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On a Mathematical Model Relative to the Doping of Semiconductors

ABSTRACT. — A mathematical model relative to the doping of semiconductors is studied and an existence and uniqueness theorem is proved.

Un modello matematico relativo al drogaggio dei semiconduttori

SUNTO. — Si studia un modello matematico relativo al drogaggio di semiconduttori e si dimostra un teorema di esistenza ed unicità.

1. - INTRODUCTION

It is well known that the process of doping semiconductors (normally silicon) has lately assumed very great importance, in particular in the manufacture of electronic devices.

A mathematical model which is widely used in applications is expressed by the equations (see for instance [1], [2])

$$u_t - \frac{\partial}{\partial x}(\Phi(u)u_x) = f \tag{1.1}$$

where u is the concentration of the dopant, Φ is the diffusion coefficient, f the quantity of dopant introduced.

If u is "small" ($< 10^{19}\text{cm}^{-3}$) Φ does not depend on u and (1.1) reduces to the well known Fick's law. For high concentrations the relationship between diffusion coefficient

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and concentration is given by the formula

$$\Phi(u) = \alpha + \beta|u| + \gamma u^2 \tag{1.2}$$

with α, β, γ positive constants, depending on the nature of the dopant. Some indications regarding values of these constants are given in the table below

TABLE FOR Si:

	α	β	γ
P	$\neq 0$	$\neq 0$	$\neq 0$
As	$\neq 0$	$\neq 0$	0
Sb	$\neq 0$	$\neq 0$	0
Bi	$\neq 0$	$\neq 0$	0

TABLE FOR GaAs:

	α	β	γ
Zn([1])	0	0	$\neq 0$

([1]) Zn is not considered a dopant

In the sequel we shall limit our study to the most common dopant, phosphorous, since the other materials can be considered as particular cases.

The model described above will in what follows be called **classical model**.

This model has been criticized owing to the fact that in its deduction the solubility limit of dopant is assumed to be infinite, a condition which is not physically verified in applications (see for instance [3]).

For a more detail discussion of the physical aspects of the problem considered see references [4] to [16].

The aim of the present paper is to introduce and study a model obtained essentially from (1.1), but which takes into account the fact that the concentration of dopant is bounded by the solid solubility constant $M_1 : |u| \leq M_1$.

Precisely, this will be done by substituting to equation (1.1) an inequality associated in a natural way to it, see for instance [17], [18], [19] .

The corresponding model will be called **inequality model**.

In what follows, we shall assume that the silicon crystal is homogeneous (i.e. the coefficients α, β, γ are constant). Since the temperature is fixed during the process, the solid solubility is also constant.

2. - The inequality model

Let us observe first of all, that both the classical and the inequality models are "atomic", precisely we assume that the material is constituted by "atoms" of a given diameter δ; hence the following two conditions hold

$$|u| \leq M_1; \quad \left|\frac{u(x+h) - u(x)}{h}\right| \leq \frac{1}{\delta} = M_3 \qquad \forall h > 0 \tag{2.1}$$

(the second condition (2.1) follows from the first; where M_3 is a constant).

Finally, since the model is not relativistic the velocity of the"atoms" must not exceed the speed of light, hence

$$|u_t| \leq M_2 \tag{2.2}$$

(M_2 is a constant).

In what follows, relations (2.1), (2.2) will be called **consistency conditions**.

Let now K_T be the closed convex set defined by

$$K_T = \left\{u \in L^2(0,T;H^1_{00}) : |u| \leq M_1, |u_x| \leq M_3,\ |u_t| \leq M_2\right\} \tag{2.3}$$

where

$$H^1_{00} = \left\{u \in H^1 \middle| u(0,t) = 0, \frac{\partial u}{\partial x}\bigg|_{x=l} = 0 \quad \forall t \in [0,T]\right\}$$

and consider the inequality associated to (1.1)

$$\frac{1}{2}\|v(t) - \varphi(t)\|^2_{L^2} + \tag{2.4}$$
$$+\int_0^t (\varphi_t, v - \varphi)_{L^2} d\zeta + \int_0^t \left\{((a + \beta|v| + \gamma v^2)v_x, v_x - \varphi_x)_{L^2}\right\} d\zeta \leq \int_0^t (f, v - \varphi)_{L^2} d\zeta$$

where φ is an arbitrary test function $\in K_T$.

The inequality model is then defined by (2.4) and by the consistency conditions introduced above.

We shall say that v is a K_T-solution in $(0,T)$ of (2.4) satisfying the initial condition

$$v(x,0) = 0 \qquad (0 \leq x \leq l) \tag{2.5}$$

and the boundary conditions

$$v(0,t) = 0 \quad \frac{\partial v}{\partial x}\bigg|_{x=l} = 0 \quad (0 \leq t \leq T) \tag{2.6}$$

if

i) $v \in K_T$

ii) v satisfies (2.4), (2.5), (2.6) $\forall\ \varphi \in K_T$.

The second condition of (2.6) means that there is no flow of dopant through the surface (see for instance [9], [23]) which is physically reasonable. Moreover we observe that the first condition of (2.6) has been taken into account by imposing that $v \in H^1_{00}$, while the second condition of (2.6) is automatically satisfied since the boundary terms, which normally appear when Green's formula is applied to (1.1), vanish.

The relationship between the classical and the inequality model is expressed by the following well known proposition (see for instance [17]). Assume that there exists $T^* > 0$ such that $v \in \overset{\circ}{K}_{T^*}$ (internal set of K_{T^*}) then the K_{T^*}-solutions are also solutions in $(0,T^*)$ of (1.1), with the same initial and boundary conditions. Thus, on $(0,T^*)$ the solutions of the two models coincide, while, when $t > T^*$ the two models may differ; in this case, however, neither model is physically acceptable, since it does not comply with the consistency conditions.

It appears therefore reasonable to substitute the classical model with the inequality model, since this last holds on the largest possible time interval.

In the next section 3 we shall prove an auxiliary theorem. Subsequently in sections 4 and 5 we shall prove an existence and uniqueness theorem for the K_T-solutions relative to the inequality model.

3. - An auxiliary theorem

Consider the regularized inequality associated to (2.4)

$$\frac{1}{2}\|v(t)-\varphi(t)\|^2_{L^2}+\int_0^t(\varphi_t, v-\varphi)_{L^2}d\zeta+ \tag{3.1}$$

$$+\int_0^t\{\varepsilon(Gv, v-\varphi)_{L^2}+((a+\beta|v|+\gamma v^2)v_x, v_x-\varphi_x)_{L^2}\}d\zeta \leq \int_0^t(f, v-\varphi)_{L^2}d\zeta$$

where G is the (positive, self-adjoint) Green's operator relative to the equation $z_{tt}=h$ with $z(0)=z(T)=0$.

We shall say that v is a K_T-solution in $(0, T)$ of (3.1) satisfying the initial and boundary conditions (2.5), (2.6) if

$i_1)$ $v \in K_T$

$ii_1)$ v satisfies (3.1), (2.5), (2.6) $\forall\varphi \in K_T$

Let us prove the following auxiliary theorem.

Theorem 1.

Assume that $f \in L^2(0, T; L^2)$.There exists then $\forall\varepsilon > 0$ in (0,T) a K_T-solution of (3.1), with the initial and boundary conditions (2.5), (2.6).

The proof is based on the classical Faedo-Galerkin method.

Let $\{g_j\}$ be a basis in $H^1_{00}(0, l)$ and set

$$v=\sum_{j=1}^{\infty}\sigma_j g_j \tag{3.2}$$

$$v_n=\sum_{j=1}^{n}\sigma_{nj} g_j \tag{3.3}$$

with

$$v_n(0)=0.$$

We consider now, for each fixed $\varepsilon > 0$, the system of n ordinary differential equations

in the unknowns $\sigma_{nj}(t)$

$$\left(v_{nt} - \frac{\partial}{\partial x}[(a + \beta|v_n| + \gamma v_n^2)v_{nx}] + \varepsilon G v_n + nP(v_n) - f, g_j\right)_{L^2} = 0 \tag{3.4}$$

where P is a penalization operator relative to the convex set K_T .

The system (3.4), thanks to well known properties, admits local solution.

Multiplying (3.4) by σ_{nj} and adding with respect to j from 1 to n, we have

$$\frac{1}{2}\frac{d}{dt}\|v_n\|_{L^2}^2 + ((a + \beta|v_n| + \gamma v_n^2)v_{nx}, v_{nx})_{L^2} + \varepsilon(Gv_n, v_n)_{L^2} + \\ + (nP(v_n), v_n)_{L^2} - (f, v_n)_{L^2} = 0. \tag{3.5}$$

Bearing in mind that by definition of penalization and Green's operators

$$(P(z), z)_{L^2} \geq 0 \ , \qquad (Gz, z\ )_{L^2} = (G^{1/2}z, G^{1/2}z)_{L^2} \ , \tag{3.6}$$

we obtain by (3.5) integrating between 0 and $t \in (0, T)$,

$$\frac{1}{2}\|v_n(t)\|_{L^2}^2 - \frac{1}{2}\|v_n(0)\|_{L^2}^2 + \int_0^t ((a + \beta|v_n| + \gamma v_n^2)v_{nx}, v_{nx})_{L^2} d\zeta + \\ + \varepsilon \int_0^t \left\|G^{1/2}v_n\right\|_{L^2}^2 d\zeta \leq \int_0^t (f, v_n)_{L^2} d\zeta \tag{3.7}$$

with

$$v_n(0) = 0 \qquad \forall n. \tag{3.8}$$

Hence, by (3.7), (3.8), we have

$$\|v_n\|_{L^2(0,T;\, H_{00}^1)\, \cap\, L^\infty(0,T;\, L^2)} \leq C_1 \tag{3.9}$$

$$\varepsilon\left\|G^{1/2}v_n\right\|_{L^2}^2 \leq \varepsilon C_2 \tag{3.10}$$

$$\|v_{nx}\|_{L^2}^2 \leq C_3 \tag{3.11}$$

with C_i independent of n and $\varepsilon, (i = 1, 2, 3)$.

By well known embedding and interpolation theorems see, for example [20], [21], [22] it follows then, $\forall\ \varepsilon$ fixed > 0

$$\lim_{n\to\infty} v_n = v \qquad \text{in } C^0((0, l) \times (0, T)). \tag{3.12}$$

Moreover, by the semicontinuity of weak convergence we have

$$\varepsilon\left\|G^{1/2}v\right\|_{L^2}^2 \leq \min\lim_{n\to\infty} \varepsilon\left\|G^{1/2}v_n\right\|_{L^2}^2 \tag{3.13}$$

$$a\|v_x\|_{L^2}^2 \leq \min\lim_{n\to\infty} a\|v_{nx}\|_{L^2}^2 \tag{3.14}$$

$$\beta\|v_x\|_{L^2}^2 \leq \min\lim_{n\to\infty} \beta\|v_{nx}\|_{L^2}^2 \tag{3.15}$$

$$\gamma\|vv_x\|_{L^2}^2 \leq \min\lim_{n\to\infty} \gamma\|v_n v_{nx}\|_{L^2}^2. \tag{3.16}$$

From (3.9), (3.12) it follows in particular that the solution of (3.4) exists globaly in $[0, T]$.

Let us prove that v is a solution (i.e. satisfies i_1), ii_1). In order to prove condition ii_1), consider an arbitrary function $\varphi \in H^2(0, T; H^2_{00}) \cap K_T$ where

$$H^2_{00} = \left\{ u \in H^2 \middle| u(0,t) = 0,\ \frac{\partial u}{\partial x}\bigg|_{x=l} = 0 \quad \forall t \in [0,T] \right\}$$

and set

$$\varphi = \sum_{j=1}^{\infty} \rho_j g_j \qquad \varphi_p(t) = \sum_{j=1}^{p} \widetilde{\rho}_j g_j$$

$$\widetilde{\rho}_j = \left\{ \begin{array}{ll} \rho_j & \text{for} \quad j \le p \\ 0 & \text{for} \quad j > p \end{array} \right\}$$

If we suppose $n > p$, multiplying (3.4) by $\sigma_{nj} - \widetilde{\rho}_j$ adding with respect to j, integrating in $(0, t)$ and bearing in mind that P is mononote ($\Rightarrow (Pv_n, v_n - \varphi_p)_{L^2} = (Pv_n - P\varphi_p, v_n - \varphi_p)_{L^2} \ge 0$) we obtain

$$\frac{1}{2}\left\|v_n(t) - \varphi_p(t)\right\|^2_{L^2} + \int_0^t ((a + \beta|v_n| + \gamma v_n^2)v_{nx}, v_{nx} - \varphi_{px})_{L^2} d\zeta + \tag{3.17}$$

$$+ \int_0^t \left\{ \varepsilon(G^{1/2}v_n, G^{1/2}v_n - G^{1/2}\varphi_p)_{L^2} d\zeta - (f, v_n - \varphi_p)_{L^2} \right\} d\zeta + \int_0^t (\varphi_{pt}, v_n - \varphi_p)_{L^2} d\zeta \le 0.$$

Let now $n \to \infty$ (keeping ε fixed); by (3.12), (3.13), (3.14), (3.15), (3.16), the semicontinuity of the weak limit, and the definition of P, v satisfies condition ii_1) $\forall \varphi \in H^2(0, T; H^2_{00}) \cap K_T$, see [23].

We shall prove now that the K_T-solution belongs to the convex set K_T.

Moreover, again from the equation (3.5), integrating in $(0, t)$ and bearing in mind conditions (3.12), (3.13), (3.14), (3.15), (3.16) we have

$$n \int_0^t (P(v_n), v_n))_{L^2} dt \le C_4, \tag{3.18}$$

and consequently $v_n \in K_T$; hence v satisfies condition i_1) (where C_4 is a constant).

By the usual density argument, inequality (3.1) is satisfied also $\forall \varphi \in K_T$.

The existence theorem of the regularized problem is then completely proved.

4. - An existence theorem

Theorem 2.

Assume that $f \in L^2(0, T; L^2)$. There exists then in $(0, T)$ a K_T-solution v of (2.4), (2.5), (2.6).

Let v_ε be a solution of (3.1), (2.5), (2.6) corresponding to the value ε. Following the same procedure as in Theorem 1, we can prove that

$$\lim_{\varepsilon\to 0} v_\varepsilon = v \tag{4.1}$$

in the weak topology of $L^2(0,T;H^1_{00}) \cap L^\infty(0,T;L^2) \cap H^1_{00}(0,T;L^2)$ and strong topology of $L^2(0,T;L^2)$.

The limit function v is a solution of (2.4), (2.5), (2.6). In fact consider the inequality

$$\begin{aligned} \frac{1}{2}\|v_\varepsilon(t)-\varphi(t)\|^2_{L^2} &+ \int_0^t ((a+\beta|v_\varepsilon|+\gamma v_\varepsilon^2)v_{\varepsilon x}, v_{\varepsilon x}-\varphi_x)_{L^2} d\zeta + \\ &+ \int_0^t \left\{\varepsilon(G^{1/2}v_\varepsilon, G^{1/2}v_\varepsilon - G^{1/2}\varphi)_{L^2} d\zeta - (f, v_\varepsilon-\varphi)_{L^2}\right\} d\zeta + \int_0^t (\varphi_t, v_\varepsilon-\varphi)_{L^2} d\zeta \le 0 \end{aligned} \tag{4.2}$$

with $\varphi \in H^2(0,T;H^2_{00}) \cap K_T$.

Let now, in (4.2) $\varepsilon \to 0$. Bearing in mind the semicontinuity of the weak limit, the definitions of P and G, v satisfies condition *ii*) $\forall\varphi \in H^2(0,T;H^2_{00}) \cap K_T$.

We can prove that v satisfies also condition *i*) $\forall\varphi \in H^2(0,T;H^2_{00}) \cap K_T$ by the same procedure of theorem 1.

Again by a density argument, inequality (2.4) is satisfied also $\forall\varphi \in K_T$.

5. - An uniqueness theorem

Theorem 3.

Let us now prove the uniqueness of the solution of

$$(u_t, u-\varphi)_{L^2} + ((a+\gamma u^2)u_x, u_x-\varphi_x)_{L^2} \le (f, u-\varphi)_{L^2} \tag{5.1}$$

under the further condition $\beta = 0$.

This condition is justified by the fact that in most pratical cases the coefficient β "is small" (see [16], [23]).

Following a classical procedure (see for instance[17]), let us assume that there exists two solutions, u, v, of (5.1), (2.5), (2.6).

$$(u_t, u-\varphi)_{L^2} + \left(\left(a+\gamma u^2\right) u_x, u_x-\varphi_x\right)_{L^2} \le (f, u-\varphi)_{L^2} \tag{5.2}$$

$$(v_t, v-\psi)_{L^2} + \left(\left(a+\gamma v^2\right) v_x, v_x-\psi_x\right)_{L^2} \le (f, v-\psi)_{L^2} \tag{5.3}$$

with $\varphi, \psi \in K_T$

Setting $\varphi = v$ and $\psi = u$ (which is obviously possible) and adding (5.2), (5.3), we obtain

$$(u_t-v_t, u-v)_{L_2} + \left((a+\gamma u^2)\, u_x, u_x-v_x\right)_{L^2} + \left((a+\gamma v^2)\, v_x, v_x-u_x\right)_{L^2} \le 0 \tag{5.4}$$

Bearing in mind that u and $v \in K_T$ it follows

$$\frac{1}{2}\frac{\partial}{\partial t}\|u-v\|_{L_2}^2 + a\|u_x - v_x\|_{L_2}^2 + ((\gamma u^2 u_x - \gamma v^2 v_x, u_x - v_x)_{L_2} \leq 0 \tag{5.5}$$

Now using a standard procedure we obtain

$$\frac{1}{2}\frac{\partial}{\partial t}\|u - v\|_{L_2}^2 + a\|u_x - v_x\|_{L_2}^2 + \gamma v^2\|u_x - v_x\|_{L_2}^2 + \gamma M((u-v), u_x - v_x)_{L_2} \leq 0 \tag{5.6}$$

$$a > 0,\ \gamma > 0,\ M > 0$$

hence

$$\frac{1}{2}\frac{\partial}{\partial t}\|u-v\|_{L_2}^2 + \frac{\gamma M}{2}\frac{\partial}{\partial x}\|u-v\|_{L_2}^2 \leq 0 \tag{5.7}$$

and consequently

$$u = v.$$

The theorem is completely prove.

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