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Stationary energy models for semiconductor devices with incompletely ionized impurities

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Mohrenstr. 39 10117 Berlin glitzky@wias-berlin.de www.wias-berlin.de June 2005 mass and charge and energy transport in heterogeneous semiconductor devices

described by

- continuity equations for densities n, p
  of electrons e^- and holes h^+
- Poisson equation for the electrostatic potential φ
- balance equation for the density of the total energy e
- reaction equations for incompletely ionized impurities
  X_j, $X_j^{+(-)}$, $j = 1, \ldots, k$
  (radiation-induced traps, other deep recombination centers)

Mathematical problems

non-smooth data:

- heterogeneous materials – physical quantities jump at material interfaces discontinuities w.r.t. space variable
- domain Ω in general non-smooth, but only Lipschitz
- mixed boundary conditions

strongly coupled PDEs:

- coefficients depend on the state variable
- ellipticity condition is not fulfilled uniformly
- equations degenerate if $n = 0$, $p = 0$ or $T = \infty$

Poisson equation singularly perturbed

constraints $n, p, T > 0$

restrict us to the stationary energy model

Stationary energy model for devices with incompletely ionized impurities

(1) $$-\nabla \cdot (\varepsilon \nabla \varphi) = f_0 - n + p + \sum_{i=1}^{2k} q_i u_i, \quad \nabla \cdot j_e = 0,$$

(2) $$\nabla \cdot j_n = R_0 + \sum_{j=1}^{k} R_{j1}, \quad \nabla \cdot j_p = R_0 + \sum_{j=1}^{k} R_{j2},$$

(3) $$R_{j1} = R_{j2}, \quad u_{2j-1} + u_{2j} = f_j, \quad j = 1, \dots, k.$$

ε	dielectric permittivity
f_0, f_j	prescribed charge density and particle densities
j_e	flux density of the total energy
j_n, j_p	particle flux densities of electrons and holes
R_{j1}, R_{j2}	reaction rates of the ionization reactions
R_0	reaction rate of the direct electron-hole recombination-generation $\mathrm{e}^- + \mathrm{h}^+ \rightleftharpoons 0$

impurities:

X_j occur in different charge states, take place ionization reactions

If X_j is an acceptor-like impurity, X_j^- its ion, the reactions are

$$e^- + X_j \rightleftharpoons X_j^-, \quad h^+ + X_j^- \rightleftharpoons X_j$$

If X_j is a donor-like impurity, X_j^+ its ion, the reactions are

$$e^- + X_j^+ \rightleftharpoons X_j, \quad h^+ + X_j \rightleftharpoons X_j^+$$

for donors X_j: u_{2j-1} – density of X_j, u_{2j} – density of X_j^+
for acceptors X_j: u_{2j-1} – density of X_j^-, u_{2j} – density of X_j

charge numbers:

$$q_{2j-1} := \begin{cases} 0 & \text{if } X_j \text{ is a donor} \\ -1 & \text{if } X_j \text{ is an acceptor} \end{cases}, \qquad q_{2j} := 1 + q_{2j-1}$$

system has to be completed by

- state equations
- kinetic relations (reactions, fluxes)
- mixed boundary conditions

denote

$\zeta_n,\ \zeta_p$	– electrochemical potentials of electrons and holes
ζ_i	– electrochemical potentials of immobile (neutral, ionized)
$i = 1, \ldots, 2k$	impurities

Elimination of the constraints (3)

state equations

$$u_i = F_i(\cdot, \varphi, T, \zeta_i), \quad i = 1, \dots, 2k, \quad n = F_n(\cdot, \varphi, T, \zeta_n), \quad p = F_p(\cdot, \varphi, T, \zeta_p)$$

kinetic relations (reaction rates)

$$R_{j1} = r_{j1}(\cdot, \varphi, T, \zeta_n, \zeta_p) \left(\exp \frac{\zeta_{2j-1}}{T} - \exp \frac{\zeta_{2j} + \zeta_n}{T} \right),$$
$$R_{j2} = r_{j2}(\cdot, \varphi, T, \zeta_n, \zeta_p) \left(\exp \frac{\zeta_{2j}}{T} - \exp \frac{\zeta_{2j-1} + \zeta_p}{T} \right),$$
$$R_0 = r_0(\cdot, \varphi, T, \zeta_n, \zeta_p) \left(1 - \exp \frac{\zeta_n + \zeta_p}{T} \right)$$

under reliable assumptions eliminate the constraints (3) by evaluating the sub-systems

$$u_{2j-1} + u_{2j} = f_j, \quad R_{j1} = R_{j2}, \quad j = 1, \dots, k$$

obtain

$$\zeta_{2j} = S_j(\cdot, \varphi, T, \zeta_n, \zeta_p, f_j), \quad \zeta_{2j-1} = \widehat{S}_j(\cdot, \varphi, T, \zeta_n, \zeta_p, f_j), \quad j = 1, \dots, k$$

Elimination of the constraints (3)

use state equations and expression for ζ_i, $i = 1, \ldots, 2k$, to write right hand sides in (1), (2):

$$f_0 - n + p + \sum_{i=1}^{2k} q_i u_i \quad \mapsto \quad H(\cdot, \varphi, T, \zeta_n, \zeta_p, f_0, f_1, \ldots, f_k),$$

$$R_0 + \sum_{j=1}^{k} R_{j1} \quad \mapsto \quad R(\cdot, \varphi, T, \zeta_n, \zeta_p, f_0, f_1, \ldots, f_k)$$

$$= r(\cdot, \varphi, T, \zeta_n, \zeta_p, f_0, f_1, \ldots, f_k) \left(1 - \exp \frac{\zeta_n + \zeta_p}{T}\right)$$

Reduced energy model

(4) $$-\nabla\cdot\begin{pmatrix}\varepsilon & 0 & 0 & 0\\ 0 & \kappa+\widehat{\omega}_0 & \omega_1 & \omega_2\\ 0 & \widehat{\omega}_1 & \sigma_n+\sigma_{np} & \sigma_{np}\\ 0 & \widehat{\omega}_2 & \sigma_{np} & \sigma_p+\sigma_{np}\end{pmatrix}\begin{pmatrix}\nabla\varphi\\ \nabla T\\ \nabla\zeta_n\\ \nabla\zeta_p\end{pmatrix}=\begin{pmatrix}H\\ 0\\ R\\ R\end{pmatrix}\quad \text{in } \Omega,$$

where

$$\begin{pmatrix}\widehat{\omega}_1\\ \widehat{\omega}_2\end{pmatrix}=\begin{pmatrix}\sigma_n+\sigma_{np} & \sigma_{np}\\ \sigma_{np} & \sigma_p+\sigma_{np}\end{pmatrix}\begin{pmatrix}P_n\\ P_p\end{pmatrix},\qquad \widehat{\omega}_0=(\zeta_n+P_nT)\,\widehat{\omega}_1+(\zeta_p+P_pT)\,\widehat{\omega}_2,$$

$$\begin{pmatrix}\omega_1\\ \omega_2\end{pmatrix}=\begin{pmatrix}\sigma_n+\sigma_{np} & \sigma_{np}\\ \sigma_{np} & \sigma_p+\sigma_{np}\end{pmatrix}\begin{pmatrix}\zeta_n+P_nT\\ \zeta_p+P_pT\end{pmatrix},$$

$$H=H(\cdot,\varphi,T,\zeta_n,\zeta_p,f_0,f_1,\ldots,f_k),\qquad R=R(\cdot,\varphi,T,\zeta_n,\zeta_p,f_0,f_1,\ldots,f_k)$$

with coefficients $\kappa>0$, $\sigma_n,\ \sigma_p>0$, $\sigma_{np}\geq 0$, $P_n,\ P_p$,
all depending in a nonsmooth way on x, smoothly on the state variables,
system strongly coupled, matrix not symmetric

Γ_D and Γ_N denote disjoint, relatively open parts of the boundary $\Gamma = \partial\Omega$ with mes$(\Gamma \setminus (\Gamma_D \cup \Gamma_N)) = 0$

mixed boundary conditions

$$(5)\qquad \begin{array}{rrrrl} \varphi = v_{D1}, & T = v_{D2}, & \zeta_n = v_{D3}, & \zeta_p = v_{D4} & \text{on } \Gamma_D \\ \nu \cdot (\varepsilon \nabla \varphi) = g_1, & -\nu \cdot j_e = g_2, & -\nu \cdot j_n = g_3, & -\nu \cdot j_p = g_4 & \text{on } \Gamma_N \end{array}$$

notation

$$v = (\varphi, T, \zeta_n, \zeta_p), \quad v_D = (v_{D1}, \dots, v_{D4}), \quad g = (g_1, \dots, g_4), \quad f = (f_0, f_1, \dots, f_k)$$

$$w = (v_D, g, f) \quad \text{(vector of data)}$$

look for weak solutions of (4), (5) in the form

$$v = V + v^D$$

where
- $v^D = L v_D$ continuation of the Dirichlet values v_D to Ω
- V fulfils homogeneous Dirichlet bcs on Γ_D

Outline of the results and methods for the reduced stationary energy model

result:

existence of a thermodynamic equilibrium

$$v_i^* = \text{const}, \; i = 2, 3, 4, \; v_3^* + v_4^* = 0$$

local existence and uniqueness result near this thermodynamic equilibrium

methods:

- prove existence of a thermodynamic equilibrium v^* with $T^*, n^*, p^* > 0$
- apply Implicit Function Theorem
- we obtain only local assertions
  but we needn't global assumptions

problems:

- suitable choice of function spaces and weak formulation
- supply requirements of Implicit Function Theorem
- differentiability properties of Nemyzki operators
- regularity results for strongly coupled lin. ell. systems with mixed bcs
- technique works in 2D only

Let $s \in [1, \infty)$, we define

$$\begin{aligned} X_s &= (W_0^{1,s}(\Omega \cup \Gamma_N))^4 \\ Y_s &= (W^{1-1/s,s}(\Gamma_D))^4 \end{aligned}$$

Lemma 1. There exists a $p_0 > 2$ such that for all $p \in [2, p_0]$ the following assertion holds true:
For all $v_D \in Y_p$ there exists a unique solution $v^D \in (W^{1,p}(\Omega))^4$ of

$$\Delta v_i^D = 0 \text{ in } \Omega, \quad v_i^D = v_{Di} \text{ on } \Gamma_D, \quad \frac{\partial v_i^D}{\partial \nu} = 0 \text{ on } \Gamma_N, \quad i = 1, 2, 3, 4.$$

v^D is given by $v^D = L v_D$ where $L \in \mathcal{L}(Y_p, (W^{1,p}(\Omega))^4)$.

necessary conditions for the existence of thermodynamic equilibrium:

data has to fulfil

$$v_{Di} = \text{const}, \;\; i = 2, 3, 4, \quad v_{D3} + v_{D4} = 0,$$

$$v_{D2} > 0, \quad g_i = 0, \;\; i = 2, 3, 4$$

corresponding equilibrium densities n, p are obtained by the state equations

$$n = F_n(\cdot, v_1, Lv_{D2}, Lv_{D3}), \quad p = F_p(\cdot, v_1, Lv_{D2}, Lv_{D4})$$

where v_1 has to satisfy the nonlinear Poisson equation

$$-\nabla \cdot (\varepsilon \nabla v_1) = H(\cdot, v_1, Lv_{D2}, Lv_{D3}, Lv_{D4}, f)$$

$$v_1 = v_{D1} \text{ on } \Gamma_D, \quad \nu \cdot (\varepsilon \nabla v_1) = g_1 \text{ on } \Gamma_N$$

Let $p \in (2, p_0]$,

$$Q = \Big\{ w = (v_D, g, f) \, : v_D \in Y_p, \; (g, f) \in Z, \\ g_i = 0, \; v_{Di} = \text{const}, \; i = 2,3,4, \; v_{D2} > 0, v_{D3} + v_{D4} = 0 \Big\}$$

$$Y_p \; = (W^{1-1/p,p}(\Gamma_D))^4, \quad Z = L^\infty(\Gamma_N)^4 \times L^\infty(\Omega) \times \{ y \in L^\infty(\Omega) \; : \; \text{essinf}_{x \in \Omega} \, y > 0\}^k$$

Theorem 1. (Existence of thermodynamic equilibria)
Let $w^* = (v_D^*, g^*, f^*) \in Q$.
Then there exist $q_0 \in (2, p]$ and $v_1^* \in W^{1,q_0}(\Omega)$ such that

$$v^* = (v_1^*, L v_{D2}^*, L v_{D3}^*, L v_{D4}^*)$$

is a thermodynamic equilibrium.

set

$$\begin{aligned} v &= V + Lv_D, & w &= (v_D, g, f) \\ v^* &= V^* + Lv_D^*, & w^* &= (v_D^*, g^*, f^*) \end{aligned}$$

Definition. Let $q \in (2, p]$. We define the open subset $M_q \subset X_q \times Y_p$,

$$M_q = \Big\{ (V, v_D) \in X_q \times Y_p \text{ with } |V_i + Lv_{Di}| < \tau, \ i = 1, 3, 4, \\ \tfrac{1}{\tau} < V_2 + Lv_{D2} < \tau \ \text{ on } \Omega \ \Big\}$$

where $\tau > 1$ is such that $(V^*, v_D^*) \in M_{q_0}$

define $\quad A_q \colon M_q \times Z \to X_{q'}^*$

$$
\begin{aligned}
\langle A_q(V,w),\psi\rangle_{X_{q'}} &= \int_\Omega \sum_{i,k=1}^{4} a_{ik}(\cdot,v)\nabla v_k\cdot\nabla\psi_i\,\mathrm{d}x \\
&+ \int_\Omega \left\{ r(\cdot,v,f)\left(\exp\frac{v_3+v_4}{T}-1\right)(\psi_3+\psi_4) - H(\cdot,v,f)\psi_1 \right\}\mathrm{d}x \\
&- \int_{\Gamma_N} \sum_{i=1}^{4} g_i\psi_i\,\mathrm{d}\Gamma, \quad \psi\in X_{q'}, \qquad v = V + Lv_D
\end{aligned}
$$

Problem (P):

find (q,V,w) such that $q\in(2,p]$, $(V,w)\in X_q\times Y_p\times Z$,

$$(V,v_D)\in M_q, \quad A_q(V,w)=0$$

Implicit Function Theorem

equilibrium:

$$A_{q_0}(V^*, w^*) = 0$$

differentiability:

$$A_q\colon M_q \times Z \to X^*_{q'} \quad \text{is continuously differentiable for all } q \in (2, p]$$

properties of the linearization in the thermodynamic equilibrium:

Let $w^* = (v_D^*, g^*, f^*) \in Q$, and $A_{q_0}(V^*, w^*) = 0$.
Then there exists a $q_1 \in (2, q_0]$ such that the Fréchet derivative

$$\partial_V A_{q_1}(V^*, w^*)\colon X_{q_1} \to X^*_{q_1'}$$

is an injective Fredholm Operator of index zero.

Theorem 2. (Local existence and uniqueness of steady states)

Let $w^* = (v_D^*, g^*, f^*) \in Q$, and let (q_0, V^*, w^*) be the equilibrium solution to Problem (P) according to Theorem 1.

Then there exists $q_1 \in (2, q_0]$ such that the following assertion holds: There exist neighbourhoods $\mathcal{V} \subset X_{q_1}$ of V^* and $\mathcal{W} \subset Y_p \times Z$ of $w^* = (v_D^*, g^*, f^*)$ and a C^1-map $\Phi\colon \mathcal{W} \to \mathcal{V}$ such that $V = \Phi(w)$ iff

$$A_{q_1}(V, w) = 0, \quad (V, v_D) \in M_{q_1}, \quad V \in \mathcal{V}, \quad w = (v_D, g, f) \in \mathcal{W}.$$

For data $w = (v_D, g, f)$ near $w^* = (v_D^*, g^*, f^*) \in Q$ there exists a locally unique solution $v = V + Lv_D$ of the stationary energy model.

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