Weierstraß-Institut für Angewandte Analysis und Stochastik

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Energiemodelle für heterogene Halbleiterstrukturen

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Introduction

mass, charge and energy transport in heterogeneous semiconductor materials

mass and charge transport of charged and uncharged particles $\Longrightarrow$
continuity equations + Poisson equation
energy transport resulting in a variation of the lattice temperature $\Longrightarrow$
heat flow equation or balance equation for the densities of entropy or energy

heterogeneity: heterogeneous materials, mixed boundary conditions

fields of application:

- application of semiconductor devices
- semiconductor technology
- other problems in electrochemistry

Instationary energy model

$X_i, \ i = 1, \ldots, n$	- species	$\overline{u}_i$	- reference density
u_i	- particle density	E_i	- reference energy
ζ_i	- electrochemical potential	φ	- electrostatic potential
q_i	- charge number	T	- lattice temperature
e	- density of the internal energy	s	- entropy density
e_i	- specific energy	s_i	- specific entropy
e_L	- lattice energy	s_L	- lattice entropy

ansatz for the state equations

$$u_i = \overline{u}_i(x, T)\, \mathrm{e}^{(\zeta_i - q_i\varphi - E_i(x,T))/T}$$

$$e = e_L(T) + \sum_{i=1}^{n} u_i e_i(x, u_i, T), \quad e_i = E_i + T(T(\ln \overline{u}_i)' - E_i'), \quad ' = \frac{\partial}{\partial T}$$

$$s = s_L(T) + \sum_{i=1}^{n} u_i s_i(x, u_i, T), \quad s_i = 1 + T(\ln \overline{u}_i)' - E_i' - \ln \frac{u_i}{\overline{u}_i}$$

Instationary energy model

reversible, charge preserving reactions

$$\alpha_1 X_1 + \ldots + \alpha_n X_n \rightleftharpoons \beta_1 X_1 + \ldots + \beta_n X_n$$

stoichiometric coefficients $(\alpha, \beta) = (\alpha_1, \ldots, \alpha_n, \beta_1, \ldots, \beta_n) \in \mathcal{R}$

reaction rates according to the mass action law

$$R_{\alpha\beta} = r_{\alpha\beta}(x, u, T, \varphi) \left(\mathrm{e}^{\sum_{i=1}^n \alpha_i \zeta_i / T} - \mathrm{e}^{\sum_{i=1}^n \beta_i \zeta_i / T} \right), \quad (\alpha, \beta) \in \mathcal{R}$$

Instationary energy model

ansatz for particle flux densities j_i and entropy flux density j_s

$$j_i = -\sum_{k=1}^{n} \sigma_{ik}(x,u,T)\,(\nabla\zeta_k + P_k(x,u,T)\nabla T)\,, \quad i = 1,\dots,n$$

$$j_s = -\frac{\kappa(x,u,T)}{T}\nabla T + \sum_{i=1}^{n} P_i(x,u,T)\,j_i$$

σ_{ik}, κ - conductivities, P_i - transported entropies

$$\sigma_{ik} = \sigma_{ki}, \quad \sum_{i,k=1}^{n} \sigma_{ik}(x,u,T) y_i y_k \geq \sigma_0(u,T)\|y\|^2 \quad \forall y \in \mathbb{R}^n, \quad \kappa(x,u,T) \geq \kappa_0(u,T)$$

with $\sigma_0(u,T)$, $\kappa_0(u,T) > 0$ for all non-degenerated states u, T, no sign condition for P_i

for isothermal case ($\nabla T = 0$): $j_s = \sum_{i=1}^{n} P_i\, j_i$
explains the meaning of P_i as transported entropies

Instationary energy model

entropy formulation

$$\begin{pmatrix} j_1 \\ \vdots \\ j_n \\ j_s \end{pmatrix} = -\begin{pmatrix} \sigma_{11} & \cdots & \sigma_{1n} & \tau_1 \\ \vdots & \ddots & \vdots & \vdots \\ \sigma_{n1} & \cdots & \sigma_{nn} & \tau_n \\ \tau_1 & \cdots & \tau_n & \frac{\kappa}{T} + \tau_{n+1} \end{pmatrix} \begin{pmatrix} \nabla \zeta_1 \\ \vdots \\ \nabla \zeta_n \\ \nabla T \end{pmatrix}$$

$$\tau_i = \sum_{k=1}^{n} \sigma_{ik} P_k, \quad i = 1, ..., n, \quad \tau_{n+1} = \sum_{i,k=1}^{n} \sigma_{ik} P_i P_k$$

matrix is symmetric, positive definite for non-degenerated states $\Longrightarrow$ Onsager's relations are fulfilled for fluxes $(j_1, \ldots, j_n, j_s)$ and generalized forces $(\nabla \zeta_1, \ldots, \nabla \zeta_n, \nabla T)$

Instationary energy model

n continuity equations, entropy balance equation, Poisson equation

$$\begin{aligned} \frac{\partial u_i}{\partial t} + \nabla \cdot j_i &= \sum_{(\alpha,\beta)\in\mathcal{R}} (\beta_i - \alpha_i) R_{\alpha\beta}, \quad i = 1, \ldots, n \\ \frac{\partial s}{\partial t} + \nabla \cdot j_s &= d \\ -\nabla \cdot (\varepsilon \nabla \varphi) &= f + \sum_{i=1}^{n} q_i u_i \end{aligned}$$

entropy production rate

$$T\, d = -\sum_{i=1}^{n} j_i \cdot \nabla \zeta_i - j_s \cdot \nabla T + \sum_{(\alpha,\beta)\in\mathcal{R}} R_{\alpha\beta} \sum_{i=1}^{n} (\alpha_i - \beta_i) \zeta_i$$

$d \geq 0$, and for non-degenerated states

$$d = 0 \quad \Longleftrightarrow \quad \begin{cases} \nabla \zeta_i = 0, \quad i = 1, \ldots, n \\ \nabla T = 0 \\ \sum_{i=1}^{n} (\alpha_i - \beta_i) \zeta_i = 0 \quad \forall (\alpha, \beta) \in \mathcal{R} \end{cases}$$

conditions characterize thermodynamic equilibrium

Instationary energy model

Reformulation of the entropy balance equation by an energy balance equation

define the energy flux density

$$j_e = T j_s + \sum_{i=1}^{n} \zeta_i j_i = -\kappa \nabla T + \sum_{i=1}^{n} (\zeta_i + P_i T) j_i$$

obtain by the state equations the balance equation for the internal energy

$$\frac{\partial e}{\partial t} + \nabla \cdot j_e = \varphi \nabla \cdot \sum_{i=1}^{n} q_i j_i$$

Instationary energy model

Onsager's relations for fluxes $(j_1, \ldots, j_n, j_e)$ and generalized forces $(\nabla\zeta_1, \ldots, \nabla\zeta_n, \nabla T)$ are not fulfilled

change of generalized forces to $(\nabla[\zeta_1/T], \ldots, \nabla[\zeta_n/T], \nabla[-1/T])$

$$\begin{pmatrix} j_1 \\ \vdots \\ j_n \\ j_e \end{pmatrix} = - \begin{pmatrix} \sigma_{11}T & \cdots & \sigma_{1n}T & \widetilde{\tau}_1 \\ \vdots & \ddots & \vdots & \vdots \\ \sigma_{n1}T & \cdots & \sigma_{nn}T & \widetilde{\tau}_n \\ \widetilde{\tau}_1 & \cdots & \widetilde{\tau}_n & \kappa T^2 + \widetilde{\tau}_{n+1} \end{pmatrix} \begin{pmatrix} \nabla[\zeta_1/T] \\ \vdots \\ \nabla[\zeta_n/T] \\ \nabla[-1/T] \end{pmatrix}$$

$$\widetilde{\tau}_i = \sum_{k=1}^{n} \sigma_{ik} T (\zeta_k + P_k T), \ \ i = 1, \ldots, n, \ \ \widetilde{\tau}_{n+1} = \sum_{i,k=1}^{n} \sigma_{ik} T (\zeta_i + P_i T)(\zeta_k + P_k T)$$

matrix is symmetric, positive definite for non-degenerated states $\Longrightarrow$ Onsager's relations are fulfilled for fluxes $(j_1, \ldots, j_n, j_e)$ and generalized forces $(\nabla[\zeta_1/T], \ldots, \nabla[\zeta_n/T], \nabla[-1/T])$

Instationary energy model

define total energy density

$$\widetilde{e} = e + \frac{\varepsilon}{2}|\nabla\varphi|^2$$

and total energy flux

$$j_{\widetilde{e}} = j_e - \varphi\frac{\partial(\varepsilon\nabla\varphi)}{\partial t}$$

balance equation for the internal energy
Poisson equation (differentiated by time)
continuity equations with charge preserving reactions

$$\left.\right\} \implies \frac{\partial\widetilde{e}}{\partial t} + \nabla\cdot j_{\widetilde{e}} = 0$$

Conservation law for the total energy

Instationary energy model

total entropy

$$S(t) = \int_\Omega s(x,t)\,\mathrm{d}x$$

If $j_i \cdot \nu = 0,\ j_e \cdot \nu = 0$ on $\partial\Omega$, then entropy balance equation and $d \geq 0 \Longrightarrow$

$$\frac{\mathrm{d}}{\mathrm{d}t} S(t) = \int_\Omega \frac{\partial}{\partial t} s(x,t)\,\mathrm{d}x = \int_\Omega d\,\mathrm{d}x + \int_{\partial\Omega} \Big(\sum_{i=1}^{n} \frac{\zeta_i}{T} j_i \cdot \nu - \frac{1}{T} j_e \cdot \nu \Big)\,\mathrm{d}\Gamma \geq 0$$

$-S$ is a Lyapunov function of the evolution system in the energy formulation (at least formally)

Stationary energy model

consider the stationary problem in the energy formulation in 2D
reactions are charge preserving $\Longrightarrow$

$$\nabla \cdot j_e = \varphi \nabla \cdot \sum_{i=1}^{n} q_i j_i = \varphi \sum_{(\alpha,\beta)\in\mathcal{R}} \sum_{i=1}^{n} q_i (\beta_i - \alpha_i) R_{\alpha\beta} = 0$$

results the system of equations

$$\left.\begin{array}{rcl} \nabla \cdot j_i &=& \sum_{(\alpha,\beta)\in\mathcal{R}} (\beta_i - \alpha_i) R_{\alpha\beta}, \quad i = 1, \ldots, n \\ \nabla \cdot j_e &=& 0 \\ -\nabla \cdot (\varepsilon \nabla \varphi) &=& f + \sum_{i=1}^{n} q_i u_i \end{array}\right\} \quad \text{in } \Omega \subset \mathbb{R}^2$$

for $(j_1, \ldots, j_n, j_e)$ and generalized forces $(\nabla[\zeta_1/T], \ldots, \nabla[\zeta_n/T], \nabla[-1/T])$ Onsager's relations are valid

Stationary energy model

introduce new variables $z = (z_1, \dots, z_{n+2}) = \left(\frac{\zeta_1}{T}, \dots, \frac{\zeta_n}{T}, -\frac{1}{T}, \varphi\right)$

reformulate the state equations, reaction rates $R_{\alpha\beta}$

$$u_i(x) = H_i(x, z), \quad R_{\alpha\beta}(x, z) = \tilde{r}_{\alpha\beta}(x, z) \left(\mathrm{e}^{\sum_{i=1}^n \alpha_i z_i} - \mathrm{e}^{\sum_{i=1}^n \beta_i z_i}\right)$$

strongly coupled nonlinear (not uniformly) elliptic system

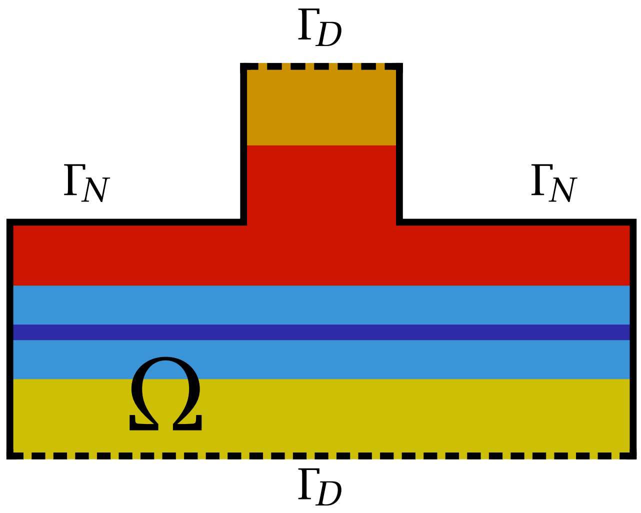
$$-\nabla \cdot \begin{pmatrix} a_{11} & \cdots & a_{1,n+1} & 0 \\ \vdots & \ddots & \vdots & 0 \\ a_{n,1} & \cdots & a_{n,n+1} & 0 \\ a_{n+1,1} & \cdots & a_{n+1,n+1} & 0 \\ 0 & 0 & 0 & \varepsilon \end{pmatrix} \begin{pmatrix} \nabla z_1 \\ \vdots \\ \nabla z_n \\ \nabla z_{n+1} \\ \nabla z_{n+2} \end{pmatrix} = \begin{pmatrix} R_1 \\ \vdots \\ R_n \\ 0 \\ f + \sum_{k=1}^n q_k H_k \end{pmatrix}$$

$$a_{ki} = a_{ik} = a_{ik}(x, z(x)), \ \varepsilon = \varepsilon(x)$$

$$R_i = \sum_{(\alpha,\beta)\in\mathcal{R}} (\beta_i - \alpha_i) R_{\alpha\beta}(x, z(x)), \ H_k = H_k(x, z(x))$$

mixed boundary conditions

$$
\begin{aligned}
z_i &= z_i^D, && i = 1, \ldots, n+2, && && \text{on } \Gamma_D \\
\nu \cdot \textstyle\sum_{k=1}^{n+1} a_{ik}(z) \nabla z_k &= g_i, && i = 1, \ldots, n+1, && \nu \cdot (\varepsilon \nabla z_{n+2}) = g_{n+2} && \text{on } \Gamma_N
\end{aligned}
$$



Stationary energy model

if a thermodynamic equilibrium satisfies the boundary conditions, the data has to fulfil

$$z_i^D = \text{const}, \;\; i = 1, \dots, n, \quad \textstyle\sum_{i=1}^n (\alpha_i - \beta_i) z_i^D = 0 \;\; \forall (\alpha, \beta) \in \mathcal{R},$$

$$z_{n+1}^D = \text{const} < 0, \quad g_i = 0, \;\; i = 1, \dots, n+1$$

corresponding equilibrium densities u_i are obtained by the state equations

$$u_i = H_i(\cdot, z_1^D, \dots, z_{n+1}^D, z_{n+2}), \quad i = 1, \dots, n$$

where z_{n+2} has to satisfy the nonlinear Poisson equation

$$-\nabla \cdot (\varepsilon \nabla z_{n+2}) = f + \sum_{i=1}^n q_i H_i(\cdot, z_1^D, \dots, z_{n+1}^D, z_{n+2})$$

$$z_{n+2} = z_{n+2}^D \text{ on } \Gamma_D, \quad \nu \cdot (\varepsilon \nabla z_{n+2}) = g_{n+2} \text{ on } \Gamma_N$$

Restricted thermodynamic equilibrium

For the Dirichlet data we suppose that there exists a $p > 2$ such that z_i^D on Γ_D are traces of functions $z_i^D \in W^{1,p}(\Omega)$, $i = 1, \ldots, n+2$, with $z_{n+1}^D < 0$ in Ω

$$Q = \Big\{ w = (z^D, g, f) \in W^{1,p}(\Omega)^{n+2} \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega):$$

$$g_i = 0,\ z_i^D = \text{const},\ i = 1,\dots,n+1,\ z_{n+1}^D < 0,\ \sum_{i=1}^{n} (\alpha_i - \beta_i)\, z_i^D = 0\ \forall(\alpha, \beta) \in \mathcal{R} \Big\}$$

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

$$z^* = (z_1^{D*}, \ldots, z_{n+1}^{D*}, z_{n+2}^*)$$

is a restricted thermodynamic equilibrium.

Weak formulation

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

$$X_s = (W_0^{1,s}(\Omega \cup \Gamma_N))^{n+2}$$
$$Y_s = (W^{1,s}(\Omega))^{n+2}$$

We set

$$z = Z + z^D, \qquad w = (z^D, g, f)$$
$$z^* = Z^* + z^{D*}, \qquad w^* = (z^{D*}, g^*, f^*)$$

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

$$M_q = \Big\{(Z, z^D) \in X_q \times Y_p \text{ with } |Z_i + z_i^D| < \tau, \ i = 1, \dots, n, n+2, \\ -\tau < Z_{n+1} + z_{n+1}^D < -\tfrac{1}{\tau} \text{ on } \Omega \Big\}$$

where $\tau > 1$ is such that $(Z^*, z^{D*}) \in M_{q_0}$

Weak formulation

define $\quad F_q \colon M_q \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega) \to X_{q'}^*$

$$\begin{aligned}\langle F_q(Z, w), \psi\rangle_{X_{q'}} &= \int_\Omega \Big\{ \sum_{i,k=1}^{n+1} a_{ik}(\cdot, z)\nabla z_k \cdot \nabla\psi_i + \varepsilon\nabla z_{n+2} \cdot \nabla\psi_{n+2}\Big\}\,\mathrm{d}x \\ &+ \int_\Omega \Big\{ \sum_{(\alpha,\beta)\in\mathcal{R}} R_{\alpha\beta}(\cdot, z) \sum_{i=1}^{n} (\alpha_i - \beta_i)\psi_i + h(\cdot, z)\psi_{n+2}\Big\}\,\mathrm{d}x \\ &- \int_\Omega f\,\psi_{n+2}\,\mathrm{d}x - \int_{\Gamma_N} \sum_{i=1}^{n+2} g_i\psi_i\,\mathrm{d}\Gamma, \quad \psi \in X_{q'}\end{aligned}$$

Problem (P):

Find (q, Z, w) such that $q \in (2, p]$, $(Z, w) \in X_q \times Y_p \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega)$,

$$(Z, z^D) \in M_q, \quad F_q(Z, w) = 0.$$

Implicit Function Theorem

equilibrium:

$$F_{q_0}(Z^*, w^*) = 0$$

differentiability:

$F_q \colon M_q \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega) \to X^*_{q'}$ is continuously differentiable for all $q \in (2, p]$.

properties of the linearization in the restricted thermodynamic equilibrium:

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

$$\partial_Z F_{q_1}(Z^*, w^*) \colon X_{q_1} \to X^*_{q_1'}$$

is an injective Fredholm Operator of index zero.

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

Let $w^* = (z^{D*}, g^*, f^*) \in Q$, and let (q_0, 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 $W \subset Y_p \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega)$ of $w^* = (z^{D*}, g^*, f^*)$ and a C^1-map $\Phi\colon W \to U$ such that $Z = \Phi(w)$ iff

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

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.

Corollary

$$Q_1 = \left\{ w = (z^D, g, f) \in Y_p \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega) : z^D_{n+1} < 0 \right\} \supset Q$$

Let $w = (z^D, g, f) \in Q_1$ be given. Then there are constants $q \in (2, p]$, $\epsilon > 0$ such that the following assertions hold: If

$$\|\nabla z_i^D\|_{L^p(\Omega)} < \epsilon, \quad i = 1, \ldots, n+1,$$

$$\|\sum_{i=1}^{n} (\alpha_i - \beta_i)\, z_i^D\|_{L^1(\Gamma_D)} < \epsilon \quad \forall (\alpha, \beta) \in \mathcal{R},$$

$$\|g_i\|_{L^\infty(\Gamma_N)} \le \epsilon, \quad i = 1, \ldots, n+1,$$

then there exists a $Z \in X_q$ such that (q, Z, w) is a solution to (P). This solution lies in a neighbourhood of an equilibrium solution (q, Z^*, w^*) to Problem (P), and in this neighbourhood there are no solutions $(q, \tilde{Z}, w)$ with $\tilde{Z} \neq Z$.

Outlook

- boundary conditions formulated in other quantities (resulting in nonlinear Dirichlet boundary conditions)
- boundary conditions of third kind are more realistic
- different types of bcs for the different equations
- different domains of definition for the several equations
- models containing traps, which are immobile but can be ionized
- anisotropic materials
- global results
- instationary problem
- 3D