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

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An electronic model for solar cells

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

(Helmholtz-Zentrum Berlin für Materialien und Energie)
An electronic model for solar cells

- **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)
  
  \[ R_0: \quad n^- + p^+ \iff \emptyset \] generation/recombination of electrons and holes
  
  \[ R_1: \quad n^- + t^{0/+} \iff t^{-/0} \] capture/escape of electrons
  
  \[ R_2: \quad p^+ + t^{-/0} \iff t^{0/+} \] capture/escape of holes

- **distribution of defects** \( N(x, E) \) defines measure \( \mu = NdE \) on \( G := \Omega \times E_G \)

- **vector of quantities:**

  \[ u = (u_1, u_2, u_3, u_4) \in Y := L^2(\Omega)^2 \times L^2(G; d\mu)^2 \]

  - \( u_1, u_2 \) 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: $\lambda_i$, $\lambda = (\lambda_1, \ldots, \lambda_4)$
- Positive reference densities: $\tilde{\mu}_i$
- Chemical activities: $b_i = \frac{\mu_i}{\tilde{\mu}_i} H^1$-functions, $i = 1, 2$,

Flux terms:

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

Reaction rates:

$$R_0(x) - G_{phot}(x) = r_0(u_1u_2 - k_0)(x),$$
$$R_1(x, E) = r_1(u_1u_4 - k_1u_3)(x, E), \quad R_2(x, E) = r_2(u_2u_3 - k_2u_4)(x, E)$$

Quantities integrated over the energy interval:

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

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Model equations

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

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

Boundary conditions

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

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

Initial conditions

\[u(0) = U\]
Weak formulation, Problem (P)

Poisson equation

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

Continuity equations

\[
\int_S \left\{ (u', \hat{b})_X + \sum_{i=1}^{2} \int_\Omega \left\{ D_i \bar{u}_i (\nabla b_i + \lambda_i b_i \nabla z) \cdot \nabla \hat{b}_i + r_0 (u_1 u_2 - k_0) \hat{b}_i \right\} \, dx \right. \\
+ \left. \int_G \left\{ r_1 (u_1 u_4 - k_1 u_3) (\hat{b}_1 + \hat{b}_4 - \hat{b}_3) + r_2 (u_2 u_3 - k_2 u_4) (\hat{b}_2 + \hat{b}_3 - \hat{b}_4) \right\} \, d\mu \right\} ds = 0,
\]

\[\hat{b} \in L^2(S, X), \quad X := \{ b \in Y: b_i \in H_0^1(\Omega \cup \Gamma_N), \ i = 1, 2 \}.\]

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

\[
0 \leq u_3(t), u_4(t) \leq 1, \quad u_3(t) + u_4(t) = U_3 + U_4 = 1 \quad \mu\text{-a.e. on } G.
\]
**Lemma (Poisson equation)**

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

- $\|z - \bar{z}\|_Z \leq c \|u - \bar{u}\|_Y \quad \forall u, \bar{u} \in Y,$

- $\|z\|_{W^{1,q}} \leq c \left(1 + \sum_{i=1}^{2} \|u_i\|_{L^2}^{2/(2+q)}\right)$ for a suitable $q > 2$.

**Free energy**

$$F(u) := \int_{\Omega} \frac{\varepsilon}{2} |\nabla (z - z^D)|^2 + \sum_{i=1}^{2} \left\{ u_i (\ln \frac{u_i}{u_i^D} - 1) + u_i^D \right\} \, dx + \sum_{i=3}^{4} \int_{G} \left\{ u_i (\ln \frac{u_i}{\bar{u}_i} - 1) + \bar{u}_i \right\} \, d\mu,$$

where $z$ is the solution to the Poisson equation with this $u$ in the right hand side,

$$u_i^D = \tilde{u}_i b_i^D, \quad u_1^D \tilde{u}_4 = k_1 \tilde{u}_3.$$

**Lower estimate of the free energy**

$$\|z - z^D\|^2_Z + \sum_{i=1}^{2} \|u_i \ln u_i\|_{L^1} + \sum_{i=1}^{2} \|u_i\|_{L^1} \leq c F(u) + \tilde{c}.$$
Energy estimates

Theorem (Energy estimate)

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

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

(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

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

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

Using

- monotonicity of the \( \ln \) function
- definition of \( \tilde{u}_3, \tilde{u}_4 \)
- boundedness of \( u_3, u_4 \)
- case by case analysis

it results

\[
F(u(t)) - F(U) \\
\leq c \int_0^t \sum_{i=1}^2 (1 + \| u_i \|_{L^1}) \left( \| \nabla (\ln b_i^D + \lambda_i z_i^D) \|_{L^\infty}^2 + \| \ln \frac{k_1 k_2}{u_1^D u_2^D} \|_{L^\infty(G,\mu)} \right) ds \\
+ c \int_0^t \| \ln \frac{u_1^D u_2^D}{k_0} \|_{L^\infty} ds
\]

- 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.
A priori estimates

Theorem (Boundedness)

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

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

$$
\|z(t)\|_{L^\infty} \leq d(\|F(u)\|_{C(S)}) \quad \forall t \in S
$$

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

Idea of the proof:

- test functions

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

where $v_i := (b_i - K)^+$, $K = \max \left( 1, \max_{i=1,2} \|U_i\|_{L^\infty}, \max_{i=1,2} \|b_i^D\|_{L^\infty} \right)$

- $L^2$ 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
Generalizations

- different kinds of defects with different trap distributions $N_j(x, E)$ leading to measures $\mu_j$ on $\Omega \times E_G$
- different kinds of traps on different subdomains of $\Omega \times E_G$
- traps with more than two charge states $\leadsto$ 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)
References


