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Energy models for semiconductor devices where the various equations are defined on different domains

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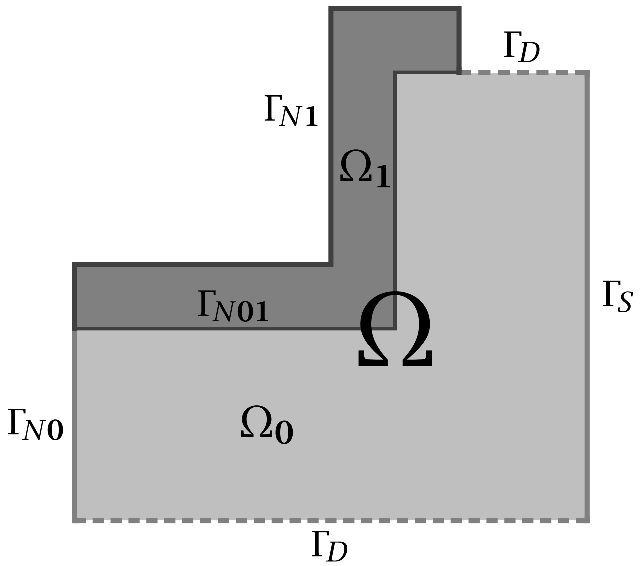
mass and charge and energy transport described by

- continuity equations for densities n, p of electrons e^- and holes h^+ on Ω_0
- balance equation for the density of the total energy e on Ω
- Poisson equation for the electrostatic potential φ on Ω



strongly coupled PDEs, different domains of definition, heterogeneous materials, mixed boundary conditions

restrict us to the **stationary energy model**

Stationary energy model

$$\nabla \cdot j_n = R, \quad \nabla \cdot j_p = R \qquad \text{in } \Omega_0$$

$$\nabla \cdot j_e = 0 \qquad \text{in } \Omega$$

$$-\nabla \cdot (\varepsilon \nabla \varphi) = \begin{cases} f - n + p & \text{in } \Omega_0 \\ f & \text{in } \Omega_1 \end{cases}$$

R	reaction rate of the direct electron-hole recombination-generation $e^- + h^+ \rightleftharpoons 0$
$j_n,\ j_p$	particle flux densities of electrons and holes
j_e	flux density of the total energy
ε	dielectric permittivity
f	prescribed charge density

system has to be completed by

state equations, kinetic relations, mixed boundary conditions

Stationary energy model: state equations, kinetic relations

$\zeta_n,\ \zeta_p$ – electrochemical potentials of electrons and holes, T – lattice temperature

use variables

$$z = \left(\frac{\zeta_n}{T}, \frac{\zeta_p}{T}, -\frac{1}{T}, \varphi\right),$$

z_1, z_2 defined on Ω_0
z_3, z_4 defined on Ω

state equations:

$$n = H_n(\cdot, z), \quad p = H_p(\cdot, z)$$

$$n - p = h(\cdot, z)$$

reaction:

$$R = r(\cdot, z)\left(\mathrm{e}^{z_1+z_2} - 1\right)$$

Stationary energy model:kinetic relations

fluxes:

$$\begin{pmatrix} j_n \\ j_p \\ j_e \end{pmatrix} = - \begin{pmatrix} \sigma_{nn} T & \sigma_{np} T & \tilde{\tau}_n \\ \sigma_{pn} T & \sigma_{pp} T & \tilde{\tau}_p \\ \tilde{\tau}_n & \tilde{\tau}_p & \kappa T^2 + \tilde{\tau}_0 \end{pmatrix} \begin{pmatrix} \nabla z_1 \\ \nabla z_2 \\ \nabla z_3 \end{pmatrix} \quad \text{on } \Omega_0$$

$$\tilde{\tau}_i = \sum_{k=n,p} \sigma_{ik} T(\zeta_k + P_k T), \; i = n, p, \quad \tilde{\tau}_0 = \sum_{i,k=n,p} \sigma_{ik} T(\zeta_i + P_i T)(\zeta_k + P_k T)$$

$$j_e = -\tilde{\kappa} T^2 \nabla z_3 \qquad \text{on } \Omega_1$$

conductivities $\tilde{\kappa}, \kappa, \sigma_{nn}, \sigma_{pp} > 0$, $\sigma_{np} = \sigma_{pn} \geq 0$ depend nonsmoothly on x and smoothly on the state variables, $P_n, \; P_p$ - transported entropies

Onsager relations are fulfilled

Stationary energy model: strongly coupled system (1)

$$-\nabla\cdot\begin{pmatrix} a_{11}(z) & a_{12}(z) & a_{13}(z) & 0\\ a_{21}(z) & a_{22}(z) & a_{23}(z) & 0\\ a_{31}(z) & a_{32}(z) & a_{33}(z) & 0\\ 0 & 0 & 0 & \varepsilon \end{pmatrix}\begin{pmatrix}\nabla z_1\\ \nabla z_2\\ \nabla z_3\\ \nabla z_4\end{pmatrix} = \begin{pmatrix} -R(z)\\ -R(z)\\ 0\\ f-h(z)\end{pmatrix} \qquad \text{on } \Omega_0$$

$$-\nabla\cdot\begin{pmatrix} \tilde{a}_{33}(z_3) & 0\\ 0 & \varepsilon\end{pmatrix}\begin{pmatrix}\nabla z_3\\ \nabla z_4\end{pmatrix} = \begin{pmatrix}0\\ f\end{pmatrix} \qquad \text{on } \Omega_1$$

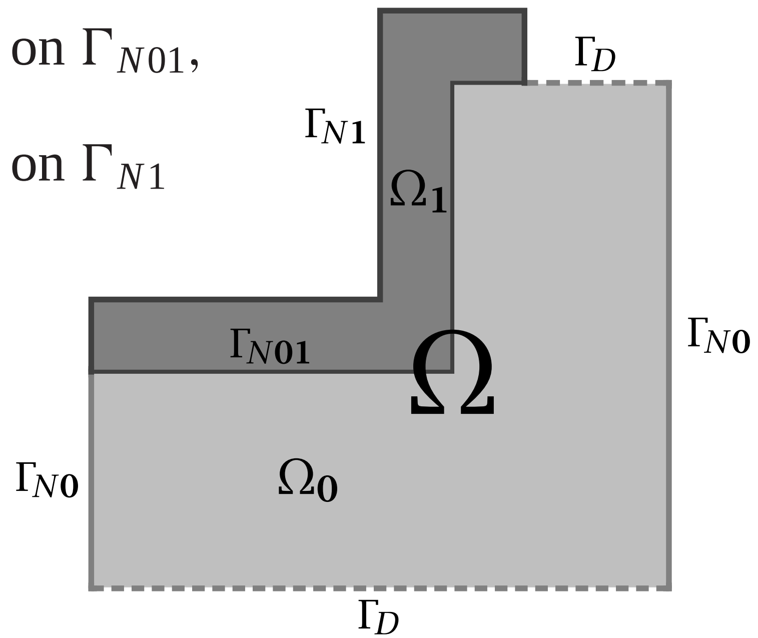
Stationary energy model: boundary conditions (2)

$$z_i = z_i^D,\ i = 1, \ldots, 4, \qquad \text{on } \Gamma_D,$$

$$\nu \cdot \textstyle\sum_{k=1,2,3} a_{ik}(x,z)\nabla z_k = g_i^{N0},\ i = 1,2,3, \qquad \text{on } \Gamma_{N0},$$
$$\nu \cdot (\varepsilon \nabla z_4) = g_4^{N0} \qquad \text{on } \Gamma_{N0},$$

$$\nu \cdot \textstyle\sum_{k=1,2,3} a_{ik}(x,z)\nabla z_k = 0,\ i = 1,2, \qquad \text{on } \Gamma_{N01},$$

$$\nu \cdot \tilde{a}_{33}(z_3) = g_3^{N1},\ \ \nu \cdot (\varepsilon \nabla z_4) = g_4^{N1} \qquad \text{on } \Gamma_{N1}$$



Notation

$$G_0 = \Omega_0 \cup \Gamma_{N0} \cup \Gamma_{N01}, \quad G = \Omega \cup \Gamma_N, \quad \Gamma_N = \Gamma_{N0} \cup \Gamma_{N1}$$

$$X_s = (W_0^{1,s}(G_0))^2 \times (W_0^{1,s}(G))^2,$$
$$W_s = (W^{1,s}(\Omega_0))^2 \times (W^{1,s}(\Omega))^2$$

define vectors of data

$$w = (z^D, g, f), \quad z^D = (z_1^D, \ldots, z_4^D), \quad g = (g_1^{N0}, \ldots, g_4^{N0}, g_3^{N1}, g_4^{N1})$$

$$\mathcal{H} = W_p \times L^\infty(\Gamma_{N0})^4 \times L^\infty(\Gamma_{N1})^2 \times L^\infty(\Omega)$$

look for solutions in the form $z = Z + z^D$, where z^D corresponds to a function fulfilling the Dirichlet boundary conditions and Z represents the homogeneous part of the solution

$$M_{q,\tau} = \Big\{(Z, z^D) \in X_q \times W_p : |Z_i + z_i^D| < \tau, \ i = 1, 2, \ \text{on } \Omega_0,$$
$$-\tau < Z_3 + z_3^D < -\frac{1}{\tau}, \quad |Z_4 + z_4^D| < \tau \text{ on } \Omega\Big\}, \quad q \in (2, p], \ \tau > 1$$

Weak formulation of the stationary energy model

$$F_{q,\tau} : M_{q,\tau} \times L^\infty(\Gamma_{N0})^4 \times L^\infty(\Gamma_{N1})^2 \times L^\infty(\Omega) \to X^*_{q'}$$

$$\begin{aligned}\langle F_{q,\tau}(Z,w),\psi\rangle_{X_{q'}} &= \int_{\Omega_0} \Big\{ \sum_{i,k=1}^{3} a_{ik}(\cdot,z)\nabla z_k \cdot \nabla\psi_i + \varepsilon\nabla z_4\cdot\nabla\psi_4 \Big\} \mathrm{d}x \\ &+ \int_{\Omega_0} \Big\{ R(\cdot,z)(\psi_1+\psi_2) + h(\cdot,z)\psi_4 \Big\} \mathrm{d}x - \int_\Omega f\,\psi_4\,\mathrm{d}x \\ &+ \int_{\Omega_1} \Big\{ \tilde{a}_{33}(\cdot,z_3)\nabla z_3\cdot\nabla\psi_3 + \varepsilon\nabla z_4\cdot\nabla\psi_4 \Big\} \mathrm{d}x \\ &- \int_{\Gamma_{N0}} \sum_{i=1}^{4} g_i^{N0}\psi_i\,\mathrm{d}\Gamma - \int_{\Gamma_{N1}} (g_3^{N1}\psi_3 + g_4^{N1}\psi_4)\,\mathrm{d}\Gamma, \quad \psi \in X_{q'}\end{aligned}$$

Problem (P):

Find (q, τ, Z, w) such that $q \in (2, p]$, $\tau > 1$, $(Z, w) \in X_q \times \mathcal{H}$,

$$F_{q,\tau}(Z,w) = 0, \quad (Z, z^D) \in M_{q,\tau}.$$

data compatible with thermodynamic equilibrium

$$Q := \Big\{ w = (z^D, g, f) \in \mathcal{H} : \; z_i^D = \text{const}, \;\; g_i^{N0} = 0, \; i = 1, 2, 3, \\ g_3^{N1} = 0, \;\; z_1^D + z_2^D = 0, \;\; z_3^D < 0 \Big\}$$

Theorem 1. Let $w^* = (z^{D*}, g^*, f^*) \in Q$ be given.

i) Then there exist $q_0 \in (2, p]$, $\tau > 1$ and $Z_4^* \in W_0^{1,q_0}(G)$ such that $(Z^*, z^{D*}) = ((0, 0, 0, Z_4^*), z^{D*}) \in M_{q_0,\tau}$ and $F_{q_0,\tau}(Z^*, w^*) = 0$.
In other words, (q_0, τ, Z^*, w^*) is a solution to (P).

ii) $z^* = Z^* + z^{D*}$ is a thermodynamic equilibrium of (1), (2).

iii) If $(\widetilde{q}, \widetilde{\tau}, \widetilde{Z}, w^*)$ is solution to (P) then $\widetilde{Z} = Z^*$ in $X_{\widehat{q}}$ with $\widehat{q} = \min\{q_0, \widetilde{q}\}$ holds.

Lemma 1. (Differentiability)
For all parameters $\tau > 1$, all exponents $q \in (2, p]$ the operator

$$F_{q,\tau} : M_{q,\tau} \times L^\infty(\Gamma_{N0})^4 \times L^\infty(\Gamma_{N1})^2 \times L^\infty(\Omega) \to X^*_{q'}$$

is continuously differentiable.

Proof: Differentiability properties of Nemyzki operators (Recke'95)

Lemma 2. (Fredholm property and injectivity of the linearization)
Let $w^* = (z^{D*}, g^*, f^*) \in Q$ be given. Let (q_0, τ, Z^*, w^*) be the equilibrium solution to Problem (P) (see Theorem 1). Then there exists a $q_1 \in (2, q_0]$ such that the operator $\partial_Z F_{q_1,\tau}(Z^*, w^*)$ is an injective Fredholm operator of index zero.

Sketch of the proof

$$\partial_Z F_{q,\tau}(Z^*, w^*) = L_q + K_q$$

$$\langle L_q\, Z, \psi\rangle_{X_{q'}} = \int_{\Omega_0} \Big(\sum_{i,k=1}^{3} a_{ik}(\cdot, z^*)\nabla Z_k \cdot \nabla \psi_i + \varepsilon\, \nabla Z_4 \cdot \nabla \psi_4 + \sum_{i=1}^{4} Z_i\, \psi_i \Big) \mathrm{d}x$$

$$+ \int_{\Omega_1} \Big(\tilde{a}_{33}(\cdot, z_3^*)\nabla Z_3 \cdot \nabla \psi_3 + \varepsilon\, \nabla Z_4 \cdot \nabla \psi_4 + \sum_{i=3}^{4} Z_i\, \psi_i \Big) \mathrm{d}x,$$

$$\langle K_q\, Z, \psi\rangle_{X_{q'}} = \int_{\Omega_0} \Big\{ r(\cdot, z^*)(Z_1 + Z_2)(\psi_1 + \psi_2) + \partial_z h(\cdot, z^*) \cdot Z\, \psi_4 - \sum_{i=1}^{4} Z_i\, \psi_i \Big\}\, \mathrm{d}x$$

$$- \int_{\Omega_1} \sum_{i=3}^{4} Z_i\, \psi_i\, \mathrm{d}x\,, \qquad \psi \in X_{q'}.$$

K_q compact
L_q injective, surjective for $q \in (2, q_1]$ (surjectivity result in Theorem 3)

Banach's open mapping theorem, Nikolsky's criterion $\Longrightarrow$
$\partial_Z F_{q_1,\tau}(Z^*, w^*)$ Fredholm operator of index zero,

$\partial_Z F_{q_1,\tau}(Z^*, w^*)$ injective □

Theorem 2. Let $w^* = (z^{D*}, g^*, f^*) \in Q$, and let (q_0, τ, Z^*, 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 $U \subset X_{q_1}$ of Z^* and $W \subset \mathcal{H}$ of $w^* = (z^{D*}, g^*, f^*)$ and a C^1-map $\Phi\colon W \to U$ such that $Z = \Phi(w)$ iff

$$F_{q_1,\tau}(Z, w) = 0, \quad (Z, z^D) \in M_{q_1,\tau}, \quad Z \in U, \quad w = (z^D, g, f) \in W.$$

For data $w = (z^D, g, f)$ near $w^* = (z^{D*}, g^*, f^*) \in Q$ there exists a locally unique solution $z = Z + z^D$ of the stationary energy model (1), (2).

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

$$\langle AZ, \psi\rangle_{X_{q'}} = \int_{\Omega_0} \Big\{ \sum_{i,k=1}^{4} d_{ik} \nabla Z_k \cdot \nabla \psi_i + \sum_{i=1}^{4} d_i Z_i \psi_i \Big\} \mathrm{d}x$$
$$+ \int_{\Omega_1} \Big\{ \sum_{i,k=3}^{4} \tilde{d}_{ik} \nabla Z_k \cdot \nabla \psi_i + \sum_{i=3}^{4} \tilde{d}_i Z_i \psi_i \Big\} \mathrm{d}x, \qquad Z \in X_q,\ \psi \in X_{q'}$$

assume:

$d_{ik}, d_i \in L^\infty(\Omega_0)$, $i, k = 1, \ldots, 4$, $\tilde{d}_{ik}, \tilde{d}_i \in L^\infty(\Omega_1)$, $i, k = 3, 4$, $\exists\, M, m > 0$ such that

$$\sum_{i,k=1}^{4} d_{ik} t_k t_i \geq m|t|^2_{\mathbb{R}^4}, \quad \sum_{i=1}^{4} \Big| \sum_{k=1}^{4} d_{ik} t_k \Big|^2 \leq M^2 |t|^2_{\mathbb{R}^4} \quad \forall t \in \mathbb{R}^4, \quad m \leq d_i \leq M \text{ a.e. in } \Omega_0$$

$$\sum_{i,k=3}^{4} \tilde{d}_{ik} t_k t_i \geq m|t|^2_{\mathbb{R}^2}, \quad \sum_{i=3}^{4} \Big| \sum_{k=3}^{4} \tilde{d}_{ik} t_k \Big|^2 \leq M^2 |t|^2_{\mathbb{R}^2} \quad \forall t \in \mathbb{R}^2, \quad m \leq \tilde{d}_i \leq M \text{ a.e. in } \Omega_1$$

Surjectivity result for L_{q_1}

$$J_{2,G} : W_0^{1,2}(G) \to W^{-1,2}(G), \quad \langle J_{2,G}u, v\rangle = \int_G (uv + \nabla u \cdot \nabla v)\mathrm{d}x$$

$q > 2$: $J_{q,G} := J_{2,G}|_{W_0^{1,q}(G)} : W_0^{1,q}(G) \to W^{-1,q}(G)$ continuous,

exists $r(G) > 2$ such that $J_{q,G}$ is onto for $q \in [2, r(G)]$ (Gröger'89)

$$M_{q,G} := \sup\{\|u\|_{W_0^{1,q}(G)} : u \in W_0^{1,q}(G),\ \|J_{q,G}u\|_{W^{-1,q}(G)} \le 1\}, \quad M_{2,G} = 1$$

analogously for G_0

$$J_q := (J_{q,G_0}, J_{q,G_0}, J_{q,G}, J_{q,G})$$

$J_q : X_q \to X_{q'}^*$ is onto for $q \in [2, \hat{r}]$, $\hat{r} = \min\{r(G_0), r(G)\}$

$$M_q := \sup\{\|u\|_{X_q} : u \in X_q,\ \|J_q u\|_{X_{q'}^*} \le 1\}$$

$$M_q \le \max\left\{(M_{\hat{r},G_0})^\theta, (M_{\hat{r},G})^\theta\right\}, \qquad \frac{1}{q} = \frac{\theta}{\hat{r}} + \frac{1-\theta}{2}$$

Theorem 3. The operator A maps X_q onto $X^*_{q'}$ provided that $q \in [2, \hat{r}]$ and

$$4^{1/2-1/q} M_q \Big(1 - \frac{m^2}{M^2}\Big)^{1/2} < 1.$$

Proof. Let $h \in X^*_{q'}$, $q \in [2, \hat{r}]$, define $Q_h : X_q \to X_q$ by

$$Q_h Z := Z - \frac{m}{M^2} J_q^{-1}(AZ - h), \quad Z \in X_q$$

$$\|Q_h Z - Q_h \bar{Z}\|_{X_q} \leq 4^{1/2-1/q} M_q \Big(1 - \frac{m^2}{M^2}\Big)^{1/2} \|Z - \bar{Z}\|_{X_q}$$

$$4^{1/2-1/q} M_q \Big(1 - \frac{m^2}{M^2}\Big)^{1/2} \to \Big(1 - \frac{m^2}{M^2}\Big)^{1/2} < 1 \quad \text{for } q \to 2$$

Banachs Fixed Point Theorem □

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Assumptions

(A1) Ω, Ω_0 are bounded Lipschitzian domains in $\mathbb{R}^2$,
G, G_0 are regular in the sense of Gröger'89

(A2) $\varepsilon \in L^\infty(\Omega),\ 0 < \varepsilon_0 \leq \varepsilon(x) \leq \varepsilon^0 < \infty$ in Ω.

Definition.
Let $V = \mathbb{R}^2 \times (-\infty, 0) \times \mathbb{R}$.
Then $b : \Omega_0 \times W \to \mathbb{R}$ is of the class D_0 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.

$b : \Omega_1 \times V_1 \to \mathbb{R}$ is of the class D_1 if in the definition V and Ω are substituted by $V_1 = (-\infty, 0)$ and Ω_1.

Assumptions

(A3) $a_{ik} : \Omega_0 \times V \to \mathbb{R}$ are of the class (D_0), $i, k = 1, 2, 3$.
For every compact subset $K \subset V$ there exists an $a_K > 0$ such that

$$\sum_{i,k=1}^{3} a_{ik}(x, z)\xi_i\xi_k \geq a_K \|\xi\|^2 \text{ for all } z \in K, \text{ all } \xi \in \mathbb{R}^3 \text{ and f.a.a. } x \in \Omega_0.$$

$\tilde{a}_{33} : \Omega_1 \times V_1 \to \mathbb{R}_+$ is of the class (D_1),
for every $k > 1$ there exists an $\tilde{a}_k > 0$ such that
$\tilde{a}_{33}(x, z) \geq \tilde{a}_k$ for all $z \in [-k, -1/k]$ and a.a. $x \in \Omega_1$.

(A4) $H_i : \Omega_0 \times V \to \mathbb{R}_+$, $i = n, p$, are of the class (D_0),
$h = H_n - H_p : \Omega_0 \times V \to \mathbb{R}$, $h(x, z_1, z_2, z_3, \cdot)$ is monotonic increasing
for all $z \in \mathbb{R}^2 \times (-\infty, 0) \times \mathbb{R}$ and a.a. $x \in \Omega_0$.
$|h(x, z)| \leq c_k e^{c|z_4|}$ for all
$(z_1, z_2, z_3) \in [-k, k]^2 \times [-k, -1/k]$, $z_4 \in \mathbb{R}$ and a.a $x \in \Omega_0$.

(A5) $R(x, z) = r(x, z)\big(e^{z_1+z_2} - 1\big)$, $r : \Omega_0 \times V \to \mathbb{R}_+$ is of the class (D_0).

Outline of the proof of Theorem 1

1. $\mathcal{E} : H_0^1(G) \to H^{-1}(G)$,

$$\langle \mathcal{E}(\phi), \bar{\phi} \rangle_{H_0^1(G)} = \int_\Omega \left\{ \varepsilon \nabla(\phi + z_4^{D*}) \cdot \nabla\bar{\phi} - f^* \bar{\phi} \right\} \mathrm{d}x - \int_{\Gamma_{N0}} g_4^{N0*} \bar{\phi} \, \mathrm{d}\Gamma - \int_{\Gamma_{N1}} g_4^{N1*} \bar{\phi} \, \mathrm{d}\Gamma$$
$$+ \int_{\Omega_0} h(\cdot, (0,0,0,\phi) + z^{D*}) \, \bar{\phi} \, \mathrm{d}x \qquad \forall \bar{\phi} \in H_0^1(G)$$

is strongly monotone, hemicontinuous, exists a unique solution $\phi \in H_0^1(G)$ of $\mathcal{E}(\phi) = 0$.

2. higher regularity $\phi \in W^{1,q_0}(G)$, $q_0 > 2$ (Gröger'89),
   exists $\tau > 0$ such that (q_0, τ, Z^*, w^*) with $Z^* = (0, 0, 0, \phi)$ is a solution to (P)
   $z^* = Z^* + z^{D*}$ is a thermodynamic equilibrium of (1), (2)

3. uniqueness (indirect proof)