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NUMERICAL APPROXIMATION OF FREE BOUNDARY PROBLEM BY VARIATIONAL INEQUALITIES. APPLICATION TO SEMICONDUCTOR DEVICES

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Abstract: In this paper we treat problem arasing in semiconductor theory from a mathematical and numerical point of view, in particular we consider a boundary value problem with unknown interfaces arising by the determination of the depletion layer in the most basic semiconductor device namely the p-n junction diode. We present the numerical approximation of free boundary problem with double obstacle treated with quasi-variational inequalities. We deal with the L^∞ convergence of the standard finite element approximation of the system of quasi-variational inequalities.

1. INTRODUCTION

Boundary-value problems are problems where the solution of a differential equation has to satisfy some conditions on the boundary of a prescribed domain. In many important case, as free boundary problems, the boundary of the domain is not known in advance but has to be determinated as a part of the solution. Typically, a free boundary problem consist of a partial differential equations of elliptic type to be satisfied within a bounded domain together with necessary boundary conditions; one section of the boundary, the free boundary, is unknown and must be determined as part of the solution. These problems have been popular subject for research in recent years, leading to a collection of new mathematical methods. Flow through porous media is an important source of free boundary problems [1], most frequently in relation to seepage phenomena that occur in nature. Examples are seepage throught earth dams; seepage out of open channels such as rivers, canals, ponds, and irrigation system. Practical interest in free boundary problems, however, is not confined to natural seepage but extends for example to topics in plasma physics, semiconductors, and electrochemical machinary. This work analyses a free boundary problem in semiconductors field, in particular the modelling of reverse-biased devices. In fact for the steady-state case of $p-n$ junction diode under reverse bias, after a singular perturbation analysis, the determination of the depletion layer leads to a free boundary problem.

For the case of $p-n$ junction diode under strong revers bias, an approximating problem which includes the same free-boundary for the potential and a mixed elliptic-hyperbolic problem for the analysis of current flow, has been derived and analyzed in a series of papers by Schmeiser [26],[27].

Without being derived as a limit of a singularly perturbed system, the double obstacle problem has already been formulated as a model for the potential distribution by Hunt and Nassif [16]. The free boundary model presented here differs from the previous one, by the definition of the obstacles which are equal to the quasi-Fermi level, obtained as a solution to the continuity equations; we give here a quasi-variational formulation of the model.

Then we deal with the L^∞ convergence of the finite element approximation of the system of quasi-variational inequalities. The L^∞- error estimate is of particular interest not only for practical reasons but also due to its inherent difficulty of convergence in this norm. Moreover, the interest in using such a norm for the approximation of obstacle problems is that they are types of free boundary problems. This fact was validated by the paper of F. Brezzi; L.A. Caffarelli, [8] and later by that of Nochetto [20], on the convergence of the discrete free boundary to the continuous one.

A lot of results on error estimates for the classical obstacle problems and variational inequalities were achieved in this norm, (cf., e.g [2], [19], [12], [21]). However, very few works concerning quasi-variational inequalities are known on this subject. (cf., [14]), [6]), Under a $W^{2,p}(\Omega)$- regularity of the continuous solution, a quasi-optimal L^∞- convergence of finite element method is established, involving a monotone algorithm of Bensoussan-Lions type and standard L^∞- error estimates known for elliptic variational inequalities.

2. REVERSE BIASED p-n JUNCTION

One of the basic properties of semiconductors is the controlled implantation of impurity atoms into a semiconductor crystal; this process is usually called *doping*. It is possible to introduce into the crystal dopant atoms which can produce one or more excess conduction electrons (called donors), or dopant atoms which can accept electrons and thus produce holes (called acceptors). This process increases the conductivity significantly, and thus the electrical properties of the crystal can be controlled by doping. The performance of a semiconductor device is mainly determined by the distributions of donors and acceptors.

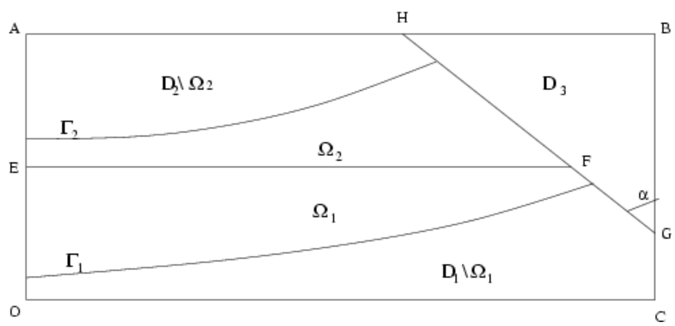

Figure 1. p-n junction with Γ_1 and Γ_2 the free boundaries of the depletion layer.

In the p-n junction the p-*side*, doped with acceptors, is positively charged and the n-*side*, doped with donors, is negatively charged. As a result of the tendency of holes to diffuse into the n region and of electrons into the p region, a nonconducting region is set up along the junction, called a *depletion layer*.

When a positive bias is applied to the junction, a large current flows through the diode, even if the voltage is small; a negative applied voltage widens the depletion layer. The unknown or free boundaries limiting the depletion layer are interfaces with another, dielectric region. The interfaces are determined by the concentrations of donors and acceptors and the potentials applied.

As in Fig. 1, let D_1 be the open set bounded by the contour $OEFGC$, D_2 the one bounded by $AHFE$, and D_3 the triangular domain bounded by $HBG : D$ consists of the whole rectangular domain $OABC$, while Ω_1 and Ω_2 are the open sets which define the depletion layer. We also let $\mathrm{C}_1 = \mathrm{D}_1 \setminus \Omega_1$ and $\mathrm{C}_2 = \mathrm{D}_2 \setminus \Omega_2$.

The model which describes potential distribution $u(x,y)$ in semiconductor device is the drift-diffusion one

$$\begin{cases} \nabla^2 u = \dfrac{q}{\varepsilon}(n - p - C) \\ \nabla \cdot (D_n \nabla n - n\mu_n \nabla u) = R_n \\ \nabla \cdot (D_p \nabla p + p\mu_p \nabla u) = R_p \end{cases} \tag{1}$$

where q and ε are the charge density and the dielectric permittivity, n and p are the concentrations of free carriers of negative and positive charge, electrons and holes, C is the predefined doping concentration, μ_n, μ_p and D_n, D_p are the mobility and diffusivity constants, R_n and R_p the recombination-generation rate for hole and electron. We suppose $R_n = R_p = 0$. We rewrite the model for the two region remembering that Ω_1 and Ω_2 are space charge regions, C_1 and C_2 are charge neutral regions $\Gamma_1 = \overline{\Omega}_1 \cap C_1$ and $\Gamma_2 = \overline{\Omega}_2 \cap C_2$ are the free boundaries. In D_1 we have:

$$\begin{cases} \Delta u = \dfrac{q}{\varepsilon}(n - N_d) \\ J_n = D_n \nabla n - n\mu_n \nabla u \\ \nabla J_n = 0 \\ J_p = 0 \end{cases} \tag{2}$$

while in D_2

$$\begin{cases} \Delta u = \dfrac{q}{\varepsilon}(N_a - p) \\ J_p = D_p \nabla p + p\mu_p \nabla u \\ \nabla J_p = 0 \\ J_n = 0 \end{cases} \tag{3}$$

with the mixed boundary conditions

$$\begin{cases} u = u_1^D & \text{on } \Gamma_1^D \\ \dfrac{\partial u_1}{\partial n} = 0 & \text{on } \Gamma_1^N \end{cases} \qquad \begin{cases} u = u_2^D & \text{on } \Gamma_2^D \\ \dfrac{\partial u_2}{\partial n} = 0 & \text{on } \Gamma_2^N \end{cases} \tag{4}$$

where $\Gamma_i^D, i = 1,2$ are the Dirichlet part of boundary, $\Gamma_i^N, i = 1,2$ the Neumann ones.

At this point we use the quasi Fermi potentials

$$n = N_d\, e^{\frac{q}{KT}(u-\phi_n)} \qquad p = N_a\, e^{\frac{q}{KT}(\phi_p-u)}$$

If $\frac{q}{KT} = k,$ inserting the last in (2), (3) we obtain

$$\Delta u = \frac{q}{\varepsilon}(n - N_d) = \frac{q}{\varepsilon}(N_d\, e^{k(u-\phi_n)} - N_d) = \frac{q}{\varepsilon} N_d\, (e^{k(u-\phi_n)} - 1) \qquad \text{in } D_1$$

$$\Delta u = \frac{q}{\varepsilon}(N_a - p) = \frac{q}{\varepsilon}(N_a - N_a\, e^{k(\phi_p-u)}) = \frac{q}{\varepsilon} N_a\, (1 - e^{k(u-\phi_n)}) \qquad \text{in } D_2$$

To simplify the model we see that $D_1 = \Omega_1 \cup C_1$ and in the charge neutral region $C_1,$ $n = N_d$ holds , so:

$$\Delta u = 0$$

and using the quasi Fermi potential we obtain

$$n = N_d\, e^{k(u-\phi_n)} = N_d$$

from the relation above follows that

$$e^{k(u-\phi_n)} = 1 \quad \Rightarrow \quad u = \phi_n$$

On the other hand in the space charge region $\Omega_1,$ $n = 0$ so

$$\Delta u = -\frac{q}{\varepsilon} N_d = -\xi_1$$

and using the quasi Fermi potential

$$n = N_d\, e^{k(u-\phi_n)} = 0$$

therefore

$$e^{k(u-\phi_n)} = 0 \quad \Rightarrow \quad u < \phi_n$$

In the same way for $D_2 = \Omega_2 \cup C_2,$ since $p = N_a$ in $C_2,$ we get

$$\Delta u = 0$$

and

$$p = N_a e^{k(\phi_p - u)} = N_a$$

therefore

$$e^{k(\phi_p - u)} = 1 \quad \Rightarrow \quad u = \phi_p$$

Since in Ω_2 we have $p = 0,$ then

$$\Delta u = \frac{q}{\varepsilon} N_a = \xi_2$$

and

$$p = N_d e^{k(\phi_p - u)} = 0$$

As a result we obtain

$$e^{k(\phi_p - u)} = 0 \quad \Rightarrow \quad \phi_p < u.$$

Then we have a free boundary problem with double obstacle, with the free boundaries

$$\Gamma_1 = \overline{\Omega}_1 \cap C_1 \qquad \Gamma_2 = \overline{\Omega}_2 \cap C_2$$

and the obstacle are represented by the quasi Fermi levels ϕ_p and ϕ_n.

3. QUASI-VARIATIONAL INEQUALITY FORMULATION

This section is devoted to define the functional spaces and variational problems. If $\mathcal{O}$ is an open bounded set of euclidean plane $\mathbb{R}^2$, we shall denote by $C^0(\overline{\mathcal{O}})$ the set of continuous functions on $\overline{\mathcal{O}}$, $C^k(\overline{\mathcal{O}})(k = 1, 2, \ldots)$ the set of all function defined on $\overline{\mathcal{O}}$ with continuous derivatives until the k order.

We denote by $D(\mathcal{O})$ the space of the functions of $C^\infty(\overline{\mathcal{O}})$, which are zero in a neighbourhood of $\partial\mathcal{O}$, the space $D'(\mathcal{O})$ of the distribtions on $\mathcal{O}$ is the dual of $D(\mathcal{O})$, and we denote by $L^p(O)(1 \leq p \leq +\infty)$ the usual space of the real functions, defined a.e. on $\mathcal{O}$, measurable and p- summable on $\mathcal{O}$ (or a.e. bounded on $\mathcal{O}$ if $p = \infty$); $W^{k,p}(O)(k = 1, 2, \ldots; 1 \leq p \leq \infty)$ denotes the Banach space:

$$\{f \in L^p(\mathcal{O}); D_x^h D_y^h f \in L^p(\mathcal{O}) \text{ per } h, l \geq 0, h + l \leq k\}$$

We have the following relations

$$(\Delta u + \xi_1)(u - \phi_n) = 0 \qquad \text{in } D_1 \tag{5}$$

because

$$\begin{aligned} &\Delta u + \xi_1 = 0 \quad \text{e} \quad u < \phi_n \quad \text{in } \Omega_1 \\ &\Delta u \geq \xi_1 \quad \text{e} \quad u = \phi_n \quad \text{in } C_1 \end{aligned}$$

In equal manner in D_2 we will write

$$(\Delta u - \xi_2)(\phi_p - u) = 0 \qquad \text{in } D_2 \tag{6}$$

since

$$\begin{aligned} &\Delta u - \xi_2 = 0 \quad \text{e} \quad u > \phi_p \quad \text{in } \Omega_2 \\ &\Delta u \leq \xi_2 \quad \text{e} \quad u = \phi_p \quad \text{in } C_2 \end{aligned}$$

Let now consider the following set:

$$U = \{v \in H^1(D), v = g \text{ on } \partial D\},$$

where $D = D_1 \cup D_2 \cup D_3$, e $g : \partial D \to \mathbb{R}$ a function with costant value on ∂D which satisfies the mathematical expression of the reverse biased conditions:

$$\begin{aligned} &g = u_1^D \text{ on } \Gamma_1^D \qquad g = u_2^D \text{ on } \Gamma_2^D \\ &u_2^D \leq g \leq u_1^D \quad \text{on } (HB) \cup (BG) \\ &\sup_{\Gamma_1^D} g \leq 0 \leq \inf_{\Gamma_2^D} g \end{aligned} \tag{7}$$

The potential u is related to ϕ_n, ϕ_p and the relation between u, ϕ_n and ϕ_p is given by a non linear operator which maps u in $M_1(u)$ and $M_2(u)$. This operator is defined by logarithmic transformations of the solutions $w_1 = w_1(u)$ and $w_2 = w_2(u)$ of the following mixed boundary value problems in the Slotboom variables:

$$\begin{cases} \nabla \cdot (e^{ku} \nabla w_1) = 0, \\ w_1 = e^{kg_1} \text{ on } \Gamma_1^D, \quad \partial w_1 / \partial n = 0 \text{ on } \Gamma_1^N \end{cases} \tag{8}$$

$$\begin{cases} \nabla \cdot (e^{-ku} \nabla w_2) = 0, \\ w_2 = e^{-kg_2} \text{ on } \Gamma_2^D, \quad \partial w_2 / \partial n = 0 \text{ on } \Gamma_2^N \end{cases} \tag{9}$$

where the values $g_i = g \,|_{\Gamma_i^D}, i = 1,2$ are related with the potential at ohmic contacts; we set

$$V = \{v \in H^1(D), v = e^{-kg} \text{ on } \partial D\}.$$

We may write the quasi Fermi potentials as:

$$\phi_n = -\frac{1}{k} \ln w_1(u) = M_1(u) \qquad \phi_p = \frac{1}{k} \ln w_2(u) = M_2(u)$$

In order to give the classical formulation of the problem, we set $\mathcal{F} = \bigotimes_{i=1}^{3} H^2(D_i) \cup C^1(\overline{D}_i)$, and we have:

Problem 1. *Find* $(u, \varphi_1, \varphi_2)$ *such that* $u = (u_1, u_2, u_3) \in \mathcal{F}$, φ_1 *e* φ_2 *monotone nondecreasing functions (representing* Γ_1 *e* Γ_2*) satisfyng*

$$\Delta u_1 = \xi_1 \quad \text{in } \Omega_1 \qquad \text{where } u < M_1(u) \tag{10}$$

$$\Delta u_1 = 0 \quad \text{in } C_1 \qquad \text{where } u = M_1(u) \tag{11}$$

$$\Delta u_2 = \xi_2 \quad \text{in } \Omega_2 \qquad \text{where } u > M_2(u) \tag{12}$$

$$\Delta u_2 = 0 \quad \text{in } C_2 \qquad \text{where } u = M_2(u) \tag{13}$$

$$\Delta u_3 = 0 \quad \text{in } D_3 \tag{14}$$

with the free interface conditions

$$\frac{\partial u_i}{\partial n} = 0 \quad \text{on } \Gamma_i, \qquad i = 1,2 \tag{15}$$

as well as interface conditions

$$u_1 = u_2 \qquad \frac{\partial u_1}{\partial n} = \frac{\partial u_2}{\partial n} \quad \text{on } (EF), \tag{16}$$

$$u_1 = u_3 \qquad \frac{\partial u_1}{\partial n} = \frac{\partial u_3}{\partial n} \quad \text{on } (FG), \tag{17}$$

$$u_2 = u_3 \qquad \frac{\partial u_2}{\partial n} = \frac{\partial u_3}{\partial n} \quad \text{on } (HF), \tag{18}$$

and boundary conditions

$$u = u_1^D \quad \text{on } \Gamma_1^D \ (OC), \qquad u = u_2^D \quad \text{on } \Gamma_2^D \ (AH). \tag{19}$$

$$\frac{\partial u}{\partial n} = 0 \qquad \text{on } \Gamma_1^N \qquad \frac{\partial u}{\partial n} = 0 \qquad \text{on } \Gamma_2^N \tag{20}$$

Let the convex set

$$K(u) = \{\varphi \in U, \varphi \le \phi_n = M_1(u) \text{ in } D_1, \phi_p = M_2(u) \le \varphi \text{ in } D_2\} \tag{21}$$

We have the following

Theorem 3.1 If u *is a solution of Problem 1 , then* $u \in K(u)$ *must satisfy the quasi-variational inequality*

$$\iint_D \nabla u\, \nabla(\varphi - u)\, dx\, dy + \iint_{D_1} \xi_1(\varphi - u) dx\, dy - \iint_{D_2} \xi_2(\varphi - u) dx\, dy \ge 0, \ \forall \varphi \in K(u) \tag{22}$$

Proof. Let $\varphi \in K(u)$, being $D = \Omega \cup C$ with $\Omega = \Omega_1 \cup \Omega_2$ e $C = C_1 \cup C_2$, we have

$$\iint_D \Delta u\,(\varphi - u)\,dx\,dy = \iint_\Omega \Delta u\,(\varphi - u)\,dx\,dy + \iint_C \Delta u\,(\varphi - u)\,dx\,dy =$$
$$\iint_{\Omega_1} \Delta u\,(\varphi - u)\,dx\,dy + \iint_{\Omega_2} \Delta u\,(\varphi - u)\,dx\,dy\; +$$
$$\iint_{C_1} \Delta u\,(\varphi - u)\,dx\,dy + \iint_{C_2} \Delta u\,(\varphi - u)\,dx\,dy$$

but for (11) and (13) we have

$$\iint_D \Delta u\,(\varphi - u)\,dx\,dy = \iint_{\Omega_1} \Delta u\,(\varphi - u)\,dx\,dy\; + \iint_{\Omega_2} \Delta u\,(\varphi - u)\,dx\,dy \tag{23}$$

moreover from (10) and (12) it follows

$$\iint_D \Delta u\,(\varphi - u)\,dx\,dy = -\iint_{\Omega_1} \xi_1\,(\varphi - u)\,dx\,dy + \iint_{\Omega_2} \xi_2\,(\varphi - u)\,dx\,dy \tag{24}$$

being $\varphi \in K(u)$ will be $\varphi \le \phi_n = M_1(u)$ and $\varphi \ge \phi_p = M_2(u)$ therefore again thanks (11) and (13) $u = M_1(u)$ in C_1 and $u = M_2(u)$ in C_2 then $\varphi \le u$ in C_1 and $\varphi \ge u$ in C_2; this gives

$$\xi_1(\varphi - u) \le 0 \text{ in } C_1 \qquad \xi_2(\varphi - u) \ge 0 \text{ in } C_2$$

therefore in C_1 will be

$$\iint_{D_1} \xi_1\,(\varphi - u)\,dx\,dy = \iint_{C_1} \xi_1\,(\varphi - u)\,dx\,dy + \iint_{\Omega_1} \xi_1\,(\varphi - u)\,dx\,dy \le \iint_{\Omega_2} \xi_1\,(\varphi - u)\,dx\,dy$$

in equal manner for C_2

$$\iint_{D_2} \xi_2\,(\varphi - u)\,dx\,dy = \iint_{C_2} \xi_2\,(\varphi - u)\,dx\,dy + \iint_{\Omega_2} \xi_2\,(\varphi - u)\,dx\,dy \ge \iint_{\Omega_2} \xi_2\,(\varphi - u)\,dx\,dy$$

From (24) we obtain

$$-\iint_D \Delta u\,(\varphi-u)\,dx\,dy = -\iint_{D_1} \Delta u\,(\varphi-u)\,dx\,dy - \iint_{D_2} \Delta u\,(\varphi-u)\,dx\,dy$$

$$\iint_{\Omega_1} \xi_1\,(\varphi-u)\,dx\,dy - \iint_{\Omega_2} \xi_2\,(\varphi-u)\,dx\,dy \geq$$

$$\iint_{D_1} \xi_1\,(\varphi-u)\,dx\,dy - \iint_{D_2} \xi_2\,(\varphi-u)\,dx\,dy$$

For Green's theorem we have

$$\iint_D \Delta u\,(\varphi-u)\,dx\,dy =$$

$$-\iint_D \nabla u\,\nabla(\varphi-u)\,dx\,dy + \int_{\partial D} (\varphi-u)\frac{\partial u}{\partial n}\,ds = -\iint_D \nabla u\,\nabla(\varphi-u)\,dx\,dy$$

for the boundary conditions because $\varphi \in K(u)$.
Therefore

$$\iint_D \nabla u\,\nabla(\varphi-u)\,dx\,dy = -\iint_D \Delta u\,(\varphi-u)\,dx\,dy \geq$$

$$\iint_{D_1} \xi_1\,(\varphi-u)\,dx\,dy - \iint_{D_2} \xi_2\,(\varphi-u)\,dx\,dy$$

then the quasi-variational inequality is satisfied

$$\iint_D \nabla u\,\nabla(\varphi-u)\,dx\,dy + \iint_{D_1} \xi_1(\varphi-u)dx\,dy - \iint_{D_2} \xi_2(\varphi-u)dx\,dy \geq 0,$$

$\forall\varphi \in K(u)$ $\quad\Diamond$

Let now

$$a(u,v) = \iint_D \nabla u\,\nabla v\,dx\,dy \qquad u,v \in U$$

we can rewrite the problem as:

Problem 2.

$$\begin{cases} \text{Find } u \in K(u) \text{ such that} \\ a(u, \varphi - u) \geq (\zeta, \varphi - u), \quad \forall \varphi \in K(u) \\ \text{with } \zeta = -\xi_1 \text{ in } D_1 \quad \zeta = \xi_2 \text{ in } D_2 \quad \zeta = 0 \text{ in } D_3 \end{cases} \tag{25}$$

We can say that the (25) in general is not a variational inequality; it is a variational inequality only when $\forall \varphi \in U, K(\varphi) = K,$, with K being a non-empty closed convex set of $H^1(D)$. In fact it is a new type of entity, we will call it, according with Bensoussan-Goursat-Lions [3], a *quasi-variational inequality*. To the quasi-variational inequality (25) we can associate in a natural way a family of variational inequalities: for z fixed in U we will call *variational section* of the quasi-variational inequality (25) along z, the variational inequality

$$a(w, \varphi - w) \geq (\zeta, \varphi - w), \quad \forall \varphi \in K(z) \tag{26}$$

under the hypothesis (which is standard in the variational case, and which we will make here too) of the coerciveness of the form a

$$a(v, v) \geq \gamma_0 \parallel v \parallel_{1,D}^2 \quad \gamma_0 > 0 \tag{27}$$

$$| \, a(u, v) \, | \leq \gamma_1 \parallel u \parallel_{1,D} \parallel v \parallel_{1,D} \qquad u, v \in U, \quad \gamma_1 > 0 \tag{28}$$

we can say that (26) has one and only one solution.

Therefore if $z \in U,$ the application $S : U \to U,$ such that $u_z = S(z)$ is a solution of (26),

$$u_z \in K(z) : a(u_z, \varphi - u_z) \geq (\zeta, \varphi - u_z), \quad \forall \varphi \in K(z)$$

We will call this application the *variational selection* associated with the quasi-variational inequality (25); under the hypothesis (27), (28), this selection is well defined.

It follows immediately that a solution of (25) is a fixed point for S. Therefore the basic idea to solve the **Problem 2** is to consider the variational selection of (25) and to find its fixed points; an inportant question is what type of fixed point theorem we can use. We do not expect a Lipschitz continuos or a monotonic situation, and thus the classical theorems are useless, more usefull is Schauder's theorem or the results of Joly and Mosco [22].

4. NUMERICAL APPROXIMATIONS

We have seen like some free boundary problem very complex in their structure can be solved through opportune modifications tied to the physical characteristics of the problem by means of variational and quasi-variational inequalities. From a numerical point of view the quasi-variational inequalities can be solved with the Bensoussan-Lions iterative scheme, which is a sequence of iterative variational inequalities, for a fixed obstacle. Quasi-variational inequalities and their applications in different areas have been investigated since the early eighties notably by Bensoussan, Lions, Mosco and Baiocchi. However, very little was known about the numerical methods for such problems till recently [10]. We show a technique for the approximation of quasi-variational inequalities.

To determinate the depletion region in a $p-n$ junction we have to solve the following model

$$\begin{cases} \text{Find } u \in K(u) \text{ such that} \\ a(u, \varphi - u) \geq (\zeta, \varphi - u), \quad \forall \varphi \in K(u) \\ \text{with } \zeta = -\xi_1 \text{ in } D_1, \quad \zeta = \xi_2 \text{ in } D_2, \zeta = 0 \text{ in } D_3 \end{cases} \tag{29}$$

with

$$K(u) = \{\varphi \in U, \varphi \leq \phi_n = M_1(u) \text{ in } D_1, \phi_p = M_2(u) \leq \varphi \text{ in } D_2\}$$

Where the obstacles $M_1(u)$ e $M_2(u)$ are defined solving the two mixed boundary value problems

$$\begin{cases} \nabla \cdot (e^{ku} \nabla w_1) = 0, \\ w_1 = e^{-kg_1} \text{ on } \Gamma_1^D, \quad \partial w_1 / \partial n = 0 \text{ on } \Gamma_1^N \end{cases} \tag{30}$$

$$\begin{cases} \nabla \cdot (e^{-ku} \nabla w_2) = 0, \\ w_2 = e^{kg_2} \text{ on } \Gamma_2^D, \quad \partial w_2 / \partial n = 0 \text{ on } \Gamma_2^N \end{cases} \tag{31}$$

by a maximum principle we obtain $w_1, w_2 > 0$, thus we can compute the obstacles as follow

$$M_1(u) = -\frac{1}{k}\ln w_1(u) \qquad M_2(u) = \frac{1}{k}\ln w_2(u)$$

Consider a regular triangulation $\mathcal{T}_h$, established over the open polygonal $D \subset \mathbb{R}^2$ such that

$$D = \bigcup_{T\in\mathcal{T}_h} T$$

Let T a triangle in $\mathcal{T}_h$, and $\mathbb{P}_1(T)$ the space of all polynomials of degree ≥ 1 restricted to the set T. We associate with $\mathcal{T}_h$ the usual finite element spaces:

$$X_h = \{v_h \in C^0(\bar{D}), v_h\,|_T \in \mathbb{P}_1(T), \forall T \in \mathcal{T}_h\}, \qquad V_{0h} = \{v_h \in X_h, v_h = 0 \text{ on } \partial D\},$$
$$U_h = \{u_h \in X_h, u_h = g_h \text{ on } \partial D\}, \qquad V_h = \{v_h \in X_h, v_h = e^{kg_h} \text{ on } \partial D\}.$$

Then we define the obstacles as

$$M_{1h} : u_h \in U_h \longrightarrow M_{1h}(u_h) = r_h(-\frac{1}{k}\ \ln w_{1h})$$

$$M_{2h} : u_h \in U_h \longrightarrow M_{2h}(u_h) = r_h(\frac{1}{k}\ \ln w_{2h})$$

with $w_{1h}, w_{2h} \in V_h$ which satisfy

$$\nabla\cdot(e^{ku_h}\nabla w_{1h}) = 0, \quad \forall u_h \in V_h$$

$$\nabla\cdot(e^{-ku_h}\nabla w_{2h}) = 0, \quad \forall u_h \in V_h$$

We introduce the convex set

$$K_h(u_h) = \{\varphi_h \in U_h, \varphi_h \leq M_{1h}(u), M_{2h}(u) \leq \varphi_h\}.$$

We have the following finite element formulation of the problem

$$\begin{cases} \text{Find } u_h \in K_h(u_h) \text{ such that} \\ a(u_h, \varphi_h - u_h) \geq (\zeta, \varphi_h - u_h), \quad \forall \varphi_h \in K_h(u_h) \\ \zeta \in L^\infty(D) \end{cases} \tag{32}$$

To update the obstacles the continuity equations can be solved and then we have a system of quasi-variational inequality and we use a Bensoussan-Lions iterative scheme to solve the problem. We shall recall some results related to elliptic variational inequalities that are necessary to prove some useful qualititive properties.

5. ASSUMPTIONS AND NOTATIONS

In this section we are concerned with the standard finite element approximation of the system of quasi-variational inequalities (QVIs): Find a vector $U = (u^1, ..., u^M)$ satisfying

$$\begin{cases} a^i(u^i, v - u^i) \geq (f^i, v - u^i) \quad \forall v \in H^1(\Omega) \\ u^i \leq \psi u^i; \quad u^i \geq 0; \quad v \leq \psi u^i \end{cases} \tag{33}$$

where Ω is a bounded smooth domain of $\mathbb{R}^N$ with boundary $\partial\Omega$, $a^i(u, v)$ are bilinear forms defined on $H^1(\Omega) \times H^1(\Omega)$, $(\cdot,\cdot)$ is the inner product in $L^2(\Omega)$ and f^i are ψ regular functions. For sake of simplicity we will treat the case of one obstacle, considering the two obstacle problem a generalization in which we replace the constraint set of (21) with the following: $K = \{v \in H^1(\Omega) \text{ such that } v \leq \psi\}$

We are given functions

$$a^i_{jk}(x), a^i_k(x), a^i_0(x) \in C^2(\overline{\Omega}), \quad x \in \overline{\Omega}, \quad 1 \leq k, \quad j \leq N, \quad 1 \leq i \leq M,$$

sufficiently smooth such that:

$$\sum_{1 \leq j,k \leq N} a^i_{jk}(x)\xi_j\xi_k \geq \alpha \parallel \xi \parallel^2, \qquad \xi \in \mathbb{R}^N; \ \alpha > 0 \tag{34}$$

$$a_{jk} = a_{kj}, \quad a^i_0(x) \geq c_0 > 0; \tag{35}$$

We define the second-order , uniformly elliptic operator of the form

$$\mathcal{A}^i = \sum_{1\le j,k\le N} a^i_{jk}(x)\frac{\partial^2}{\partial x_j \partial x_k}\sum_{k=1}^{N} b^i_k(x)\frac{\partial}{\partial x_k} + a^i_0(x) \tag{36}$$

and the bilinear forms associated with $\mathcal{A}^i$: for any $u, v \in H^1(\Omega)$

$$a^i(u,v) = \int_\Omega \left(\sum_{1\le j,k\le N} a^i_{jk}(x)\frac{\partial u}{\partial x_j}\frac{\partial v}{\partial x_k} + \sum_{k=1}^{N} a^i_k(x)\frac{\partial u}{\partial x_k} v + a^i_0(x)uv \right) dx \tag{37}$$

that we assume to be coercive, i.e., there exist $\gamma > 0$ such that

$$a^i(v,v) \ge \gamma \parallel v \parallel^2_{H^1(\Omega)}; \quad \forall v \in H^1(\Omega). \tag{38}$$

The right hand sides $f^1,\ldots,f^M$ are also given such that

$$f^i \in L^\infty(\Omega); \;\; f^i \ge 0 \tag{39}$$

We shall also need the following norm:

$$\forall W = (w^1,\ldots,w^M) \in \prod_{i=1}^{M} L^\infty(\Omega), \tag{40}$$

$$\parallel W \parallel_\infty = \max_{1\le i\le M} \parallel w^i \parallel_{L^\infty}, \tag{41}$$

where $\parallel \cdot \parallel_{L^\infty}$ denotes the classic L^∞ norm.

5.1 Elliptic Variational inequalities

Let f be a function in L^∞ and ψ an obstacle in $W^{2,\infty}$ such that $\psi \ge 0$ on $\partial\Omega$. Let also $\mathcal{A}$ be an elliptic operator and $a(\cdot,\cdot)$ its associated coercive bilinear form of the same forms as those defined in (36) and (37), respectively. We consider the following elliptic variational inequality (VI): Find $u \in K$ such that

$$a(u, v-u) \ge (f, v-u) \quad \forall v \in K \tag{42}$$

where $K=\{v\in H1(\Omega)$ such that $v\le\psi$ a.e.$\}$ Thanks to [23,5], the VI (42) has one and only one solution. Moreover, $u\in W^{2,p}, 1\le p\le\infty$ and satisfies

$$\| u \|_{W^{2,p}} \le C(\| f \|_\infty + \| \mathcal{A}\psi \|_\infty) \tag{43}$$

Definition 1. *$z\in K$ is said to be a subsolution for VI (42) if*

$$a(z,v)\le(f,v)\quad \forall v\in K,\qquad v\ge 0 \tag{44}$$

Let X denote the set of such subsolutions, then (see [5]) the solution of VI (42) is the maximum element of X.

Consider now the following mapping:

$$\begin{aligned}\sigma: L^\infty(\Omega) &\longrightarrow L^\infty(\Omega)\\ \psi &\longrightarrow \sigma(\psi)=u\end{aligned}$$

where u is the solution to VI (42). The mapping σ is increasing, concave, and Lipschitz continuos with respect to ψ [7].

Existence of a unique solution to system (33) can be proved, adapting the approach developed in [4].

Indeed, let $H^+=(L_+^\infty(\Omega))^M=\{V=(v^1,\ldots,v^M)$ such that $v^i\in L_+^\infty(\Omega)\}$, equipped with the norm: $\| V \|_\infty=\max\limits_{1\le i\le M}\| v^i \|_{L^\infty(\Omega)}$ where $L_+^\infty(\Omega)$ is the positive cone of $L^\infty(\Omega)$. We consider the mapping

$$\begin{aligned}T: H^+ &\longrightarrow H^+\\ W &\longrightarrow TW=\zeta=(\zeta^1,\ldots,\zeta^M)\end{aligned}$$

where $\zeta^i=\sigma(\psi w^i)\in H^1(\Omega)$ is solution to the following VI:

$$\begin{cases}a^i(\zeta^i,v-\zeta^i)\ge(f^i,v-\zeta^i)\ \forall v\in H^1(\Omega)\\ \zeta^i\le\psi w^i\quad ;\quad v\le\psi w^i\end{cases} \tag{45}$$

Problem (45) being a coercive VI, thanks to [23], [5] has one and only one solution.

Consider now $\overline{U}^0=(\overline{u}^{1,0},\ldots,\overline{u}^{M,0})$, where $\overline{u}^{i,0}$ is the solution to the following variational equation:

$$a^{i}(\overline{u}^{i,0}, v) = (f^{i}, v) \forall v \in H^{1}(\Omega) \tag{46}$$

Due to (39), problem (46) has a unique solution. Moreover, $\overline{u}^{i,0} \in W^{2,p}(\Omega);\ 2 \leq p < \infty$

Proposition 5.1 *Let* $\mathbb{C} = \{W \in H^{+}$ such that $0 \leq W \leq \overline{U}^{0}\}$, *then* T *maps* $\mathbb{C}$ *into itself. Moreover is* T *increasing, concave and Lipschitz continuous on* H^{+}.

We notice that the solutions $U = (u^{1}, \ldots, u^{M})$ of system (33) correspond to fixed points of mapping T, that is $U = TU$. In this view it is natural to consider the following iterative scheme.

5.2 A Continuous Iterative Scheme of Bensoussan-Lions Type

An iterative scheme for the solution of system of QVIs is given as follows.

Starting from $\overline{U}^{0}$ defined in (46) (resp. $\underline{U}^{0} = (0, \ldots, 0)$), we define the sequences

$$\overline{U}^{n+1} = T\overline{U}^{n}\ ;\ n = 0, 1, \ldots \tag{47}$$

respectively

$$\underline{U}^{n+1} = T\underline{U}^{n}; n = 0, 1, \ldots. \tag{48}$$

Making use of properties of mapping T we have the following convergence result.

Theorem 5.2 *The sequences* $(\overline{U}^{n})$ *and* $(\underline{U}^{n})$ *are monotone and well defined in* $\mathbb{C}$. *Moreover, they converge respectively from above and below to the unique solution of system (33), (cf. [4] p.453).*

The following estimations provide a rate of convergence for sequences.

Lemma 5.3 *There exist a constant* $\mathbb{C}$ *independent of* n *such that for any* $i = 1, 2, \ldots, M$, *[15]*

$$\max_{n \geq 0} (\| \overline{u}^{i,n} \|_{W^{2,p}(\Omega)}, \| \underline{u}^{i,n} \|_{W^{2,p}(\Omega)}) \leq C\ ;\ 2 \leq p < \infty$$

Theorem 5.4 *Assume* $a^i_{jk}(x)$ *in* $C^{1,\alpha}(\overline{\Omega})$, $a^i(x)$, $a^i_0(x)$ *and* f^i *in* $C^{0,\alpha}(\Omega)$. *Then* $(u^1,...,u^M) \in (W^{2,p}(\Omega))^M;\ 2 \leq p < \infty$.

Proposition 5.5 *There exist a positive constant* $0 \leq \mu \leq 1$ *such that*

$$\| \overline{U}^n - U \|_\infty \leq \mu^n \| \overline{U}^0 \|_\infty \tag{49}$$

$$\| \underline{U}^n - U \|_\infty \leq \mu^n \| \overline{U}^0 \|_\infty \tag{50}$$

5.3 The Discrete Problem

Let Ω be decomposed into triangles and let $\mathcal{T}_h$ denote the set of all those elements; $h > 0$ is the mesh size. We assume the family $\mathcal{T}_h$ is regular and quasi-uniform.

Let V_h denote the standard finite element space, $A^i, 1 \leq i \leq M$ be the matrices with generic coefficients $a^i(\varphi_l, \varphi_s)$, where $\varphi_s, s = 1,2,...m(h)$ are the nodal basis functions. Let also r_h be the usual interpolation operator.

In the sequel of the paper, we shall use the discrete maximum assumption (d.m.p.). Under the d.m.p., we shall achieve a similar study to that devoted to the continuos problem, therefore the qualitative properties and results stated in the continuous case are conserved in the discrete case.

The discrete system of QVIs is then defined as follows: Find $U_h = (u^1_h,...,u^M_h) \in (V_h)^M$ such that

$$\begin{cases} a^i(u^i_h, v - u^i_h) \geq (f^i, v - u^i_h) \quad \forall v \in V_h \\ \qquad u^i_h \leq r_h \psi u^i_h \ ; u^i_h \geq 0 ;\ v \leq r_h \psi u^i_h \end{cases} \tag{51}$$

Existence and uniqueness of a solution of system (51) can be shown similarly to that of the continuous case provided the discrete maximum principle is satisfied. Indeed, the idea for proving that consists of associating with the system (51) the following discrete fixed point mapping:

$$\begin{aligned} T_h : H^+ &\longrightarrow (V_h)^M \\ W &\longrightarrow T_h W = \zeta_h = (\zeta^1_h, ..., \zeta^M_h) \end{aligned}$$

where $\zeta^i_h = \sigma_h(\psi w^i)$ is the solution of the following discrete VI:

$$\begin{cases} a^i(\zeta_h^i, v - \zeta_h^i) \geq (f^i, v - \zeta_h^i) \quad \forall v \in V_h \\ \zeta_h^i \leq r_h \psi w^i \text{ , } v \leq r_h \psi w^i \end{cases} \tag{52}$$

Under the d.m.p the mapping T_h possesses analogous properties to that of mapping T.

Let $\overline{U}_h^0 = (\overline{u}_h^{1,0},...,\overline{u}_h^{M,0})$ be the discrete analogue to the solution of problem (46) :

$$a^i(\overline{u}_h^{i,0}, v) = (f^i, v) \forall v \in V_h \quad 1 \leq i \leq M \tag{53}$$

Proposition 5.6 *T_h maps $\mathbb{C}_h$ into itself, where $\mathbb{C}_h = \{W \in (L^\infty(\Omega))^M$ such that $0 \leq W \leq \overline{U}_h^0\}$, moreover T_h is increasing, concave and Lipschitz continuous on H^+.*

It is not hard to see that the solution of system of QVIs (51) is a fixed point of T_h, that is $U_h = T_h U_h$. Therefore, as in the continuous problem, one can define the following discrete iterative scheme.

Starting from $\overline{U}_h^0$ solution of (53) (resp. from $\underline{U}_h^0 = (0,...,0)$), one can compute

$$\overline{U}_h^{n+1} = T_h \, \overline{U}_h^n \quad n = 0,1,... \tag{54}$$

(resp.)

$$\underline{U}_h^{n+1} = T_h \underline{U}_h^n \quad n = 0,1,... \tag{55}$$

Theorem 5.7 *Under the d.m.p. the sequences $(\overline{U}_h^n)$ and $(\underline{U}_h^n)$ are monotone and well defined in $\mathbb{C}_h$. Moreover, they converge respectively from above and below to the unique solution of system (51)*

Using the above result, we are able to establish the geometric convergence of sequence $(\overline{U}_h^n)$ and $(\underline{U}_h^n)$.

Proposition 5.8 *There exist a positive constant $0 \leq \mu \leq 1$ such that*

$$\| \overline{U}_h^n - U_h \|_\infty \leq \mu^n \, \| \overline{U}_h^0 \|_\infty \tag{56}$$

$$\| \underline{U}_h^n - U_h \|_\infty \leq \mu^n \, \| \overline{U}_h^0 \|_\infty \tag{57}$$

5.4 The Finite Element Error Analysis

We recall some known L^{∞}-error estimates result and introduce an auxiliary problem. From now on C will denote a constant independent of both h and n.

Theorem 5.9 *Let $\overline{u}^{i,0}$ (respectively, $\overline{u}_h^{i,0}$), be the solution of problem (46), (respectively (53)). Then (see [11,19]]*

$$\| \overline{u}^{i,0} - \overline{u}_h^{i,0} \|_{L^{\infty}(\Omega)} \leq Ch^2 \mid log \ h \mid^{3/2} \qquad \forall i = 1, 2, \ldots, M \tag{58}$$

Theorem 5.10 *Let the d.m.p. and regularity result (43) hold. Then (see [14])*

$$\| u - u_h \|_{L^{\infty}(\Omega)} \leq Ch^2 \mid log \ h \mid^2 \tag{59}$$

We introduce the following discrete sequence

$$\begin{cases} \widetilde{U}_h^{n+1} = T_h \overline{U}^n; \quad n = 0, 1, \ldots \\ \text{with } \ \widetilde{U}_h^0 = \overline{U}_h^0 \end{cases} \tag{60}$$

where $\overline{U}_h^0$ is defined in (53) and for any $n \geq 1$, $\tilde{u}_h^{i,n}$ is a solution to following discrete variational inequality:

$$\begin{cases} a^i(\tilde{u}_h^{i,n+1}{}_h, v - \tilde{u}_h^{i,n+1}) \geq (f^i, v - \tilde{u}_h^{i,n+1}) \qquad \forall v \in V_h \\ \tilde{u}_h^{i,n+1} \leq r_h \psi \overline{u}^{i,n} \ , \ v \leq r_h \psi \overline{u}^{i,n} \end{cases} \tag{61}$$

$\overline{U}^n = (\overline{u}^{1,n}, \ldots, \overline{u}^{M,n})$ being the sequence defined by (48). Again, thanks to [5], (61) has one and only one solution.

We notice that $\tilde{u}_h^{i,n}$ solution of (61) represents the standard finite element approximation of $\overline{u}^{i,n}$. Therefore, using the regularity result provided by Lemma 4.2 and next adapting [12], we have the following uniform error estimate.

Proposition 5.11

$$\| \overline{U}^n - \widetilde{U}_h^n \|_{\infty} \leq Ch^2 \mid log \ h \mid^2 \tag{62}$$

with the use of the result seen above we introduce the following :

Lemma 5.12

$$\| \overline{U}^n - \overline{U}_h^n \|_\infty \leq \sum_{p=0}^{n} \| \overline{U}^p - \widetilde{U}_h^p \|_\infty \tag{63}$$

Now guided by Propositions 5, 8, 11, Lemma 12 Theorem 9 we are in a position to prove the main result.

Theorem 5.13

$$\| U - U_h \|_\infty \leq Ch^2 \mid log \ h \mid^3 \tag{64}$$

$$\| U - U_h \|_{1,\infty} \leq Ch \mid log \ h \mid^3 \tag{65}$$

where: $\| U \|_{1,\infty} = \max_{1 \leq i \leq M} \| u^i \|_{W^{1,\infty}(\Omega)}$

Proof. Using estimations (49), (56) we have:
$\| U - U_h \|_\infty \leq \| U - \overline{U}^n \|_\infty + \| \overline{U}^n - \overline{U}_h^n \| + \| \overline{U}_h^n - U_h \|_\infty$

$$\leq \| U - \overline{U}^n \|_\infty + \sum_{p=0}^{n} \| \overline{U}^p - \overline{U}_h^p \|_\infty + \| \overline{U}_h^n - U_h \|_\infty \leq$$

$$\| U - \overline{U}^n \|_\infty + \| \overline{U}^0 - \overline{U}_h^0 \|_\infty + \sum_{p=1}^{n} \| \overline{U}^p - \overline{U}_h^p \|_\infty + \| \overline{U}_h^n - U_h \|_\infty$$

$$\leq \mu^n \ \| \overline{U}^0 \|_\infty + \mu^n \ \| \overline{U}_h^0 \|_\infty + Ch^2 \mid log \ h \mid^{3/2} + nCh^2 \mid log \ h \mid^2$$

Finally, letting $\mu^n = h^2$ we get the desired result.

The $W^{1,\infty}$-error estimate (65) follows immediately from the standard inverse inequality (cf. [11]). It is important to notice that the error estimate obtained contains an extra power in $(log \ h)$ than expected, due to the approach followed.

6. RESULTS AND CONCLUSIONS

The variational method presented is an alternative approach to the classical drift-diffusion model which can be described by a nonlinear Poisson equation for the electrostatic potential coupled with a system of convection-diffusion equations for the transport of charge

$$\begin{cases} \nabla^2 \psi = \dfrac{q}{\varepsilon}(n - p - C) \\ \nabla \cdot (-n\mu_n \nabla\psi + D_n \nabla n) = R(\psi, n, p) \\ \nabla \cdot (p\mu_p \nabla\psi + D_p \nabla p) = R(\psi, n, p) \end{cases}$$

In the context of semiconductor device modelling, the presence of strong variation of the convection term $\nabla\psi$ is a source of numerical troubles since it give rise to sharp internal layers.

This equations can be solved with Gummel like process to decouple the system and Newton's method to obtain the resulting sequences of linear systems.

The Poisson problem leads to a symmetric, positive definite system which can be solved iteratively using BCG.

The transport equation leads to nonsymmetric indefinite systems; moreover their solutions exibit steep layers and are subject to numerical oscillations and instabilities if standard Galerkin-type discretization strategies are used.

We present numerical result for Variational Method and Drift Diffusion model for a two dimensional p-n junction with the following parameters: $\xi_1 = \xi_2 = 4, u^D = |V_a|$ where V_a is the applied potential with value $-5V, -4V, -2V$.

Variational Method					**Drift-Diffusion**		
$h = 1/6 = 0.16$							
Appl.Pot.(V)	-5	-4	-2		-5	-4	-2
Iter. num.	253	175	120		296	225	167
Esec. time (sec)	25	18	13		42	31	23
Depletion layer size (μm)	1.19	1.01	0.78		1.18	1.02	0.79

Table 1. Numerical results with $h = 1/6$

Variational Method					**Drift-Diffusion**		
$h = 1/12 = 0.083$							
Appl.Pot.(V)	-5	-4	-2		-5	-4	-2
Iter. num.	615	524	392		712	638	453
Esec. time(sec)	224	192	133		370	321	235
Depletion layer size(μm)	1.22	1.00	0.76		1.18	1.01	0.80

Table 2. Numerical results with h = 1/2

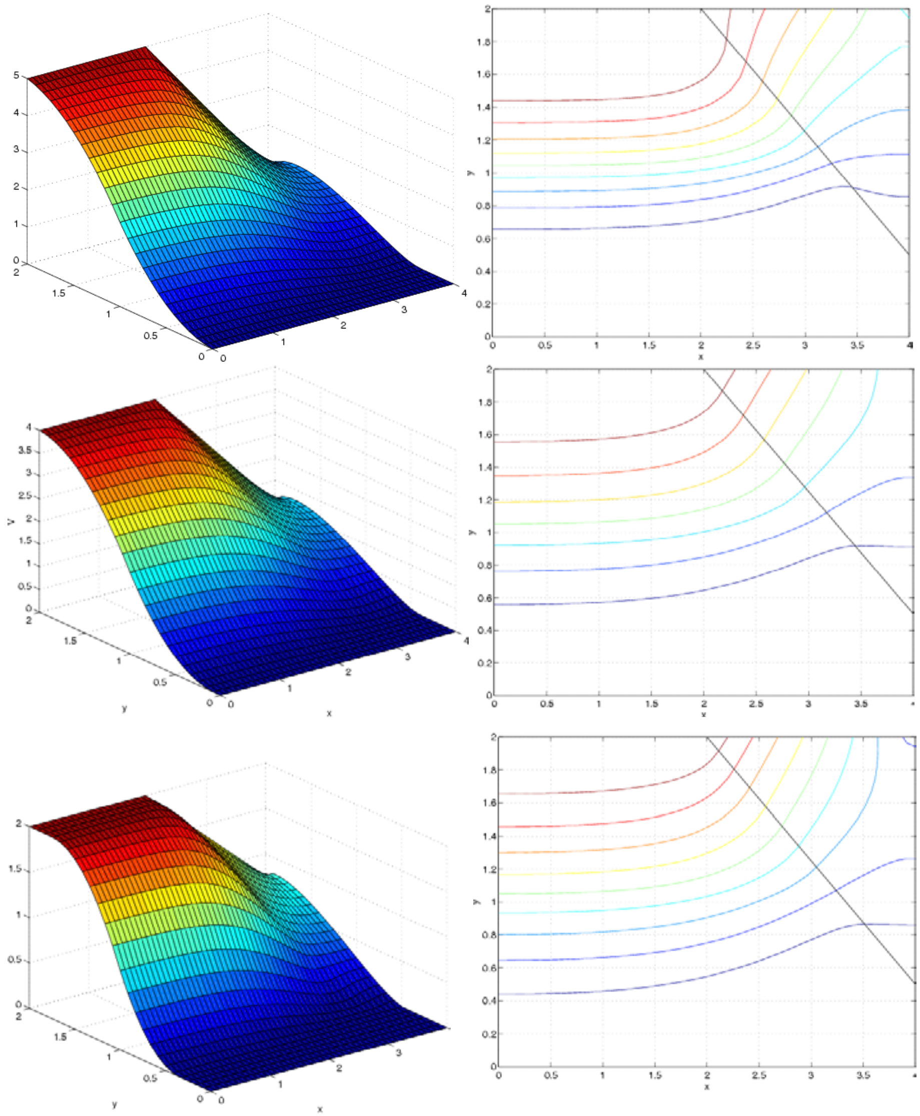

Figure 2. Varational Method. Numerical solution and depletion layer $V_a = -5V, -4V, -2V$

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