



Weierstraß-Institut für Angewandte Analysis und Stochastik

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Annegret Glitzky

Analysis of Spin-Polarized Drift-Diffusion Models

Spin-resolved drift-diffusion model

consider **spin-resolved carriers** $e_{\uparrow}, e_{\downarrow}, h_{\uparrow}, h_{\downarrow}$

spin-resolved densities for electrons and holes

$$n_{\uparrow\downarrow} = \frac{N_c}{2} \exp\left[\frac{-E_{c0} \pm qg_c}{k_B T}\right] \exp\left[\frac{\varphi_{n\uparrow\downarrow} + q\psi}{k_B T}\right]$$

$$p_{\uparrow\downarrow} = \frac{N_v}{2} \exp\left[\frac{E_{v0} \mp qg_v}{k_B T}\right] \exp\left[\frac{-\varphi_{p\uparrow\downarrow} - q\psi}{k_B T}\right]$$

N_c, N_v effective densities of state

E_{c0}, E_{v0} band edge energies

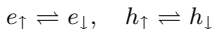
$\varphi_{n\uparrow\downarrow}, \varphi_{p\uparrow\downarrow}$ spin-resolved quasi-Fermi energies

q, ψ elementary charge, electrostatic potential

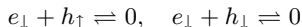
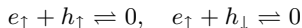
g_c, g_v **splitting of carrier bands** due to magnetic impurities or an applied magnetic field

T, k_B Temperature, Boltzmann constant

spin relaxation reactions



recombination/generation of electrons and holes



Spin-resolved drift-diffusion model

charge current densities

$$j_{n\uparrow\downarrow} = \mu_{n\uparrow\downarrow} n_{\uparrow\downarrow} \nabla \varphi_{n\uparrow\downarrow},$$

$$j_{p\uparrow\downarrow} = \mu_{p\uparrow\downarrow} p_{\uparrow\downarrow} \nabla \varphi_{p\uparrow\downarrow},$$

- ▷ system of **4 continuity equations** containing spin-relaxation as well as generation-recombination terms
- ▷ coupled with a **Poisson equation**
- ▷ completed by boundary from device simulation and initial conditions
- ▷ obtain a **generalization of the classical van Roosbroeck system**
- ▷ introduce scaled variables

Model equations in scaled variables

X_i	species: $e_{\uparrow}, e_{\downarrow}, h_{\uparrow}, h_{\downarrow}$	γ_i	charge numbers $\gamma = (-1, -1, 1, 1)$
u_i	densities	\bar{u}_i	reference densities
v_i	chemical potentials	v_0	electrostatic potential
		$\zeta_i = v_i + \gamma_i v_0$	electrochemical potentials

state equation for species X_i

$$u_i = \bar{u}_i e^{v_i}$$

particle flux density for species X_i

$$J_i = -D_i u_i \nabla \zeta_i = -D_i \left(\bar{u}_i \nabla \frac{u_i}{\bar{u}_i} + u_i \gamma_i \nabla v_0 \right)$$

$-R_i$ net production rate of species X_i

$$R_1 = r_{13}(e^{v_1+v_3} - 1) + r_{14}(e^{v_1+v_4} - 1) + r_{12}(e^{v_1} - e^{v_2}),$$

$$R_2 = r_{23}(e^{v_2+v_3} - 1) + r_{24}(e^{v_2+v_4} - 1) - r_{12}(e^{v_1} - e^{v_2}),$$

$$R_3 = r_{13}(e^{v_1+v_3} - 1) + r_{23}(e^{v_2+v_3} - 1) + r_{34}(e^{v_3} - e^{v_4}),$$

$$R_4 = r_{14}(e^{v_1+v_4} - 1) + r_{24}(e^{v_2+v_4} - 1) - r_{34}(e^{v_3} - e^{v_4})$$

Model equations

continuity equations

$$\begin{aligned} \frac{\partial u_i}{\partial t} + \nabla \cdot J_i &= -R_i \text{ in } \mathbb{R}_+ \times \Omega, \\ \nu \cdot J_i &= 0 \text{ on } \mathbb{R}_+ \times \Gamma_N, \quad v_i = v_i^D \text{ on } \mathbb{R}_+ \times \Gamma_D, \\ u_i(0) &= U_i \text{ in } \Omega, \quad i = 1, \dots, 4. \end{aligned}$$

Poisson equation

$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla v_0) &= f + \sum_{i=1}^4 \gamma_i u_i \text{ in } \mathbb{R}_+ \times \Omega, \\ \nu \cdot (\varepsilon v_0) &= 0 \text{ on } \mathbb{R}_+ \times \Gamma_N, \quad v_0 = v_0^D \text{ on } \mathbb{R}_+ \times \Gamma_D \end{aligned}$$

use vectors $v = (v_0, \dots, v_4)$, $u = (u_0, \dots, u_4)$, $u_0 = \sum_{i=1}^4 \gamma_i u_i$

Assumptions

- (A1)** $\Omega \subset \mathbb{R}^2$ bounded Lipschitzian domain, Γ_D, Γ_N are disjoint open subsets of $\partial\Omega$, $\partial\Omega = \Gamma_D \cup \Gamma_N \cup (\overline{\Gamma_D} \cap \overline{\Gamma_N})$, $\text{mes } \Gamma_D > 0$, $\overline{\Gamma_D} \cap \overline{\Gamma_N}$ consists of finitely many points ($\Omega \cup \Gamma_N$ is regular in the sense of Gröger);
- (A2)** $D_i \in L^\infty(\Omega)$, $D_i \geq c > 0$ a.e. on Ω , $i = 1, \dots, 4$;
- (A3)** $r_{ij} : \Omega \times \mathbb{R} \times \mathbb{R}_+^4 \rightarrow \mathbb{R}_+$, $r_{ij}(x, \cdot)$ Lipschitzian uniformly w.r.t. $x \in \Omega$, $r_{ij}(\cdot, y)$ measurable for all $y \in \mathbb{R} \times \mathbb{R}_+^4$, $r_{ij}(\cdot, 0) \in L^\infty(\Omega)$, $ij = 13, 14, 23, 24$, $r_{ij} \in L_+^\infty(\Omega)$, $ij = 12, 34$;
- (A4)** $\varepsilon, \bar{u}_i \in L^\infty(\Omega)$, $\varepsilon \geq c > 0$, $\bar{u}_i \geq \underline{c} > 0$ a.e. on Ω , $i = 1, \dots, 4$, $f \in L^2(\Omega)$, $v_i^D \in W^{1,\infty}(\Omega)$, $i = 0, \dots, 4$, $\gamma = (-1, -1, 1, 1)$;
- (A5)** $u_i^0 \in L^\infty(\Omega)$, $u_i^0 \geq c > 0$ a.e. on Ω , $i = 1, \dots, 4$, $u_0^0 = \sum_{i=1}^4 \gamma_i u_i^0$.

Weak formulation

$$V = H_0^1(\Omega \cup \Gamma_N)^5, \quad U = \{u \in V^* : u_i \in L^2(\Omega), \ln u_i \in L^\infty(\Omega), i = 1, \dots, 4\}$$

define operators $E : V + v^D \rightarrow V^*, A : U \times (V + v^D) \rightarrow V^*$

$$\langle Ev, \bar{v} \rangle = \langle E_0 v_0, \bar{v}_0 \rangle + \int_{\Omega} \sum_{i=1}^4 \bar{u}_i \mathbf{e}^{v_i} \bar{v}_i \, dx, \quad \bar{v} \in V,$$

$$\langle E_0 v_0, \bar{v}_0 \rangle = \int_{\Omega} \{ \varepsilon \nabla v_0 \cdot \nabla \bar{v}_0 - f \bar{v}_0 \} \, dx, \quad \bar{v}_0 \in H_0^1(\Omega \cup \Gamma_N),$$

$$\begin{aligned} \langle A(u, v), \bar{v} \rangle = & \int_{\Omega} \left\{ \sum_{i=1}^4 D_i u_i \nabla \zeta_i \cdot \nabla \bar{\zeta}_i + \sum_{ij=12,34} r_{ij} (\mathbf{e}^{v_i} - \mathbf{e}^{v_j}) (\bar{v}_i - \bar{v}_j) \right. \\ & \left. + \sum_{ij=13,14,23,24} r_{ij}(\cdot, u) (\mathbf{e}^{v_i+v_j} - 1) (\bar{v}_i + \bar{v}_j) \right\} \, dx, \quad \bar{\zeta}_i = \bar{v}_i + \gamma_i \bar{v}_0. \end{aligned}$$

Problem (P):

$$u' + A(u, v) = 0, \quad u = Ev \text{ a.e. on } \mathbb{R}_+, \quad u(0) = u^0,$$

$$u \in H_{\text{loc}}^1(\mathbb{R}_+, V^*), \quad v - v^D \in L_{\text{loc}}^2(\mathbb{R}_+, V) \cap L_{\text{loc}}^\infty(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^5)).$$

Energy functionals

E is a strict monotone potential operator with potential $G : V + v^D \rightarrow \mathbb{R}$,

$$G(v) = \int_{\Omega} \left\{ \frac{\varepsilon}{2} |\nabla v_0|^2 - \frac{\varepsilon}{2} |\nabla v_0^D|^2 - f(v_0 - v_0^D) + \sum_{i=1}^4 \bar{u}_i (\mathbf{e}^{v_i} - \mathbf{e}^{v_i^D}) \right\} dx.$$

- $\Omega \subset \mathbb{R}^2$, Trudingers imbedding result $\implies \text{dom } G = V + v^D$
- G is continuous, strictly convex, Gateaux differentiable, subdifferentiable, $\partial G = E$

free energy $F : V^* \rightarrow \overline{\mathbb{R}}$,

$$F(u) = G^*(u) = \sup_{w \in V} \left\{ \langle u, w \rangle - G(w + v^D) \right\}.$$

- F is proper, lower semicontinuous, convex
- if $u = Ev \implies F(u) = \langle u, v - v^D \rangle - G(v)$, $v - v^D \in \partial F(u)$
- if $u \in V^*$ and $u_i \in L^2(\Omega)$, $u_i \geq 0$, $i = 1, \dots, 4$, $E_0 v_0 = u_0 \implies$

$$F(u) = \int_{\Omega} \left\{ \frac{\varepsilon}{2} |\nabla(v_0 - v_0^D)|^2 + \sum_{i=1}^4 \left\{ u_i \left(\ln \frac{u_i}{\bar{u}_i} - v_i^D - 1 \right) + \bar{u}_i \mathbf{e}^{v_i^D} \right\} \right\} dx.$$

Energy estimates

Theorem. Let (A1) – (A5) be satisfied. Then there exists a $c_1 > 0$ depending only on the data such that

$$F(u(t)) \leq (F(u^0) + 1)e^{c_1 t} \quad \forall t \in \mathbb{R}_+$$

for any solution (u, v) to (P). If

$$\nabla(v_k^D + \gamma_k v_0^D) = 0, \quad k = 1, \dots, 4, \quad v_i^D = v_j^D, \quad ij = 12, 34, \quad v_i^D + v_j^D = 0, \quad ij = 13, 14, 23, 24,$$

then $F(u(t))$ is bounded and decays monotonously (and exponentially).

Idea of the proof: $v(t) - v^D \in \partial F(u(t))$ a.e. on \mathbb{R}_+ , Brézis formula \implies

$$\begin{aligned} F(u(t)) - F(u(s)) &= \int_s^t \langle u'(\tau), v(\tau) - v^D \rangle \, d\tau = - \int_s^t \langle A(u, v), v(\tau) - v^D \rangle \, d\tau \\ &\leq c \int_s^t \sum_{k=1}^4 (\|u_k\|_{L^1} + 1) \left\{ \|\nabla \zeta_k^D\|_{L^\infty}^2 + \sum_{ij=12,34} \|v_i^D - v_j^D\|_{L^\infty} + \sum_{ij=13,14,23,24} \|v_i^D + v_j^D\|_{L^\infty} \right\} \, d\tau \end{aligned}$$

$s = 0$: since $\|u_k\|_{L^1} \leq F(u) + c$, Gronwall's lemma $\implies F(u(t)) \leq (F(u^0) + ct)e^{ct}$

Existence and uniqueness result

Theorem. We assume (A1) – (A5). Then there exists a unique solution to Problem (P).

Guideline for the proof

- regularized problem (P_M) on arbitrarily chosen finite time interval $S = [0, T]$
regularize state equations, reaction terms (parameter M)
- solvability of (P_M)
by time discretization, passing to the limit
- a priori estimates
 - energy estimates (F_M)
 - Moser techniques to get upper and lower bounds independent of M
- solution to (P_M) is a solution to (P) if M is chosen sufficiently large
- uniqueness result

Regularized problem (P_M) on a finite time interval

Problem (P_M):

$$\begin{aligned} u' + A_M(u, v) &= 0, \quad u = E_M v \text{ f.a.a. } t \in S, \\ u(0) &= u^0, \quad v - v^D \in L^2(S, V), \quad u \in H^1(S, V^*). \end{aligned}$$

where

$$\begin{aligned} \langle E_M v, \bar{v} \rangle &= \langle E_0 v_0, \bar{v}_0 \rangle + \int_{\Omega} \sum_{i=1}^4 \bar{u}_i e^{P_M v_i} \bar{v}_i \, dx, \quad \bar{v} \in V, \\ \langle A_M(u, v), \bar{v} \rangle &= \int_{\Omega} \left\{ \sum_{i=1}^4 D_i u_i \nabla \zeta_i \cdot \nabla \bar{\zeta}_i + \sum_{ij=12,34} r_{ij} \left[\left(e^{P_M v_i} - \frac{u_j}{\bar{u}_j} \right) \bar{v}_i - \left(\frac{u_i}{\bar{u}_i} - e^{P_M v_j} \right) \bar{v}_j \right] \right. \\ &\quad \left. + \sum_{ij=13,14,23,24} r_{ij}(\cdot, u) \left(e^{P_{2M}(v_i+v_j)} - 1 \right) (\bar{v}_i + \bar{v}_j) \right\} dx, \quad \bar{v} \in V, \end{aligned}$$

with

$$\zeta_i = v_i + \gamma_i v_0, \quad \bar{\zeta}_i = \bar{v}_i + \gamma_i \bar{v}_0, \quad P_k(y) = \begin{cases} k, & \text{if } y > k \\ y, & \text{if } |y| \leq k \\ -k, & \text{if } y < -k \end{cases}$$

Upper and lower bounds

Estimates from above

testing $u' + A_M(u, v) = 0$ (or $u' + A(u, v) = 0$) by

- $2e^{2t} (0, z_1, z_2, z_3, z_4), \quad z_i := \left(\frac{u_i}{u_i} - K\right)^+$

where $K \geq \widehat{K} := \max\left(1, e^{\max_{i=1, \dots, 4} \|v_i^D\|_{L^\infty}}, \max_{i=1, \dots, 4} \left\|\frac{u_i^0}{u_i}\right\|_{L^\infty}\right)$ suitable chosen

- $p e^{pt} (0, z_1^{p-1}, z_2^{p-1}, z_3^{p-1}, z_4^{p-1}), \quad z_i := \left(\frac{u_i}{u_i} - \widehat{K}\right)^+, \quad p = 2^n, \quad n \geq 1$

+ Moser iteration

Estimates from below

fix some $i \in \{1, 2, 3, 4\}$, testing by

- $-p e^{pt} (0, \dots, 0, z^{p-1} \frac{\bar{u}_i}{u_i}, 0, \dots, 0), \quad z := \left(\ln \frac{u_i}{u_i} + \widetilde{K}\right)^-, \quad p = 2^n, \quad n \geq 1$

where $\widetilde{K} := \sum_{i=1}^4 \left(\|\ln\left(\frac{u_i}{u_i} + 1\right)\|_{L^\infty(S, L^\infty)} + \|v_i^D\|_{L^\infty}\right) + \max_{i=1, \dots, 4} \left\|\left(\ln \frac{u_i^0}{u_i}\right)^-\right\|_{L^\infty}$

+ Moser iteration

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