Weierstrass Institute for
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Analysis of electronic models for solar cells including energy resolved defect densities

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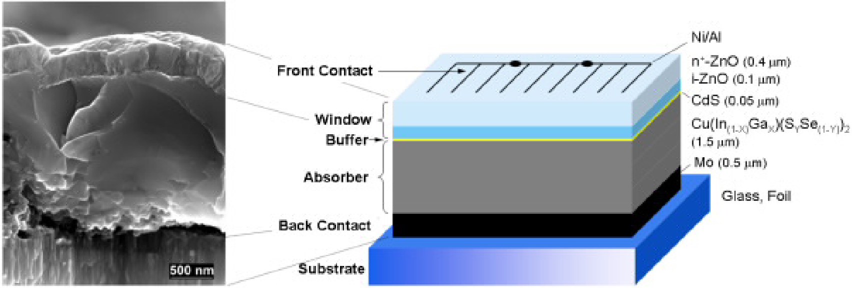
GAMM 82nd Annual Meeting Graz

Content

An electronic model for solar cells



(Helmholtz-Zentrum Berlin für Materialien und Energie)

Situation:

- semiconductor heterostructure with mixed boundary conditions
- technological treatment leads to energy resolved defect distributions
- besides electron/hole generation/recombination there occur special recombinations at defects

- species: $n^-(x), p^+(x)$ electrons and holes
  $t^{-/0}(x,E), t^{0/+}(x,E)$ defects occupied/unoccupied by electrons
- reactions: (for acceptor like defects)

R_0:	$n^- + p^+ \rightleftharpoons \emptyset$	generation/recombination of electrons and holes
R_1:	$n^- + t^{0/+} \rightleftharpoons t^{-/0}$	capture/escape of electrons
R_2:	$p^+ + t^{-/0} \rightleftharpoons t^{0/+}$	capture/escape of holes

- distribution of defects $N(x,E)$ defines measure $\mu = N\mathrm{d}E$ on $G := \Omega \times E_G$
- vector of quantities:

$$u = (u_1, u_2, u_3, u_4) \in Y := L^2(\Omega)^2 \times L^2(G; \mathrm{d}\mu)^2$$

  - $u_1,\ u_2$ densities of electrons and holes
  - u_3 occupation probability by an electron for defects with trap distribution $N(x,E)$, $u_4 = 1 - u_3$

Notation

electrostatic potential	z
charge numbers	$\lambda_i, \quad \lambda = (\lambda_1, \ldots \lambda_4)$
positive reference densities	$\widetilde{u}_i$
chemical activities	$b_i = \frac{u_i}{\widetilde{u}_i} \quad H^1$- functions, $i = 1, 2,$

flux terms

$$j_i = -D_i \widetilde{u}_i (\nabla b_i + \lambda_i b_i \nabla z), \quad i = 1, 2$$

reaction rates

$$R_0(x) - G_{phot}(x) = r_0(u_1 u_2 - k_0)(x),$$

$$R_1(x, E) = r_1(u_1 u_4 - k_1 u_3)(x, E), \quad R_2(x, E) = r_2(u_2 u_3 - k_2 u_4)(x, E)$$

quantities integrated over the energy interval

$$\langle\langle g \rangle\rangle(x) := \int_{E_G} g(E) \mu(x, \mathrm{d}E)$$

Drift-diffusion system

$$-\nabla\cdot(\varepsilon\nabla z) = f - u_1 + u_2 + \sum_{i=3}^{4}\lambda_i\langle\langle u_i\rangle\rangle \quad \text{on } \mathbb{R}_+\times\Omega,$$

$$\frac{\partial}{\partial t}u_i + \nabla\cdot j_i = G_{phot} - R_0 - \langle\langle R_i\rangle\rangle \quad \text{on } \mathbb{R}_+\times\Omega, \quad i=1,2,$$

ODEs for defects

$$\frac{\partial}{\partial t}u_3 = R_1 - R_2, \quad \frac{\partial}{\partial t}u_4 = -\frac{\partial}{\partial t}u_3 \quad \text{on } \mathbb{R}_+\times\operatorname{supp}\mu,$$

Boundary conditions

$$z = z^D,\ b_i = b_i^D \quad \text{on } \mathbb{R}_+\times\Gamma_D,\ i=1,2,$$

$$\nu\cdot(\varepsilon\nabla z) = 0,\ \nu\cdot j_i = 0 \quad \text{on } \mathbb{R}_+\times\Gamma_N,\ i=1,2.$$

Initial conditions

$$u(0) = U$$

Poisson equation

$$\int_\Omega \left\{ \varepsilon \nabla z \cdot \nabla \widehat{z} - \Big[f + \sum_{i=1}^{2} \lambda_i u_i \Big] \widehat{z} \right\} \mathrm{d}x - \sum_{i=3}^{4} \int_G \lambda_i u_i \widehat{z} \, \mathrm{d}\mu = 0, \quad \widehat{z} \in Z = H_0^1(\Omega \cup \Gamma_N).$$

Continuity equations

$$\int_S \Big\{ (u', \widehat{b})_X + \sum_{i=1}^{2} \int_\Omega \left\{ D_i \bar{u}_i (\nabla b_i + \lambda_i b_i \nabla z) \cdot \nabla \widehat{b}_i + r_0 (u_1 u_2 - k_0) \widehat{b}_i \right\} \mathrm{d}x$$

$$+ \int_G \left\{ r_1 (u_1 u_4 - k_1 u_3)(\widehat{b}_1 + \widehat{b}_4 - \widehat{b}_3) + r_2 (u_2 u_3 - k_2 u_4)(\widehat{b}_2 + \widehat{b}_3 - \widehat{b}_4) \right\} \mathrm{d}\mu \Big\} \mathrm{d}s = 0,$$

$$\widehat{b} \in L^2(S, X), \quad X := \left\{ b \in Y \colon \; b_i \in H_0^1(\Omega \cup \Gamma_N), \; i = 1, 2 \right\}.$$

For all $t \in \mathbb{R}_+$ the solutions (u, z) to (P) fulfill

$$0 \le u_3(t), \, u_4(t) \le 1, \quad u_3(t) + u_4(t) = U_3 + U_4 = 1 \quad \mu\text{-a.e. on } G.$$

Lemma (Poisson equation)

For all $u \in Y$ *there is exactly one solution* z *to the Poisson equation,* $z - z^D \in Z$.

- $\|z - \bar{z}\|_Z \le c\|u - \bar{u}\|_Y \quad \forall u, \bar{u} \in Y,$
- $\|z\|_{W^{1,q}} \le c\Big(1 + \sum_{i=1}^{2} \|u_i\|_{L^{2q/(2+q)}}\Big)$ *for a suitable* $q > 2$ *N=2!!.*

Free energy

$$F(u) := \int_\Omega \frac{\varepsilon}{2}|\nabla(z - z^D)|^2 + \sum_{i=1}^{2} \Big\{u_i(\ln \frac{u_i}{u_i^D} - 1) + u_i^D\Big\}\,\mathrm{d}x + \sum_{i=3}^{4} \int_G \Big\{u_i(\ln \frac{u_i}{\widetilde{u}_i} - 1) + \widetilde{u}_i\Big\}\,\mathrm{d}\mu,$$

where z is the solution to the Poisson equation with this u in the right hand side,
$u_i^D = \widetilde{u}_i b_i^D, \quad u_1^D \widetilde{u}_4 = k_1 \widetilde{u}_3.$

Lower estimate of the free energy

$$\|z - z^D\|_Z^2 + \sum_{i=1}^{2} \|u_i \ln u_i\|_{L^1} + \sum_{i=1}^{2} \|u_i\|_{L^1} \le cF(u) + \widetilde{c}.$$

Theorem (Energy estimate)

Let (u, z) be a solution to (P) *and $T \in \mathbb{R}_+$. Then*

$$F(u(t)) \leq (F(U) + c_0)\, e^{c_0 t} \quad \forall t \in [0, T], \tag{1}$$

where the constant $c_0 > 0$ does not depend on U and T. If the data is compatible with thermodynamic equilibrium, meaning that

$$\ln b_i^D + \lambda_i z^D \text{ is constant on } \Omega,\ u_1^D u_2^D = k_0 \text{ a.e. on } \Omega,\ k_1 k_2 = k_0\ \mu\text{-a.e. on } G,$$

then (1) *holds true with $c_0 = 0$.*

Idea of the proof:

formally test by

$$\lambda(z - z^D) + \left(\ln \frac{b_1}{b_1^D}, \ln \frac{b_2}{b_2^D}, \ln b_3, \ln b_4\right), \quad b_i = \frac{u_i}{\widetilde{u}_i}, \quad i = 1, \dots, 4,$$

more precise, use $\left(\ln \frac{b_1^\delta}{b_1^D}, \ln \frac{b_2^\delta}{b_2^D}, \ln b_3^\delta, \ln b_4^\delta\right)$, where $b_i^\delta = \max\{b_i, \delta\}$, let $\delta \to 0$

A priori estimates

Using
- monotonicity of the $\ln$ function
- definition of $\widetilde{u}_3, \widetilde{u}_4$
- boundedness of u_3, u_4
- case by case analysis

it results

$$
\begin{aligned}
&F(u(t)) - F(U) \\
&\leq c \int_0^t \sum_{i=1}^{2} (1 + \|u_i\|_{L^1}) \Big(\|\nabla(\ln b_i^D + \lambda_i z^D)\|_{L^\infty}^2 + \|\ln \tfrac{k_1 k_2}{u_1^D u_2^D}\|_{L^\infty(G,\mathrm{d}\mu)} \Big) \mathrm{d}s \\
&\quad + c \int_0^t \|\ln \tfrac{u_1^D u_2^D}{k_0}\|_{L^\infty} \, \mathrm{d}s
\end{aligned}
$$

- BCs compatible with thermodynamic equilibrium: $F(u(t)) \leq F(U)$
- More general case: use lower estimate of the free energy and Gronwall's Lemma.

Theorem (Boundedness)

There exists a monotonously increasing function $d : \mathbb{R}_+ \to \mathbb{R}_+$, depending on the data, but independent of T, such that

$$\|u_i(t)\|_{L^\infty} \le d(\|F(u)\|_{C(S)}), \quad i = 1, 2,$$
$$\|z(t)\|_{L^\infty} \le d(\|F(u)\|_{C(S)}) \quad \forall t \in S$$

for all solutions (u, z) to (P).

Idea of the proof:

- test functions

$$p\,\mathrm{e}^{pt}\,(v_1^{p-1}, v_2^{p-1}, 0, 0) \in L^2(S, X),\ p = 2^m,\ m \ge 1,$$

  where $v_i := (b_i - K)^+$, $K = \max\big(1, \max_{i=1,2} \|\frac{U_i}{\bar{u}_i}\|_{L^\infty}, \max_{i=1,2} \|b_i^D\|_{L^\infty}\big)$
- L^2 estimate: $m = 1$: regularity results for the solution to the Poisson equation (Gröger), lower estimate of the free energy, and energy estimate
- Moser iteration

Theorem (Existence and uniqueness)

There is exactly one solution to problem (P).

Steps of the proof

- consider regularized problem (P$_M$) on arbitrarily fixed time interval $S = [0, T]$
  regularize flux terms, reaction terms (parameter M)
- show solvability of (P$_M$) by
  decomposition into problems with partly frozen arguments for
  ☐ Poisson equation ☐ immobile species ☐ mobile species
  iteration
  Schauder's Fixed Point Theorem for densities of the mobile species
- a priori estimates (independent of M !)
  - ☐ energy estimates for (F_M)
  - ☐ Moser technique for getting upper bounds
- solution to (P$_M$) is a solution to (P) if M is chosen sufficiently large
- uniqueness result

Comments

Generalizations

- different kinds of defects with different trap distributions $N_j(x, E)$ leading to measures μ_j on $\Omega \times E_G$
- different kinds of traps on different subdomains of $\Omega \times E_G$
- traps with more than two charge states $\rightsquigarrow$ other types of ionization reactions

Outlook

- heterostructures with active interfaces:
  - traps confined at interfaces
  - defects capture/escape the electrons/holes from both sides
  - thermionic emission of electrons/holes at the active interface
- derivation of the resulting interface-model as limit model of models with volume-traps in thin layers (M. Liero)
- formulation of the system as generalized gradient flow (together with A. Mielke)
- investigations of the stationary (continuous and discretized) problem (together with K. Gärtner)

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