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# An application of the Implicit Function Theorem to stationary energy models for semiconductor devices

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**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 $\varphi$
- balance equation for the density of the total energy $e$
- reaction equations for incompletely ionized impurities
  (radiation-induced traps, other deep recombination centers)
  $X_j,\ X_j^{+(-)},\ j = 1, \ldots, k$

## Energy models with incompletely ionized impurities

Mathematical problems

non-smooth data:

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

strongly coupled PDEs:

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

constraints $n,\ p,\ T > 0$

restrict us to the **stationary energy model**

# Energy models with incompletely ionized impurities

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

| | |
|---|---|
| $\varepsilon$ | 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 $\mathrm{e}^- + \mathrm{h}^+ \rightleftharpoons 0$ |

## Energy models with incompletely ionized impurities

impurities: $X_j$ occur in two charge states, take place ionization reactions

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

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

$u_{2j-1}$ – density of $X_j^-$, $u_{2j}$ – density of $X_j$, $q_{2j-1} = -1$, $q_{2j} = 0$

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

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

$u_{2j-1}$ – density of $X_j$, $u_{2j}$ – density of $X_j^+$, $q_{2j-1} = 0$, $q_{2j} = 1$

## Energy models with incompletely ionized impurities

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 |
| $\zeta_i$ | – electrochemical potentials of immobile (neutral, ionized) |
| $i = 1, \ldots, 2k$ | impurities |

## Elimination of the constraints (3)

state equations

$$u_i = F_i\left(\cdot, T, \frac{\zeta_i - q_i\varphi}{T}\right), \quad i = 1, \dots, 2k, \quad n = F_n\left(\cdot, T, \frac{\zeta_n + \varphi}{T}\right), \quad p = F_p\left(\cdot, T, \frac{\zeta_p - \varphi}{T}\right)$$

kinetic relations (reaction rates)

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

under reliable assumptions eliminate the constraints (3) by evaluating the subsystems

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

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 $\zeta_i$, $i = 1, \ldots, 2k$, to write right hand sides in (1), (2):

$$
\begin{aligned}
f_0 - n + p + \sum_{i=1}^{2k} q_i u_i \quad &\mapsto \quad H(\cdot, \varphi, T, \zeta_n, \zeta_p, f_0, f_1, \ldots, f_k), \\
R_0 + \sum_{j=1}^{k} R_{j1} \quad &\mapsto \quad R(\cdot, \varphi, T, \zeta_n, \zeta_p, f_0, f_1, \ldots, f_k) \\
&\qquad = r(\cdot, \varphi, T, \zeta_n, \zeta_p, f_0, f_1, \ldots, f_k) \left(1 - \exp \tfrac{\zeta_n + \zeta_p}{T}\right)
\end{aligned}
$$

## Reduced energy model

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

where

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

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

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

possible to change the generalized forces of the fluxes to symmetrize the matrix

for the generalized forces

$$\nabla\left(-\frac{1}{T}\right), \nabla\left(\frac{\zeta_n}{T}\right), \nabla\left(\frac{\zeta_p}{T}\right)$$

and the fluxes $(j_e, j_n, j_p)$ the Onsager relations are fulfilled

## Reduced energy model

$\Gamma_D$ and $\Gamma_N$ denote disjoint, relatively open parts of the boundary $\Gamma = \partial\Omega$ with
$\mathrm{mes}\,(\Gamma \setminus (\Gamma_D \cup \Gamma_N)) = 0$, $\quad \Omega \cup \Gamma_N$ regular in the sense of Gröger

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

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

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

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 $\Omega$
- $V$ fulfils homogeneous Dirichlet bcs on $\Gamma_D$

# 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

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 $p \in [1, \infty)$, we define

$$X_p = (W_0^{1,p}(\Omega \cup \Gamma_N))^4$$
$$Y_p = (W^{1-1/p,p}(\Gamma_D))^4$$

**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 $L \in \mathcal{L}(Y_p, (W^{1,p}(\Omega))^4)$.

## Thermodynamic equilibrium

necessary conditions for the existence of thermodynamic equilibrium:

data has to fulfil

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

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

evaluate thermodynamic equilibrium $\quad v = V + L v_D$

set

$$V_i = 0, \qquad v_i = L v_{Di}, \qquad i = 2, 3, 4$$

$v_1$ has to satisfy the nonlinear Poisson equation

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

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

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

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

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

**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

$$v = V + Lv_D, \qquad w = (v_D, g, f)$$
$$v^* = V^* + Lv_D^*, \qquad w^* = (v_D^*, g^*, f^*)$$

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

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

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

## Weak formulation

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

$$\langle A_q(V, w), \psi\rangle_{X_{q'}} = \int_\Omega \sum_{i,k=1}^{4} a_{ik}(\cdot, v)\nabla v_k \cdot \nabla \psi_i \,\mathrm{d}x$$

$$+ \int_\Omega \left\{ r(\cdot, v, f)\left(\exp\frac{v_3 + v_4}{T} - 1\right)(\psi_3 + \psi_4) - H(\cdot, v, f)\psi_1 \right\} \mathrm{d}x$$

$$- \int_{\Gamma_N} \sum_{i=1}^{4} g_i \psi_i \,\mathrm{d}\Gamma, \quad \psi \in X_{q'}, \qquad v = V + L v_D$$

**Problem (P):**

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

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

# Setting for the 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 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

$$\partial_V A_{q_1}(V^*, w^*) \in \mathcal{LIS}(X_{q_1}, X^*_{q_1'}).$$

## Sketch of the proof

$B_q \, : \, X_q \to X^*_{q'},$

$$B_q := \partial_V A_q(V^*, w^*) \circ D(v^*), \quad D(v^*) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & v_2^{*2} & 0 & 0 \\ 0 & v_2^* v_3^* & v_2^{*2} & 0 \\ 0 & v_2^* v_4^* & 0 & v_2^{*2} \end{pmatrix} \in \mathcal{LIS}(X_q, X_q)$$

main part of $B_q$: strongly coupled, symmetric, strongly elliptic

$B_q = L_q + K_q$

$L_q$ injective, surjective for $q \in (2, q_1]$ (regularity result in Gröger’89)
$K_q$ compact

$B_{q_1}$ Fredholm operator of index zero, $B_{q_1}$ injective

$B_{q_1}, \; \partial_V A_{q_1}(V^*, w^*) \in \mathcal{LIS}(X_{q_1}, X^*_{q_1'})$

**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 $v = V + L v_D$ of the stationary energy model.

## References

G. Albinus, H. Gajewski, and R. Hünlich, *Thermodynamic design of energy models of semiconductor devices*, Nonlinearity **15** (2002), 367–383.

A. Glitzky, R. Hünlich, *Stationary solutions of two-dimensional heterogeneous energy models with multiple species*, Banach Center Publ. **66** (2004), 135-151.

A. Glitzky, R. Hünlich, *Stationary energy models for semiconductor devices with incompletely ionized impurities*, to appear in ZAMM 11-2005.

K. Gröger, *Initial–boundary value problems describing mobile carrier transport in semiconductor devices*, Math. Univ. Carolin. **26** (1985), 75–89.

K. Gröger, *A* $W^{1,p}$*–estimate for solutions to mixed boundary value problems for second order elliptic differential equations*, Math. Ann. **283** (1989), 679–687.

L. Recke, *Applications of the Implicit Function Theorem to quasi-linear elliptic boundary value problems with non-smooth data*, Comm. Partial Differential Equations **20** (1995), 1457–1479.

## Assumptions

(A1) $\Omega$ is a bounded Lipschitzian domain in $\mathbb{R}^2$, $\Gamma = \partial\Omega$,
$\Gamma_D,\ \Gamma_N$ are disjoint open subsets of $\Gamma$, mes $\Gamma_D > 0$,
$\Gamma = \Gamma_D \cup \Gamma_N \cup (\overline{\Gamma_D} \cap \overline{\Gamma_N})$, $\overline{\Gamma_D} \cap \overline{\Gamma_N}$ consists of finitely many points,
$\Sigma \subset \Omega$ with mes $\Sigma = 0$.

(A2) $\varepsilon \in L^\infty(\Omega),\ 0 < \varepsilon_0 \le \varepsilon(x) \le \varepsilon^0 < \infty$ in $\Omega \setminus \Sigma$.

**Definition.**
Let $W \subset \mathbb{R}^m$ be an open set.
$b : \Omega \times W \to \mathbb{R}$ is of the class $D(W)$ iff $b$ is a Caratheodory function, which is continuously differentiable with respect to the second argument and for which the function itself as well as its derivative with respect to the second argument are locally bounded and locally uniformly continuous.

## Assumptions

(A3) $\kappa,\ \sigma_n,\ \sigma_p,\ \sigma_{np},\ P_n,\ P_p : \Omega \times W_1 \to \mathbb{R}$ are of the class $D(W_1)$ with $W_1 = (0,\infty) \times \mathbb{R}^2$.
For all $K > 1$ there exists a $c_K > 1$ such that
$\kappa(x,T,\zeta_n,\zeta_p),\ \sigma_n(x,T,\zeta_n,\zeta_p), \sigma_p(x,T,\zeta_n,\zeta_p) \in [1/c_K, c_K]$
for $x \in \Omega \setminus \Sigma$, $(T,\zeta_n,\zeta_p) \in [1/K,K] \times [-K,K]^2$.
$\sigma_{np}(x,T,\zeta_n,\zeta_p) \geq 0$ for $x \in \Omega \setminus \Sigma$, $(T,\zeta_n,\zeta_p) \in W_1$.

(A4) $F_i : \Omega \times W_2 \to \mathbb{R}_+$ are of the class $D(W_2)$ with $W_2 = (0,\infty) \times \mathbb{R}$.
For all $K > 1$ there exist $\widehat{c}_K > 0$, $c_K > 1$ such that $\frac{\partial F_i}{\partial y}(x,T,y) \geq \widehat{c}_K$, $F_i(x,T,y) \in [1/c_K, c_K]$ for $x \in \Omega \setminus \Sigma$, $(T,y) \in [1/K,K] \times [-K,K]$, $\lim_{y\to-\infty} F_i(x,T,y) = 0$, $\lim_{y\to+\infty} F_i(x,T,y) = +\infty$ for $x \in \Omega \setminus \Sigma$, $T \in (0,\infty)$, $i = n,p$ and $i = 1,\ldots,2k$.
For all $K > 1$ there exists $c_K > 0$ such that $F_i(x,T,y) \leq c_K \mathrm{e}^{c_K|y|}$ for $x \in \Omega \setminus \Sigma$, $(T,y) \in [1/K,K] \times \mathbb{R}$, $i = n,p$.

(A5) $r_0,\ r_{ji} : \Omega \times W_3 \to \mathbb{R}_+$ are of the class $D(W_3)$ with $W_3 = \mathbb{R} \times (0,\infty) \times \mathbb{R}^2$.
For all $K > 1$ there exists a $c_K > 1$ such that $r_{ji}(x,\varphi,T,\zeta_n,\zeta_p) \in [1/c_K, c_K]$ for $x \in \Omega \setminus \Sigma$, $(\varphi,T,\zeta_n,\zeta_p) \in [-K,K] \times [1/K,K] \times [-K,K]^2$, $j = 1,\ldots,k$, $i = 1,2$.