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MIXED FINITE ELEMENT APPROXIMATION OF THE STATIONARY SEMICONDUCTOR CONTINUITY EQUATIONS

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Abstract: In this paper we discuss two discretisation methods for the stationary semiconductor continuity equations based on the mixed finite element approach. Both of them can be regarded as extensions of the wellknown Scharfetter–Gummel scheme to two dimensions. The existence and uniqueness of the solution are presented and error estimates are given. The associated linear systems are perturbations of those obtained from the conventional box method. We propose a method for the evaluation of the terminal currents which we show to be convergent and conservative.

1. Introduction

The stationary behaviour of semiconductor devices is governed by a set of nonlinear elliptic partial differential equations. This includes a nonlinear Poisson equation and two nonlinear continuity equations. Using Gummel's method [5] we can decouple the nonlinear elliptic system so that at each step we solve an equation of the form

$$-\nabla \cdot (a(x)\nabla u) + G(x,u) = F(x) \text{ in } \Omega \qquad (1.1)$$

with the boundary conditions $u|_{\partial\Omega_D} = \gamma(x)$ and $\nabla u \cdot \mathbf{n}|_{\partial\Omega_N} = 0$, where $\Omega \subset I\!R^m$, $(m = 1,2,3)$, $\partial\Omega = \overline{\partial\Omega_D} \cup \overline{\partial\Omega_N}$ is the boundary of Ω, $\mathbf{n}$ denotes the unit normal vector on $\partial\Omega$, $a \in C(\overline{\Omega})$ and $a(x) \geq a_0 > 0$.

In the following we consider only the case $m = 2$ and we take $G(x,u) = 0$, which corresponds to the two continuity equations.

As in [8], introducing a new variable $\mathbf{f} = a\nabla u$, we get a first order system of PDE's in the variables [u,f]. We consider only homogeneous Dirichlet boundary conditions. For the inhomogeneous case we can subtract a special function satisfying the Dirichlet boundary condition and change the problem into a homogeneous one. The corresponding variational problem is
Problem 1.1: Find a pair $[u,\mathbf{f}] \in V = H_D^1(\Omega) \times \mathbf{L}^2(\Omega)$ such that for all $[v,\mathbf{g}] \in V$

$$(\nabla u, \mathbf{g}) - (a^{-1}\mathbf{f}, \mathbf{g}) = 0 \qquad (1.2a)$$

$$(\mathbf{f}, \nabla v) = (F, v) \qquad (1.2b)$$

Here $H^1_D(\Omega) = \{v \in H^1(\Omega) : v|_{\partial\Omega_D} = 0\}$, $\mathbf{L}^2(\Omega) = (L^2(\Omega))^2$ and $(\cdot,\cdot)$ indicates the inner product on $\mathbf{L}^2(\Omega)$ or $L^2(\Omega)$. We comment that the solution to **Problem 1.1** exists and is unique (cf.[10]).

To discuss the finite element approximation to the solution of **Problem 1.1** we first define a partition of Ω.

Let T_h denote a triangulation of the region $\overline{\Omega}$ with each triangle t of diameter less than or equal to h. Assume that $\{T_h\}_h$ is regular, *i.e.* there is a constant $\sigma_1 > 0$ such that

$$\max_{t\in T} \frac{h_t}{\rho_t} \le \sigma_1 \qquad \forall h$$

where h_t and ρ_t denote the diameters and the incircle of t respectively. This is eqivalent to saying that the set of angles of $t \in T_h$ has a positive lower bound.

Let $X = \{x_i\}_1^{N_V}$ denote the set of vertices of T_h and $E = \{e_i\}_1^{N_E}$ the set of all edges of T_h. Let N denote the number of nodes in X not on $\partial\Omega_D$ and M the number of edges in E not on $\partial\Omega_D$. We say that T_h is a Delaunay triangulation if for any $t \in T_h$, the circumcircle of t contains no other vertices in X. The Dirichlet tessellation $\{D_i\}_1^{N_V}$ is defined by

$$D_i = \{x : \|x - x_i\| < \|x - x_j\|, x_j \in X, j \neq i\}$$

for all $x_i \in X$.

2. The Galerkin Approximation

In this section we discuss the mixed finite element method partly based on Brezzi *et al* [2]. Introducing finite dimensional subspaces $H_h, \mathbf{L}_h$ such that $V_h = H_h \times \mathbf{L}_h \subset V$, we define the following discrete problem

Problem 2.1: Find $[u_h, \mathbf{f}_h] \in V_h$ such that for all $[v_h, \mathbf{g}_h] \in V_h$

$$(\nabla u_h, \mathbf{g}_h) - (a^{-1}\mathbf{f}_h, \mathbf{g}_h) = 0 \qquad (2.1a)$$

$$(\mathbf{f}_h, \nabla v_h) = (F, v_h) \qquad (2.1b)$$

We choose $H_h = \text{span}\{\phi_i\}_1^N$, where ϕ_i is the standard piecewise linear basis function associated with x_i. For the construction of $\mathbf{L}_h$ we choose

$$\mathbf{L}_h = \{\mathbf{q} \in \mathbf{L}^2(\Omega) : \mathbf{q}|_t \in (P_0)^2, \forall t \in T_h\}$$

where P_0 is the space of zero–order polynomials. Obviously $\mathbf{L}_h$ is the space of vector–valued piecewise constants.

Corresponding to this choice of subspaces we have the following theorem:

Theorem 2.1. *Problem 2.1 has a unique solution.*

The proof of the theorem is trivial since $\nabla H_h = \{\nabla v : v \in H_h\} \subset \mathbf{L}_h$. The inf–sup condition holds trivially in this case [1, 4 (p.134)].

Introducing the piecewise constant a_A^{-1} such that

$$a_A^{-1}|_t = \frac{1}{|t|}\int_t a^{-1} dx \qquad \forall t \in T_h \tag{2.2}$$

we obtain from (2.1a)

$$\mathbf{f}_h = \frac{1}{a_A^{-1}} \nabla u_h \tag{2.3}$$

where, and hereafter, $|\cdot|$ denotes the measure or absolute value. Substituting (2.3) into (2.1b), we get a problem as follows

Problem 2.2: Find $u_h \in H_h$ such that for all $v_h \in H_h$

$$\left(\frac{1}{a_A^{-1}}\nabla u_h, \nabla v_h\right) = (F, v_h) \tag{2.4}$$

Problem 2.2 is similar to the standard conforming finite element discretisation but with the harmonic average approximation to the coefficient function $a(x)$ in each element, as in the one–dimensional Scharfetter–Gummel scheme [11].

To obtain an error estimate for the discrete solution of **Problem 2.2**, we first define a norm on $\mathbf{L}^2(\Omega)$ by $\|\cdot\|_a = (a^{-1}\cdot, \cdot)$. We then have the following error estimate

Theorem 2.2. *Let* $[u, \mathbf{f}]$ *and* $[u_h, \mathbf{f}_h]$ *be the solutions of Problem 1.1 and Problem 2.1 respectively. Let* $\mathbf{f}_I$ *and* $\tilde{\mathbf{f}}$ *be the approximations of* $\mathbf{f}$ *by*

$$\mathbf{f}_I \in \mathbf{L}_h, \qquad (\mathbf{f} - \mathbf{f}_I, \mathbf{g}) = 0, \qquad \forall \mathbf{g} \in \mathbf{L}_h$$

$$\tilde{\mathbf{f}} = a\nabla u_I$$

where u_I *is the piecewise linear interpolant of* u. *Then*

$$\|\mathbf{f} - \mathbf{f}_h\|_a \le 2(\|\mathbf{f} - \mathbf{f}_I\|_a + \|\mathbf{f} - \tilde{\mathbf{f}}\|_a)$$

Proof. See [2]. □

If we let $u_h = \sum_1^N u_i\phi_i$ and $v_h = \phi_j$, then (2.4) reduces to the following linear system.

$$\sum_{i=1}^{N} u_i\left(\frac{1}{a_A^{-1}}\nabla\phi_i, \nabla\phi_j\right) = (F, \phi_j) \qquad j = 1, 2, \ldots, N. \tag{2.5}$$

The linear system (2.5) can be reduced again using the following lemma. Before giving the lemma we define some notation. For any $e_{jk} \in E$ which is the edge connecting x_j and x_k, let $w_{jk}^{(1)}$ and $w_{jk}^{(2)}$ denote the distances from the circumcentres of the two triangles sharing e_{jk} to the midpoint of e_{jk} respectively. Here $w_{jk}^{(i)}$ $(i = 1, 2)$ is negative if the circumcentre lies outside of the triangle in question. The restrictions of a function b on the two triangles sharing e_{jk} are denoted respectively $b_{jk}^{(1)}$ and $b_{jk}^{(2)}$. Let $I_j = \{k : \overline{x_j x_k} \in E\}$ denote the index set of all neighbour nodes of x_j.

Lemma 2.2. *Let b be a function which takes constant value on each triangle $t \in T_h$. Then for all $v = \sum_1^N v_i \phi_i \in H_h$ we have*

$$(b\nabla v, \nabla \phi_j) = \sum_{k \in I_j} (b_{jk}^{(1)} w_{jk}^{(1)} + b_{jk}^{(2)} w_{jk}^{(2)}) \frac{v_j - v_k}{|e_{jk}|} \tag{2.6}$$

Proof. See Ikeda (1983). □

Applying Lemma 3.2 to (2.5) we obtain

$$\sum_{k \in I_j} (a_{jk}^{(1)} w_{jk}^{(1)} + a_{jk}^{(2)} w_{jk}^{(2)}) \frac{u_j - u_k}{|e_{jk}|} = (F, \phi_j) \quad j = 1, 2, \ldots, N \tag{2.7}$$

where $a_{jk}^{(1)}$ and $a_{jk}^{(2)}$ are respectively the restrictions of $1/a_A^{-1}$ on the two triangles sharing e_{jk}. From (2.2) we know that $(1/a_A^{-1})|_t$ is an average value of a on t. We thus perturb $a_{jk}^{(1)}$ and $a_{jk}^{(2)}$ and apply the mass lumping method based on the circumcentric domain (cf. [6]) to the right–hand side of (2.7) so that (2.7) reduces to

$$\sum_{k \in I_j} \frac{1}{a_{jk}^{-1}} w_{jk} \frac{u_j - u_k}{|e_{jk}|} = F(x_j)|D_j| \tag{2.8}$$

where $w_{jk} = w_{jk}^{(1)} + w_{jk}^{(2)}$ is the distance between the two circumcentres of the two triangles sharing e_{jk}, D_j is the Dirichlet tesselation associate with x_j and $a_{jk}^{-1} = \frac{1}{|e_{jk}|} \int_{e_{jk}} a^{-1} ds$ is an average value of a on e_{jk}. The linear system (2.8) coincides with that obtained from the conventional box scheme (cf. [3,7,9]). If T_h is a Delaunay triangulation, the weights w_{jk}'s are nonnegative. In this case the system matrix of (2.8) is a Stieltjes matrix.

3. The Petrov–Galerkin Approximation

In this section we present a Petrov–Galerkin finite element method for **Problem 1.1** We first define two other meshes associated with T_h.

With each $x_i \in X$ we associate a region $\Omega(x_i)$ consisting of all the triangles $t \in T_h$ with the common vertix x_i and an open region $b(x_i) \subset \Omega(x_i)$ constructed as follows: for each $t \subset \Omega(x_i)$, choose a point $p \in t$ arbitrarily and connect it to the two midpoints of the two edges of t sharing x_i, as show in Fig.3.1. For the sake of convenience, we sometimes denote $b(x_i)$ simply by b. The set of all such $b(x_i)$ is denoted by B_N which is a dual mesh of T_h

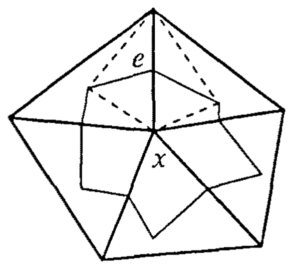

Fig.3.1: *$b(x) \subset \Omega(x)$, $\Omega(e)$*

With each edge $e_i \in E$ we also associate an open region $\Omega(e_i)$ by connecting the two end-nodes of e_i with the two chosen points in the two triangles sharing e_i generated during the construction of B_N, shown in Fig.3.1 by dashed lines. This mesh is denoted B_E. We comment that B_E is determined uniquely by B_N and *vice versa* and B_E divides each $t \in T$ into three parts t_1, t_2, t_3. We assume that B_E is regular in the sense that there is a positive constant σ_2 such that for any $i, j \in \{1, 2, 3\}, i \neq j$

$$\min_{t \in T} \frac{|t_i| + |t_j|}{|t|} \geq \sigma_2 \tag{3.1a}$$

This is equivalent to fact that for the chosen $p \in t$, the minimal distance between p and the vertices of t has a lower positive bound. The regularity of B_E implies that there is a positive constant σ_3 such that

$$\min_{x_i \in X} \frac{|b(x_i)|}{|\Omega(x_i)|} \geq \sigma_3 \tag{3.1b}$$

For the three meshes T_h, B_N, B_E, we construct three corresponding finite-dimensional spaces $U_h \subset H_0^1(\Omega), V_h \subset L^2(\Omega)$ and $\mathbf{L}_h \subset \mathbf{L}^2(\Omega)$ as follows.

Let $\{\phi_i\}_1^{N_V}$ be the conventional piecewise linear basis functions for T_h. We choose $U_h = \text{span}\{\phi_i\}_1^N$.

To construct V_h, we define a set of basis functions corresponding to the mesh B_N by

$$\psi_i = \begin{cases} 1 & x \in b(x_i) \\ 0 & x \notin b(x_i) \end{cases} \qquad i = 1, 2, \ldots, N$$

i.e. for each i, ψ_i is piecewise constant on Ω. We then choose $V_h = \text{span}\{\psi_i\}_1^N$.

For $i = 1, 2, \ldots, N_E$, define

$$\mathbf{q}_i = \begin{cases} \mathbf{e}_i & x \in \Omega(e_i) \\ 0 & x \notin \Omega(e_i) \end{cases}$$

where $\mathbf{e}_i$ is the unit tangential vector long edge e_i. Obviously we have $(\mathbf{q}_i, \mathbf{q}_j) = \delta_{ij}|\Omega(e_j)|$, where δ_{ij} is the Kronecker notation. We choose $\mathbf{L}_h = \text{span}\{\mathbf{q}_i\}_1^M$.

With these subspaces. we define the following discrete problem.

Problem 3.1: Find a pair $[u_h, \mathbf{f}_h] \in U_h \times \mathbf{L}_h$ such that for all $[v_h, \mathbf{q}_h] \in V_h \times \mathbf{L}_h$

$$(\nabla u_h, \mathbf{q}_h) - (a^{-1}\mathbf{f}_h, \mathbf{q}_h) = 0 \tag{3.2}$$

$$-\sum_{b \in B_N} \int_{\partial b} \mathbf{f}_h \cdot \mathbf{n}_{\partial b} \gamma_0 v_h|_b ds = (F, v_h) \tag{3.3}$$

where γ_0 denotes the conventional trace operator, $v_h|_b$ denotes the restriction of v_h to b and $\mathbf{n}_{\partial b}$ the outward unit normal vector along ∂b. We comment that the left–hand side of (3.3) is meaningful because $\mathbf{f}_h \cdot \mathbf{n}_{\partial b}$ is integrable on ∂b for all $\mathbf{f}_h \in \mathbf{L}_h$. It is a bilinear form on $\mathbf{L}_h \times V_h$ as follows

$$a(\mathbf{f}_h, v_h) = \sum_{b \in B_N} \int_b \mathbf{f}_h \cdot \nabla v_h dx - \sum_{b \in B_N} \int_{\partial b} \mathbf{f}_h \cdot \mathbf{n}_{\partial b} \gamma_0 v_h|_b ds \tag{3.4}$$

The first term on the right–hand side of (3.4) vanishes when $v_h \in V_h$. For simplicity, we write $\gamma_0 v_h|_b$ in the integrand of (3.3) as v_h hereafter.

The existence and uniqueness of the solution to **Problem 3.1** is contained in the following theorem.

Theorem 3.1. *Assume (3.1a–b) are satisfied. The* **Problem 3.1** *has a unique solution for the choice of* $\mathbf{L}_h, U_h$ *and* V_h.

Proof. See [12]. □

Let $\mathbf{f}_h = \sum_{i=1}^M f_i \mathbf{q}_i, u_h = \sum_{i=1}^N u_i \phi_i$, where $\{f_i\}_1^M, \{u_i\}_1^N$ are two sets of constants. Substituting these into (3.2) and letting $\mathbf{q}_h = \mathbf{q}_j$ ($j = 1, \ldots, M$), we get

$$\sum_{i=1}^N u_i (\nabla \phi_i, \mathbf{q}_j) - \sum_{i=1}^M f_i (a^{-1}\mathbf{q}_i, \mathbf{q}_j) = 0$$

This has the following solution

$$f_j = \frac{1}{a_j^{-1}} \frac{u_{j2} - u_{j1}}{|e_j|}$$

where $a_j^{-1} = \frac{1}{|\Omega(e_j)|} \int_{\Omega(e_j)} a^{-1} dx$ and u_{j1}, u_{j2} are as shown in Fig.3.2.

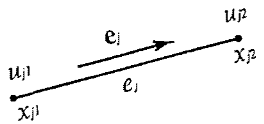

Fig.3.2

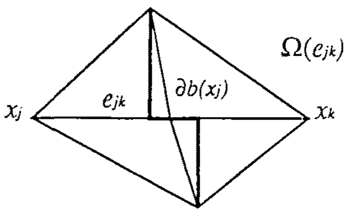

Fig.3.3

We thus have

$$\mathbf{f}_h = \sum_{i=1}^{M} \frac{1}{a_i^{-1}} \frac{u_{i2} - u_{i1}}{|e_i|} \mathbf{q}_i \tag{3.5}$$

Substituting (3.5) into (3.3) and letting $v_h = \psi_j$ $(j = 1, 2, \ldots, N)$, we obtain

$$-\sum_{i=1}^{M} \frac{1}{a_i^{-1}} \frac{u_{i2} - u_{i1}}{|e_i|} \int_{\partial b(x_j)} \mathbf{q}_i \cdot \mathbf{n}_{\partial b(x_j)} ds = (F, \psi_j) \tag{3.6}$$

Recalling the definitions of $\{\mathbf{q}_i\}_1^M$ and B_N, and using the subscripts in Fig.3.3 we finally obtain

$$\sum_{k \in I_j} \frac{1}{a_{jk}^{-1}} \frac{u_j - u_k}{|e_{jk}|} \frac{2|\Omega(e_{jk})|}{|e_{jk}|} = (F, \psi_j) \quad j = 1, 2, \ldots, N \tag{3.7}$$

where I_j is the index set of all neighbour nodes of x_j as defined in the previous section. In the above we have made use of the fact that the line integral of $\mathbf{q}_i \cdot \mathbf{n}_{\partial b(x_j)}$ is independent of path in $\Omega(e_i)$ and chosen the path shown in Fig.3.3 by heavy lines.

Let $[u, \mathbf{f}]$ be the solution of **Problem 1.1**. Let u_I be the piecewise linear interpolant of u and $\mathbf{f}_I = \frac{1}{a_A^{-1}} \nabla u_I$, where a_A^{-1} is defined in (2.2). Then we have the the following theorem for the convergence of the approximate solution u_h.

Theorem 3.2. *Assume that (3.1a–b) hold. If T_h is a Delaunay triangulation and B_N is the corresponding Dirichlet tessellation, then there is a constant $C > 0$, independent of h such that*

$$\|u_I - u_h\|_1 \leq \frac{C}{a_0} h(\|\mathbf{f} - \mathbf{f}_I\|_0 + \|F\|_0) \tag{2.10}$$

where a_0 is the positive lower bound of a defined in Section 1.

The proof of this theorem will be published elsewhere. We comment that the approximate flux $\mathbf{f}_h$ does not converge to $\mathbf{f}$ as $h \to 0$ because of the choice of $\mathbf{L}_h$.

When T_h is a Delaunay triangulation and B_N is the corresponding Dirichlet tessellation, (3.7) reduces to the conventional box scheme (cf. [3,7,9]) if we perturb a_{jk}^{-1} in (3.7) such that $a_{jk}^{-1} = \frac{1}{|e_{jk}|} \int_{e_{jk}} a^{-1} ds$.

4. Evaluation of the Terminal Currents

In this section we present a method for the evaluation of terminal currents. The approximate terminal currents are shown to be convergent and conservative. Notation in the section is the same as that in section 3.

Assume $\partial\Omega_D$ consists of finite number of disjoint segments, each of which is physically an ohmic contact. At this stage $\partial\Omega_D$ is viewed as the set of all ohmic contacts. For any $C \in \partial\Omega_D$, let $\{x_i^C\}_1^{N_C}$ denote the set of nodes on C. Let ψ_C be a function defined as

$$\psi_C(x) = \begin{cases} 1 & x \in \cup_{i=1}^{N_C} b(x_i^C) \\ 0 & \text{otherwise} \end{cases} \tag{4.1}$$

Multiplying (1.1) by ψ_C and integrating by parts on each box we have

$$-\int_C \mathbf{f} \cdot \mathbf{n} ds - \sum_{b \in B_N} \int_{\partial b \setminus (\partial b \cap C)} \psi_C \mathbf{f} \cdot \mathbf{n} ds = (F, \psi_C)$$

We thus have the outflow current through C as

$$J_C = \int_C \mathbf{f} \cdot \mathbf{n} ds = -\sum_{b \in B_N} \int_{\partial b \setminus (\partial b \cap C)} \psi_C \mathbf{f} \cdot \mathbf{n} ds - (F, \psi_C) \tag{4.2}$$

The approximate outflow current through C is then defined as

$$J_C^h = -\sum_{b \in B_N} \int_{\partial b \setminus (\partial b \cap C)} \psi_C \mathbf{f}_h \cdot \mathbf{n} ds - (F, \psi_C) \tag{4.2}$$

Using (4.1) and (3.5) we finally obtain

$$J_C^h = \sum_{i=1}^{N_C} [\sum_{j \in I_i, x_j \notin C} \frac{1}{a_{ij}^{-1}} \frac{2|\Omega(e_{ij})|}{|e_{ij}|} \frac{u_i - u_j}{|e_{ij}|} - \int_{b(x_i)} F dx] \tag{4.4}$$

Here we have used the same arguement as that for the derivation of (3.7).

The convergence and conservation of the approximate terminal currents are contained in the following theorem.

Theorem 4.1. *Assume J_C and J_C^h are defined by (4.2) and (4.3) and u_h is the solution to* **Problem 3.1**. *Let $\bar{\mathbf{f}}$ be a piecewise constant vector–valued function and a_B^{-1} a piecewise constant functions such that for all $e_i \in E$*

$$\bar{\mathbf{f}}|_{\Omega(e_i)} = \frac{1}{|\partial b_i|} \int_{\partial b_i} \mathbf{f} ds, \quad \partial b_i = \Omega(e_i) \cap (\cup_{b \in B_N} \partial b)$$

$$a_B^{-1}|_{\Omega(e_i)} = \frac{1}{|\Omega(e_i)|} \int_{\Omega(e_i)} a^{-1} dx$$

Then there is a constant $\alpha > 0$, independent of h, such that

$$|J_C - J_C^h| \leq \alpha \|\bar{\mathbf{f}} - \frac{1}{a_B^{-1}} \nabla u_h\|_0$$

Furthermore

$$\sum_{C \in \partial\Omega_D} J_C^h = - \int_\Omega F dx$$

The proof will be published elsewhere.

5. Conclusion

In this paper we have discussed two discretisation methods for the stationary semiconductor continuity equatins. One is based on the Galerkin mixed finite element appraoch and the other is based on the Petrov–Galerkin mixed finite element appraoch. The existence and uniqeness of the solution for both methods were presented and error estimates were also given. Both methods can be regarded as extensions of the well–known Scharfetter–Gummel scheme [11] to two dimensions. The resulting linear systems are perturbations of the conventional box scheme [3,7,9]. We also presented a method for the evaluation of the terminal currents and showed that the approximate terminal currents are convergent and conservative.

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