

AN HYBRID FINITE ELEMENT METHOD FOR A QUASI-VARIATIONAL INEQUALITY MODELING A SEMICONDUCTOR

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Abstract. A problem of determining the characteristics of a semiconductor can be reduced to the study of the quasi-variational inequality, (J. Abouchabaka, R. Aboulaïch, A. Nachaoui and A. Souissi, *COMPEL* **18** (1999) 143–164.) where the obstacle $\mathcal{M}(u)$ is the solution of an elliptic problem depending on u . We present here an hybrid finite element method for the computation of obstacle $\mathcal{M}(u)$ and we discuss some numerical aspects appearing in its approximation.

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1. INTRODUCTION

The stationary distribution of the carrier motions inside a semiconductor device is described by the following system of nonlinear elliptic partial differential equations:

$$\nabla \cdot \varepsilon \nabla u = q(n - p - N) \quad (1)$$

$$\nabla \cdot J_n = 0, \quad J_n = D_n \nabla n - \mu_n n \nabla u \quad \text{in } \Omega \quad (2)$$

$$\nabla \cdot J_p = 0, \quad J_p = -(D_p \nabla p + \mu_p p \nabla u) \quad (3)$$

where (1) is the Poisson equation, (2) is the continuity equations for electrons and (3) is the continuity equations for holes.

The domain Ω is an open of \mathbb{R}^2 corresponding to the interior of the semiconductor device, of lipchitzian boundary $\partial\Omega$ with $\partial\Omega = \Gamma_D \cup \Gamma_N$. These equations are subject to the following boundary conditions:

$$\nu \cdot \nabla u = \nu \cdot \nabla n = \nu \cdot \nabla p = 0 \quad \text{on } \Gamma_N \quad (4)$$

$$u = u_d, \quad n = n_d, \quad p = p_d; \quad \text{on } \Gamma_D, \quad (5)$$

where u_d, n_d, p_d are given functions on Γ_D and ν denotes the external normal vector of $\partial\Omega$.

Keywords. Semiconductor device, quasi-variational inequality, finite elements method, topological degree.

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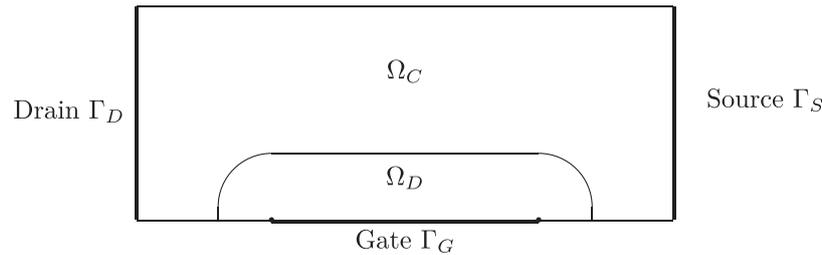


FIGURE 1. Junction field effect transistor.

In the van Roosbroeck model (1)–(3), the potential u , the electron density n and the hole density p are the unknowns; the doping function N , the charge constant q and the permittivity ε are given. In the expression of the current density J_n the quantities D_n , μ_n represent the mobility and the diffusivity of the electrons. This problem has been studied by several authors [19, 20, 30, 31], especially in a fairly general framework, [13, 15, 16, 29] and for more realistic boundary conditions by the author [13, 16]. Uniqueness is not possible in general, it is obtained under restrictive hypotheses [14, 17, 23].

Several authors are interested in the approximation of this system. For example, a finite element approximation is done in [22, 24, 28, 34], mixed finite elements is in [32], and several approximations based on the use of finite volumes can be consulted in [4, 6, 7] and the references therein. A finite-difference approximation is used in [2] for the equilibrium electrostatic potential.

Concerning the convergence of approximations, we refer the reader to [24] where he will find a general framework for the study of the convergence of approximations whatever their types. An application of this study to finite elements can be found in [22].

Under physical assumptions, we show that the system (1)–(2) leads as a limit case to a quasi-variational equation [1, 12, 25], given in the case of a unipolar field-effect semiconductor, by

$$\int_{\Omega} \nabla u \nabla (\varphi - u) dX \geq \xi \int_{\Omega} (\varphi - u) dX \quad \forall \varphi \in K(u) \quad (6)$$

with $K(u) = \{v \in H^1(\Omega), v = u \text{ on } \Gamma_D \text{ and } v \leq \mathcal{M}(u) \text{ a.e. dans } \Omega\}$ where $\mathcal{M}(u)$ is the solution of problem

$$\begin{cases} \nabla e^u \nabla e^{-w} = 0 \\ w = w_d \text{ on } \Gamma_D, \\ \frac{\partial w}{\partial \nu} = 0 \text{ sur } \Gamma_N, \end{cases} \quad (7)$$

with $u_d = w_d = 0$ on the source, $u_d = w_d = V^+ \geq 0$ on the drain, $u_d = V^- \leq 0$ and $w_d = V^+$ on the grid (see Fig. 1).

This IQV model is a formulation of a free boundary problem where we have to find the unknown boundary separating two sets Ω_C and Ω_D , corresponding to the charge neutrality region where the potential u and the Fermi quasi-potential $w = \mathcal{M}(u)$ are identical and the depletion region where $u < w$ [1, 21, 25].

The existence and uniqueness of the solution to the problem (6)–(7) are discussed in [1] where the authors propose a technique based on topological degree theory which extends the results of [20] to cases where the solution is not regular. The solution of the quasi-variational inequality being obtained as the limit of a series of variational inequalities where the two problems (6) and (7) are decoupled

$$u_m \in K(u_{m-1}), \quad \int_{\Omega} \nabla u_m \nabla (\varphi - u_m) dX \geq \xi \int_{\Omega} (\varphi - u_m) dX \quad \forall \varphi \in K(u_{m-1}). \quad (8)$$

The approximation of (6) poses no problem, any reasonable approximation scheme works. The difficulty appears in the discretization of (7) where it is necessary to take into account the electric field which can be very important in certain regions of the semiconductor. We are interested here in a hybrid discretization, [5], whose main property is the preservation of electric current, which is a particularly important property in practice, and an exact computation of the integral of the exponential. For recent use of this type of approximation in different fields see [3, 9, 18, 26, 27, 33] and the references therein.

2. HYBRID METHOD FOR THE OBSTACLE APPROXIMATION

Using the change of variable $\eta = e^{-\mathcal{M}(u)}$, we obtain new expressions of the equations verified by the electric current J :

$$e^{-u} J - \nabla \eta = 0 \text{ and } \nabla \cdot J = 0. \tag{9}$$

The multiplication of the first equation of (9) by $\varphi \in [L_2(\Omega)]^2$ and the second equation by $\psi \in H^1(\Omega)$, $\psi = 0$ sur Γ_D and integration on Ω gives rise to the following problem: find $u \in H^1(\Omega)$ and $J \in [L_2(\Omega)]^2$ such that

$$\left\{ \begin{aligned} \int_{\Omega} e^{-u} J \cdot \varphi \, dX - \int_{\Omega} \nabla \eta \cdot \varphi \, dX &= 0 \quad \forall \varphi \in [L_2(\Omega)]^2 \\ \int_{\Omega} J \cdot \nabla \psi \, dX &= 0 \quad \forall \psi \in H^1(\Omega), \psi = 0 \text{ on } \Gamma_D. \end{aligned} \right. \tag{10}$$

The hybrid discretization will be based on the approximation of (10). For this, consider a regular triangulation \mathcal{T}_h of Ω and define the following finite-dimensional spaces:

$$\begin{aligned} M_h &= \{ \mu_h \in C^0(\bar{\Omega}), \mu_h|_T \in \mathbb{P}_1(T), \forall T \in \mathcal{T}_h \} \\ M_h^\zeta &= \{ \mu_h \in M_h, \mu_h = \zeta \text{ sur } \Gamma_D \} \\ X_h &= \{ q_h \in [L_2(\Omega)]^2, q_h|_T \in [\mathbb{P}_0(T)]^2 \forall T \in \mathcal{T}_h \} \end{aligned}$$

where $\mathbb{P}_k(T)$ is the set of polynomials in x, y of degree less than or equal to k , restricted to T . The current J and the function η are then approximated by $J_h \in X_h$ and $\eta_h \in M_h^{\eta_d}$ such that

$$\left\{ \begin{aligned} \int_{\Omega} e^{-u} J_h \cdot q_h \, dX - \int_{\Omega} \nabla \eta_h \cdot q_h \, dX &= 0 \quad \forall q_h \in X_h \\ \int_{\Omega} J_h \cdot \nabla \mu_h \, dX &= 0 \quad \forall \mu_h \in M_h^0. \end{aligned} \right. \tag{11}$$

The choice of X_h and M_h^0 results in the uniqueness of the solution of (11), (see [5]).

On each triangle T , q_h and J_h are constant, the system (11) is then written

$$\left\{ \begin{aligned} \sum_{T \in \mathcal{T}_h} q_h \cdot (J_h \int_T e^{-u} \, dX - \int_T \nabla \eta_h \, dX) &= 0 \\ \sum_{T \in \mathcal{T}_h} J_h \cdot \int_T \nabla \mu_h \, dX &= 0. \end{aligned} \right. \tag{12}$$

The choice in the first equation of (12) of an element of X_h not zero on the triangle T and vanishing elsewhere results in:

$$J_h \int_T e^{-u} \, dX - \int_T \nabla \eta_h \, dX = 0,$$

hence

$$J_h = \frac{\int_T \nabla \eta_h \, dX}{\int_T e^{-u} \, dX}. \tag{13}$$

The introduction of the relation (13) in the second equation of (12) gives a system where the unique unknown is η_h

$$\eta_h \in M_h^{\eta_d}, \quad \sum_{T \in \mathcal{T}_h} \alpha_T \int_T \nabla \eta_h \cdot \nabla \mu_h \, dX = 0, \quad \forall \mu_h \in M_h^0. \tag{14}$$

where α_T is defined by $\alpha_T = mes(T) \left(\int_T e^{-u} \, dX \right)^{-1}$.

The following proposition allows us to define an approximation of $\mathcal{M}(u)$

Proposition 2.1. *Suppose that the triangulation \mathcal{T}_h is such that for all $T \in \mathcal{T}_h$ the angles of T are $\leq \frac{\pi}{2}$, then $\min_{\Gamma_D}(\eta_h) \leq \eta_h \leq \max_{\Gamma_D}(\eta_h)$.*

Proof. The matrix A associated with the system (14) is unreduced, symmetric with strictly dominant diagonal. These coefficients verify the following relation

$$\sum_j A_{ij} \geq 0, \quad \forall i, \quad A_{ij} \leq 0 \text{ pour } i \neq j.$$

As the second member of (14) is zero, we can deduce (cf. Ciarlet [8]) that the principle of discrete maximum can be applied to η_h , that is:

$$\min \eta_d \leq \eta_h \leq \max \eta_d.$$

□

Since $\eta_d(x) > 0 \quad \forall x \in \Gamma_D$, we then define an approximation M_h de M by $\mathcal{M}_h(u) = r_h\{-\ln \eta_h(u)\}$.

3. APPROXIMATION OF Q. V. I.

Consider now the convex $K_h(u)$ defined by

$$K_h(u) = \{\varphi_h \in M_h^{u_d}, \varphi_h \leq \mathcal{M}_h(u)\},$$

the finite element approximation of Q.V.I. is then given by

$$u_h \in K_h(u_h), \quad \int_{\Omega} \nabla u_h \nabla (\varphi_h - u_h) \, dX \geq \xi \int_{\Omega} (\varphi_h - u_h) \, dX \quad \forall \varphi_h \in K_h(u_h). \tag{15}$$

Proposition 3.1. *The approximate problem (15) admits a solution in $M_h^{u_d}$.*

Proof. Let w_{hs} be the solution of

$$w_{hs} \in M_h^{w_d}, \quad \int_{\Omega} \nabla w_{hs} \nabla \varphi_h \, dX = 0, \quad \forall \varphi_h \in M_h^0,$$

and let S_t be the operator who with $z_h \in M_h$ associates z'_h solution of the variational equation

$$z'_h \in K_{ht}(z_h), \int_{\Omega} \nabla u_h \nabla (\varphi - u_h) dX \geq \xi \int_{\Omega} (\varphi_h - u_h) dX \forall \varphi \in K_{ht}(z_h). \tag{16}$$

where

$$K_{ht}(z_h) = \{\varphi_h \in M_h^{u_d}, \varphi_h \leq w_{ht}(z_h)\},$$

with

$$w_{ht}(z_h) = (1 - t)w_{hs} + t\mathcal{M}_h(z_h) \forall t \in [0, 1].$$

Any fixed point of S_1 is a solution of (15). As for the problem (1)–(5) (see [23]), the fact that $S_t(z) \in K_{ht}$ and an argument of the principle of the discrete maximum [8] implies that any fixed point z_h of S_t is such that $V^- \leq z_h \leq V^+$. Let B be the open defined by:

$$B = \{\varphi_h \in M_h, \|\varphi_h\|_{\infty} < C\},$$

where C is a constant much greater than $\max(|V^-|, V^+)$, it is clear that no fixed point of S_t belongs to ∂B therefore $\text{deg}[I - S_t, B, 0]$ is defined and independent of t , where $\text{deg}[\cdot, \cdot, \cdot]$ is the topological degree of Brouwer [10, 11] and I is the identity of M_h .

For $t = 0$, $K_{h0}(z_h) = K_{h0} = \{\varphi_h \in M_h^{u_d}, \varphi_h \leq w_{hs}\}$. The operator S_0 matches to any $z_h \in M_h$ the solution of the variational inequality

$$u_h \in K_{h0}, \int_{\Omega} \nabla u_h \nabla (\varphi - u_h) dX \geq \xi \int_{\Omega} (\varphi_h - u_h) dX, \forall \varphi \in K_{h0}.$$

Consequently S_0 is trivial and therefore $\text{deg}[I - S_0, B, 0] = 1$, which implies $\text{deg}[I - S_t, B, 0] = 1, \forall t \in [0, 1]$. Hence S_1 admits a fixed point in B which is solution of (15). □

The questions concerning the convergence of u_h towards u are natural and will be published in a future work. We will treat the case where the operator \mathcal{M} is approached by a classical finite element method as well as the case of the new hybrid finite element approach.

4. NUMERICAL ASPECTS

To solve (15) which is also a Q.V.I., we use an iterative scheme based on the operator S_1 , specifically we define the following

$$u_h^m \in B \cap M_h^{u_d}, \text{ telle que } u_h^m = S_1(u_h^{m-1}), \tag{17}$$

u_h^0 being chosen as the solution of the variational inequality

$$\int_{\Omega} \nabla u_h^0 \nabla (\varphi - u_h^0) dX \geq \xi \int_{\Omega} (\varphi_h - u_h^0) dX, \varphi \in M_h^{u_d}, \varphi \leq w^0,$$

where w^0 is the Fermi quasi-potential called the Shokley approximation.

4.1. Treatment of exponential nonlinearity

The computation of the Fermi quasi-potential w_h , which serves as an obstacle in the computation of the potential u_h , solution of the variational inequation (17), is reduced to solving the system of linear equations

$$\sum_{j \in E_{hi}} b_{ij} \eta_{hj} = 0 \tag{18}$$

$$b_{ij} = \sum_{T \in T_h^{ij}} C_{hT} \alpha_{hT} \tag{19}$$

where $\alpha_{hT} = \text{mes}(T) \left(\int_T e^{-u_h} dX \right)^{-1}$, C_{hT} is the contribution of the triangle T to the discretization of the Laplacian, T_h^i is the set of triangles having the node i as vertex, E_{hi} is the set of nodes which are vertices of a triangle $T \in T_h^i$, $T_h^{ij} = T_h^i \cap T_h^j$, and u_{hl} the value of u_h at node l . In the form (19) the computation of the coefficients b_{ij} leads to capacity overruns (underflow-overflow), especially for the computation of the diagonal terms.

To eliminate this problem we will describe a technique which does not require any additional storage and which is very efficient for sufficiently small h steps.

Multiply equation (18) by $e^{u_{hi}}$ we get

$$\sum_{j \in E_{hi}} b_{ij} e^{u_{hi}} \eta_{hj} = 0,$$

that we write in the form

$$\sum_{j \in E_{hi}} b'_{ij} \eta_{hj} = 0. \tag{20}$$

Typically, the coefficients b'_{ij} keep the properties of b_{ij} , *i.e.*, the property of the dominant diagonal. However, the system of linear equation (20) is no longer symmetric. But we can still manipulate this system, by storing only the upper part of the matrix (b'_{ij}). Indeed, the non-zero subdiagonal terms can be obtained as follows:

The coefficient b'_{ji} , $j > i$; is obtained from the coefficient b'_{ij} , $j > i$, by the relation

$$b'_{ji} = b'_{ij} e^{(u_{hj} - u_{hi})}.$$

This means that the solution of the system of equation (20) does not require any additional storage than that of the upper part of the matrix (b_{ij}) and the vector $[u_{hi}]_i$. System (20) therefore preserves the main characteristics of (18), with the following properties:

Proposition 4.1. *For h sufficiently small, the calculation of all the coefficients b'_{ij} is done without any capacity overrun (neither underflow nor overflow).*

Proof. The proof of the proposition is obtained from the relation

$$b'_{ij} = \sum_{T \in T_h^{ij}} C_{hT} \text{mes}(T) \left(\int_T e^{(u_{hi} - u_h)} dX \right)^{-1}.$$

Since $u_h \in \mathbb{P}_1(T)$, we can calculate in an exact way the integral I appearing in the previous relation. For simplicity we assume that

$$I = \sum_{l \in V(T)} a_l e^{(u_{hi} - u_{hl})}$$

where $V(T)$ is the set of vertices of the triangle T . Since $i \in V(T)$, $\forall T \in \mathcal{T}_h^{ij}$, there is an $l_0 \in V(T)$ such as $e^{(u_{hi}-u_{hl_0})} = 1$, which eliminates any division by zero in the calculation of α_{hT} . Furthermore, $u_h \in \mathbb{P}_1(T)$ leads to

$$|u_{hi} - u_{hl}| \leq Ch, \quad \forall i, \forall l \in V(T).$$

It is clear that the sign of $(u_{hi} - u_{hl})$ can be negative or positive. However, for h small enough we can ensure that $-\chi < (u_{hi} - u_{hl}) < \chi$ où χ is the lower limit value acceptable by the machine for e^x , this guarantees that the capacity is not exceeded in the calculation $e^{(u_{hi}-u_{hl})}$. □

4.2. Computation of Drain current

The following proposition expresses the weak continuity of the electric current.

Proposition 4.2. *Let (η_h, J_h) be the solution of the system (11), let i be a node of \mathcal{T}_h , $i \notin \Gamma_d$ and let L_h^i be the set of sides having i as vertex. Then*

$$\sum_{e \in L_h^i} \int_e J_h \cdot \nu \, d\sigma = 0.$$

Proof. Integration by parts, the second equation of the system (12) leads to the equation

$$\sum_{T \in \mathcal{T}_h} \int_{\partial T} J_h \cdot \nu \mu_h \, d\sigma = 0, \quad \forall \mu_h \in M_h^0.$$

For the basis element φ_i associated with the node i we obtain $\sum_{e \in L_h^i} \int_e J_h \cdot \nu \, d\sigma = 0$. □

In semiconductor device technology the most important feature is the computation of the current flowing along a given contact. For FETs, it is the current of Drain J_d defined by

$$J_d = \int_{\Gamma_d} J \cdot \nu \, d\sigma,$$

where Γ_d is the Drain contact. To computation of J_d by this formula requires the computation of the electric field and a numerical integration. In the following we describe how we can get around this problem by using a method that does not require any additional calculation.

Let θ_h be the function of M_h defined by

$$\theta_h = \sum_{l \in V_d} \omega_l$$

where ω_l is the base function associated with node number l and V_d is the set of nodes belonging to the Drain. By construction $\theta_h = 1$ on Γ_d and it is identically zero on the remainder of $\partial\Omega$, hence

$$\begin{aligned} J_d &= \int_{\partial\Omega} \theta_h J \cdot \nu \, d\sigma \\ &= \int_{\Omega} \theta_h \nabla \cdot J \, dX + \int_{\Omega} J \cdot \nabla \theta_h \, dX. \end{aligned}$$

Since J has zero divergence, we get

$$J_d = \sum_{l \in V_d} \int_{\Omega} J \cdot \nabla \omega_l \, dX.$$

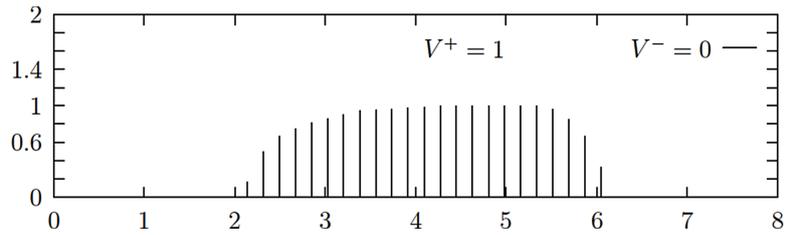


FIGURE 2. Depletion region $V^- = -0$ and $V^+ = 1$.

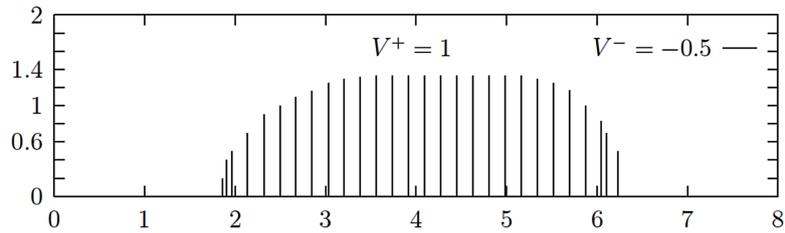


FIGURE 3. Depletion region $V^- = -0.5$ and $V^+ = 1$.

We approach the current J by J_h , the current of Drain J_d is then approached by

$$\begin{aligned}
 J_{dh} &= \sum_{l \in V_d} \sum_{T \in \mathcal{T}_h} \alpha_{hT} \int_T \nabla \eta_h \cdot \nabla \omega_l \, dX \\
 &= \sum_{l \in V_d} \left(\sum_{i=1} b_{li} \eta_{hi} \right)
 \end{aligned} \tag{21}$$

where $B = (b_{ij})$ is the matrix associated with the system (14).

Remark 4.3. The calculation of J_{dh} by the formula (21) is reduced to the product of the matrix B by the vector $[\eta_{hi}]$, whose elements are already computed and stored.

5. NUMERICAL RESULTS

Numerical simulation is made using the following value of the main parameters: $\frac{Nq}{\epsilon} = 1$, $DA = 8$ microns and $AB = 2$ microns.

We set the gate voltage to 0 V and we apply a positive voltage to the drain contact thus the current flow through the channel and we can calculate J_d , the current of the Drain contact.

We increased the drain voltage, the current J_d increases up to the value 2.8 mA, then it becomes stationary. The same remark when $Vg = -1$ V the limit value of J_d approaches 1.2 mA. Then, the limit value only reaches 0.5 mA when $Vg = -1.5$ V. The current therefore becomes increasingly weak when the absolute value of Vg becomes increasingly large. This is consistent with the Figures 2-4 which show that the depth of the depletion region increases, when the value of Vg becomes smaller and smaller, until this zone extends through the active channel which stops the current movement in the channel. This gate-source potential phenomenon is known in physics as ‘‘Pinch-off voltage’’.

We set the drain voltage to +1 V and we vary the Gate voltage from 0 V to -1.8 V. The depth of the depletion region becomes higher when we increase the gate voltage. This continues until the boundary of the depletion

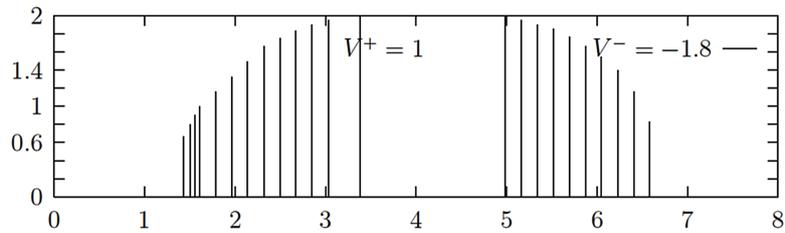


FIGURE 4. Depletion region $V^- = -1.8$ and $V^+ = 1$.

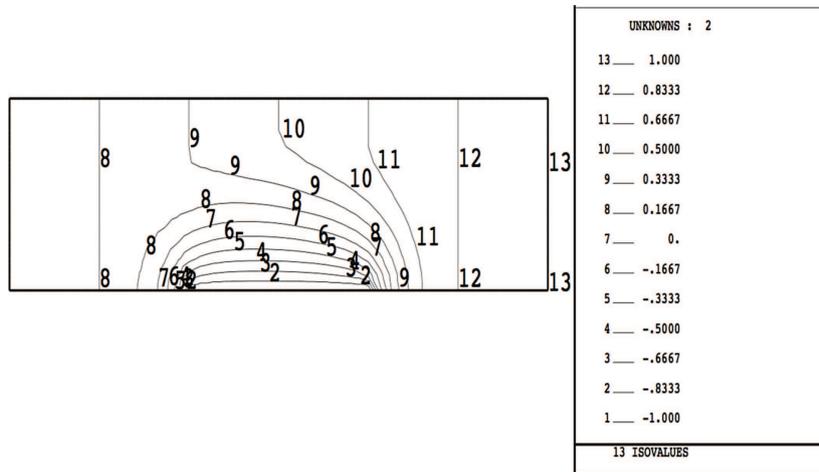


FIGURE 5. MESFET n -type, equipotentials $V^- = -1$, $V^+ = 1$.

layer touches the side opposite the Gate. The channel is then closed, which causes the flow of current to stop (2)–(4).

We observe from Figure 5 that the negative equipotentials do not cross the free boundary. They all remain confined inside line 7, equipotential of value equal to 0 V. The positive equipotentials go around line 7, cross the channel and therefore allow current to flow.

In Figure 6, where only the positive equipotentials have been represented, it can be seen that there are no more lines around the line number 1, where the potential is of value 0 V, which is no longer a closed curve. This shows that the channel is closed and there is no more current flow.

6. CONCLUSION

From these numerical results we have observed, (see the following figures), that

- The depletion region is localized around the gate contact.
- As is known from physical experience, when applying a positive potential difference between source and drain contacts, an electric current flows from one end to an other. The gate contact allows us to control the drain current by modifying the thickness of the depletion zone: a sufficiently negative gate-source voltage cuts the conducting channel and thereby switches off the drain current.

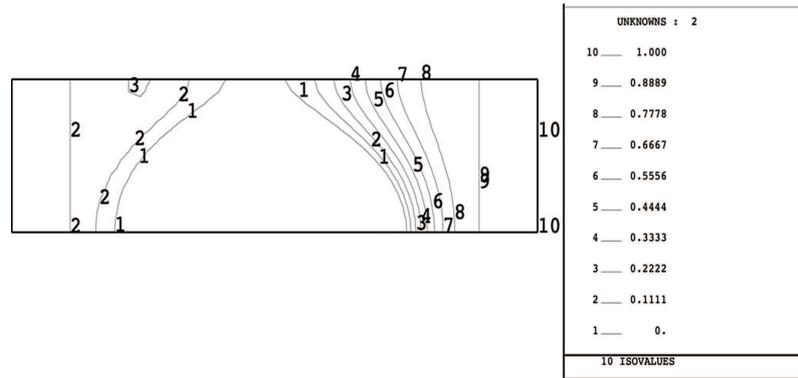


FIGURE 6. MESFET n -type, equipotentials $V^- = -1.8$, $V^+ = 1$.

We can conclude that for the semiconductor device, used in the numerical experiments, the simplified model described in section introduction does not change the behavior of the full system. Also, we can conclude that the proposed hybrid finite element method provides a good alternative for solving free boundary problems arising in the depletion approximation model. This method combined with the scaling technique makes it possible to avoid capacity overruns and leads to a correct calculation of the current.

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