(IC_\delta)$  on  $S$  and the initial-value conditions  $(IVC_\delta)$  ; 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  $(Q_\delta)$ , and set

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

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

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

Notice that

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

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

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

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

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

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

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

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

From Fatou's Lemma we deduce that

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

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 :

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

$$(2.28) \quad \begin{cases} u_{1\delta}^\Gamma = C_0 \text{ on } \Gamma_1^h, & u_{1\delta}^\Gamma = 0 \text{ on } \Gamma_1^f, \\ u_{2\delta}^\Gamma = m_\delta C_0 \text{ on } \Gamma_2^h, \\ u_{1\delta}^\Gamma = u_{2\delta}^\Gamma \text{ on } S, \end{cases}$$

$$(2.29) \quad U_\delta^\Gamma \text{ is uniformly bounded in } H^1(\Omega) \text{ (independently from } \delta)$$

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

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

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

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

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

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

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

and set  $u_{1\delta}^\Gamma \equiv C_0$ . 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  $(u_1^\delta, u_2^\delta)$  be the solution of problem  $(Q_\delta)^*$ , and set

$$u_1^\delta = u_{1\delta}^\Gamma + z_\delta, \quad u_2^\delta = u_{2\delta}^\Gamma + y_\delta,$$

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

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

Since  $\{u_{1\delta}^\Gamma, u_{2\delta}^\Gamma\}$  is uniformly bounded in  $H^1(\Omega)$ , there exists a constant  $C_5 > 0$  depending on  $\Omega, m, D_1(\cdot), C_0, \varepsilon$  and  $D_2$ , but independent from  $\delta$  such that

$$(2.32) \quad \|\{u_1^\delta, u_2^\delta\}\|_{H^1} \leq C_5 \quad \forall \delta > 0. \quad \blacksquare$$

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  $\delta$ ,

$$(2.33a) \quad u_1^\delta \rightharpoonup u_1^* \text{ weakly in } H^1(\Omega_1),$$

$$(2.33b) \quad u_2^\delta \rightharpoonup u_2^* \text{ weakly in } H^1(\Omega_2).$$

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,  $u^* = C_0$  on  $\Gamma_1^h$  and  $u^* = 0$  on  $\Gamma_1^f$ . Taking limits as  $\delta \rightarrow 0$  in the identities

$$\begin{cases} u_2^\delta = m_\delta C_0 \text{ on } \Gamma_2^h, \\ u_1^\delta = u_2^\delta \text{ on } S, \end{cases}$$

we also obtain :

$$\begin{cases} v^* = C_0 \text{ on } \Gamma_2^h, \\ u^* = m v^* \text{ on } S. \end{cases}$$

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

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

From the identity

$$\int_{\Omega_1} (D_1(u_1) \nabla u_1 - D(\bar{u}_1) \nabla \bar{u}_1) \cdot \nabla \phi + \varepsilon \rho D_2 m \int_{\Omega_2} \frac{|\nabla(u_2 - \bar{u}_2)|^2}{\rho + |u_2 - \bar{u}_2|} = 0$$

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

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

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  $\Omega, m, D_1(\cdot), C_0, \varepsilon, D_2$  and  $T$ , but is independent from  $\delta$ . 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  $u_0 \leq \bar{u}$  and  $v_0 \leq \bar{v}$  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

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

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

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

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

and choose

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

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

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

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

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

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

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

and the Lemma holds. ■

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

$$u_0 = 0 \text{ in } \Omega_1, \quad v_0 = 0 \text{ in } \Omega_2.$$

Lemma 3.2 : *The function*

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

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 :

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

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

$$(3.2) \quad u(t_n) \rightarrow \bar{u}, \quad v(t_n) \rightarrow \bar{v} \text{ a.e.}$$

Let us consider the following test functions

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

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 :

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

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 :

$$\left\{ \begin{aligned} & \int_{\Omega_1} [(\bar{u}-u(t)) - \rho \text{Log} \frac{\rho+(\bar{u}-u(t))}{\rho}] + m \int_{\Omega_2} [(\bar{v}-v(t)) - \rho \text{Log} \frac{\rho+(\bar{v}-v(t))}{\rho}] \\ & + \int_0^t \left\{ \frac{\alpha \rho}{2} \int_{\Omega_1} \frac{(|\nabla(\bar{u}-u(s))|)^2}{\rho+(\bar{u}-u(s))} + \varepsilon D_2 \rho m \int_{\Omega_2} \frac{(|\nabla(\bar{v}-v(s))|)^2}{\rho+(\bar{v}-v(s))} \right\} ds \\ & \leq \rho t + \int_{\Omega_1} [(\bar{u}-u_0) - \rho \text{Log} \frac{\rho+(\bar{u}-u_0)}{\rho}] + m \int_{\Omega_2} [(\bar{v}-v_0) - \rho \text{Log} \frac{\rho+(\bar{v}-v_0)}{\rho}] , \end{aligned} \right.$$

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

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

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

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

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

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

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

Proof of Lemma 3.3 : For instance, let us prove that the function

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

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. - THE LIMIT ANALYSIS AS $\varepsilon \downarrow 0$ .

This Section is concerned with the behaviour of the solutions  $U_\varepsilon = \{u_\varepsilon, v_\varepsilon\}$  of problems  $(P_\varepsilon)$  as  $\varepsilon$  approaches zero. It will be proved that  $u_\varepsilon$  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 :*

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

together with the boundary conditions

$$(BC)_3 \quad \left\{ \begin{array}{l} \hat{u} = C_0 \text{ on } \Gamma_1^h, \hat{u} = 0 \text{ on } \Gamma_1^f, \\ \frac{\partial \hat{u}}{\partial n_1} = 0 \text{ on } \Gamma_1^l \cup S, \end{array} \right.$$

and the initial-value condition

$$\hat{u}|_{t=0} = u_0 \text{ in } \Omega_1. \quad \blacksquare$$

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

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

where  $V$  is given by :

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

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

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

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

Proof :

Step 1 : "A priori" estimates.

Let us put

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

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

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

Then one has

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

with  $C_{11}$  being a positive constant not depending on  $\epsilon$ . Hence,

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

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

$$(4.3a) \quad u_\epsilon \text{ is uniformly bounded in } L^2(0, T; H^1(\Omega_1)) \cap L^\infty(\Omega_1 \times (0, T)),$$

$$(4.3b) \quad v_\epsilon \text{ is uniformly bounded in } L^\infty(\Omega_2 \times (0, T)),$$

$$(4.3c) \quad \sqrt{\epsilon} v_\epsilon \text{ is uniformly bounded in } L^2(0, T; H^1(\Omega_2)). \blacksquare$$

Step 2 : Extraction of a subsequence

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

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

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

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

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

$$(4.5) \quad \left\{ \begin{array}{l} u_{\mu} \rightarrow u^* \text{ weakly in } L^2(0,T;H^1(\Omega_1)) \cap L^{\infty}(\Omega_1 \times (0,T)), \\ u_{\mu} \rightarrow u^* \text{ strongly in } L^2(\Omega_1 \times (0,T)) \text{ and a.e.}, \\ \frac{\partial u_{\mu}}{\partial t} \rightarrow \frac{\partial u^*}{\partial t} \text{ weakly in } L^2(0,T;V'), \end{array} \right.$$

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

Step 3 : Conclusion

Let  $\phi$  be an arbitrary function in  $V$ , and choose  $\psi$  such that

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

Then one has :

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

for all  $t_1, t_2$ , satisfying

$$(4.6) \quad 0 \leq t_1 \leq t_2 \leq T.$$

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

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

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]).

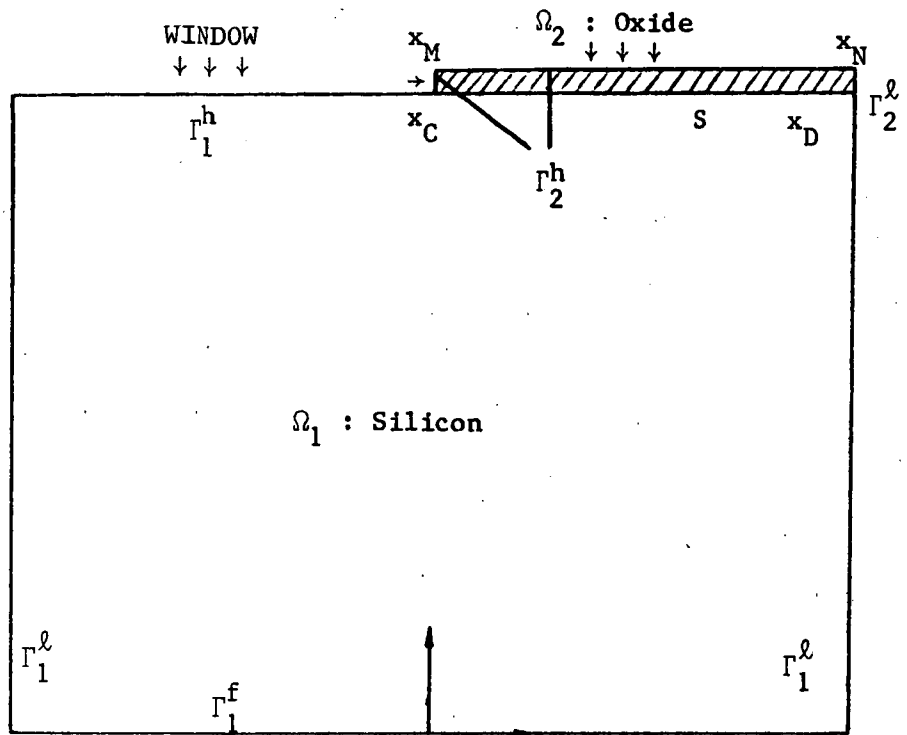


Fig. 1 : The idealized structure

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