Weierstraß-Institut
für Angewandte Analysis und Stochastik

Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint ISSN 2198-5855

Analysis of a hybrid model for the electrothermal behavior of semiconductor heterostructures

Annegret Glitzky, Matthias Liero, Grigor Nika

submitted: October 21, 2019

Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: annegret.glitzky@wias-berlin.de
matthias.liero@wias-berlin.de
grigor.nika@wias-berlin.de

No. 2636
Berlin 2019

2010 *Mathematics Subject Classification.* 35J57, 35K05, 35R05, 78A35.

Key words and phrases. Drift-diffusion, charge & heat transport, electro-thermal interaction, semiconductor heterostructures, hybrid modeling, weak solutions.

The authors gratefully acknowledge the funding by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – The Berlin Mathematics Research Center MATH+ (EXC-2046/1, project ID: 390685689) in project AA2-1.

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20372-303
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Analysis of a hybrid model for the electrothermal behavior of semiconductor heterostructures

Annegret Glitzky, Matthias Liero, Grigor Nika

Abstract

We prove existence of a weak solution for a hybrid model for the electro-thermal behavior of semiconductor heterostructures. This hybrid model combines an electro-thermal model based on drift-diffusion with thermistor type models in different subregions of the semiconductor heterostructure. The proof uses a regularization method and Schauder's fixed point theorem. For boundary data compatible with thermodynamic equilibrium we verify, additionally, uniqueness. Moreover, we derive bounds and higher integrability properties for the electrostatic potential and the quasi Fermi potentials as well as the temperature.

1 Introduction

One of the most substantial challenges in todays semiconductor devices is the modeling and simulation of electro-thermal effects as they can crucially limit the performance of devices. There exist many technical examples where self-heating effects have a potent impact. For instance, thermal lensing can affect the output power and beam quality in lasers [2] and in power electronic devices safe-operating area limits have to be identified [14]. In large-area organic light emitting diodes (OLEDs), where the conductivity additionally increases with temperature, selfheating can lead to catastrophic snapback effects in luminance [5, 6].

Most interesting semiconductor devices are usually composed from two or more different kinds of semiconductor material with different types of doping. The numerical simulation for the electro-thermal behavior in semiconductor devices plays a crucial role in the development of new, reliable, and efficient devices in order to reduce development time and production costs. A widely used modelling approach is to consider a drift-diffusion based electro-thermal model on the entire domain of the semiconductor heterostructure. Another possible approach would be to decompose the device structure into different subregions. Then, on subregions of the device where simplifications can be justified, reduced models are applied and only on the remaining subregion the full drift-diffusion and electro-thermal description is used. Any numerical simulation, therefore, must not only be computationally efficient but it must also reflect models that accurately mirror relevant physical properties. It is, thus, of great interest to provide a sound analytical treatment of hybrid models for the electro-thermal behavior of semiconductor heterostructures.

Starting from a drift-diffusion based electro-thermal model we construct a hybrid model that retains the strong coupling of the electro-thermal effects but uses different depths in the description of the current flow. Combining models for device substructures that are limiting cases of electron or hole densities resulting in thermistor-like models for highly n-doped or highly p-doped regions and the full drift-diffusion type model on the electronic relevant subregions, leads to hybrid models with different complexity and coupling interface conditions among these different subregions. We first consider a drift-diffusion type model for the interplay of electronic and heat transport in semiconductor devices, where we take into account the thermoelectric effects of Joule heating resulting from both electron and hole current, and reaction heat as source terms in the heat flow equation. Moreover, we confine our analytical investigations to the case of Boltzmann statistics.

DOI 10.20347/WIAS.PREPRINT.2636 Berlin 2019

In the device domain Ω we study the following coupled system,

$$\begin{aligned} -\nabla\cdot(\varepsilon\nabla\psi) &= C - n + p,\\ -\nabla\cdot j_n &= -R,\ j_n = -n\mu_n\nabla\varphi_n,\\ \nabla\cdot j_p &= -R,\ j_p = -p\mu_p\nabla\varphi_p,\\ -\nabla\cdot(\lambda\nabla T) &= n\mu_n|\nabla\varphi_n|^2 + p\mu_p|\nabla\varphi_p|^2 + R(\varphi_p-\varphi_n), \end{aligned} \tag{1.1}$$

where ψ is the electrostatic potential, φ_n, φ_p are the electrochemical potentials, T is the temperature, ε is the dielectric permittivity, and $C(T) := N_D^+(T) - N_A^-(T)$ represents the charged donor and acceptor densities, respectively. The mobilities of electrons $\mu_n = \mu_n(T,n)$ and holes $\mu_p = \mu_p(T,p)$ are considered to be both temperature and density dependent functions, and λ represents the thermal conductivity. Moreover, with the chemical potentials defined by $v_n := \psi - \varphi_n$ and $v_p := -(\psi - \varphi_p)$, the generation/recombination term R and the charge carrier densities n and p are given by,

$$\begin{aligned} R &= r_0(\cdot,n,p,T)\,n\,p\,\Big(1-\exp\frac{\varphi_n-\varphi_p}{T}\Big),\\ n &= N_{n0}(T)\exp\Big(\frac{\psi-\varphi_n-E_C(T)}{T}\Big) =: e_n(v_n;T),\\ p &= N_{p0}(T)\exp\Big(\frac{E_V(T)-(\psi-\varphi_p)}{T}\Big) =: e_p(v_p;T), \end{aligned} \tag{1.2}$$

with E_C, E_V denoting the band edges and N_{p0}, N_{n0} the densities of state. In particular, they are assumed to be temperature dependent.

System (1.1) is closed by mixed boundary conditions on $\Gamma := \partial\Omega$ for the stationary drift-diffusion system combined with Robin boundary conditions for the heat flow equation,

$$\begin{aligned} \psi = \psi^D,\quad \varphi_n = \varphi_n^D,\quad \varphi_p = \varphi_p^D \quad &\text{on } \Gamma_D,\\ \varepsilon\nabla\psi\cdot\nu = j_n\cdot\nu = j_p\cdot\nu = 0 \quad &\text{on } \Gamma_N,\\ \lambda\nabla T\cdot\nu + \kappa(T-T_a) = 0 \quad &\text{on } \partial\Omega, \end{aligned} \tag{1.3}$$

where Γ_D and Γ_N denote the Dirichlet and Neumann boundary parts, respectively and ν is the outer unit normal. Equations (1.1), (1.2), and (1.3) are already written in scaled form. A similar scaled model frame was used in [12]. For a discussion on the scaling of equations (1.1), (1.2), and (1.3) we refer the interested reader to [11, Section 3].

We remark that in our model, as well as in [12], the thermoelectric powers are neglected such that additional thermoelectric effects (Peltier, Thomson, and Seebeck) are not included in model (1.1). For fully thermodynamically designed energy models including all these effects we refer e.g. to [1, 2, 14, 16, 8, 9, 10], where the first four references concentrate on thermodynamically consistent modeling, [2, 14] discuss also numerical aspects. The last three references supply a local unique solution for boundary data nearly compatible with the thermodynamic equilibrium by an application of the implicit function theorem in a $W^{1,p}$, $p > 2$, setting in two spatial dimensions. In [12] the existence and uniqueness of Hölder continuous weak solutions near thermodynamic equilibria is proved by using the implicit function theorem. To ensure the continuous differentiability of the corresponding maps, regularity results from the theory of nonsmooth linear elliptic boundary value problems in Sobolev-Campanato spaces were applied.

The aims of the paper are twofold. First, to construct a hybrid model for the electro-thermal behavior of semiconductor heterostructures by applying coarser models in subregions which reduce the number of coupled equations in (1.1) from four to two equations in the corresponding subregions. In particular, the coarser model features an equation for the net current flow coupled to the heat equation, namely

$$\begin{aligned} -\nabla\cdot(\sigma(T)\nabla\varphi) &= 0,\\ -\nabla\cdot(\lambda\nabla T) &= \sigma(T)|\nabla\varphi|^2, \end{aligned} \tag{1.4}$$

with an effective electrical conductivity σ depending on temperature.

The coarsening has the added benefit of producing computationally efficient models for the numerical simulation of semiconductor devices while maintaining a degree of physical accuracy. Second, to study the analytical properties of the hybrid model. The key idea is to use for device regions with high doping of one charge carrier type (e.g. near to contacts) a coarser description by a thermistor model combining heat flow and a simpler model for the current flow. The more detailed electro-thermal drift-diffusion modelling should be restricted to electronically relevant substructures where one balances electron and hole currents and generation/recombination processes. Furthermore, the decomposition of the semiconductor device into different subregions where different models are applied, requires a formulation of transfer conditions at the interfaces among these different subregions to ensure that the total current in the normal direction to the interface is continuous. Moreover, we have to guarantee that at the interface between the highly n-doped (p-doped) subregions and the subregions where a full drift-diffusion type model is applied, the electrochemical potentials of electrons (holes) as well as the normal component of the electron (hole) current density is continuous. In conclusion, we remark that model (1.1) allows for an existence result for a large class of boundary data. Additionally, it has the property that the heat source terms in the heat flow equation in (1.1) are always nonnegative. This in connection with the Robin boundary conditions ensures that the temperature for solutions to the model equations (1.1), (1.3) has to fulfill $T \geq T_a$.

The paper is organized as follows: In Section 2 we derive the hybrid model, the associated assumptions, and the functional setting for the model, Section 3 deals with the a priori estimates regarding the hybrid model, in Section 4 we state the main theorem of the paper concerning the solvability of the hybrid problem and give a guideline of the corresponding proof, in Section 5 we introduce a regularized problem and related a priori estimates, and in Section 6 we prove the existence of a weak solution to the regularized problem using Schauder's fixed point theorem. Lastly, Section 7 contains conclusions.

2 Hybrid modeling of the electro-thermal behavior of semiconductor devices

2.1 Reduced model for strongly n- or p-doped regions

For the derivation of the coarser model, we suppose that the band edges $E_C,\ E_V$, the densities of state $N_{n0},\ N_{p0}$ in (1.2) as well as the doping densities $N_D,\ N_A$ are spatially constant and only depending on temperature.

We discuss the case of a strongly n-doped region, where the hole density is negligible. The opposite case runs analogously. We consider for the model equations (1.1), (1.3) the limit $p \to 0$ whereas the quantities $\nabla\varphi_p,\ \nabla\varphi_n,\ \psi,\ \nabla\psi,\ v_n,\ n,\ T$ and ∇T remain bounded. Having in mind that $T \geq T_a$, because of $p = N_{p0}\exp((v_p + E_V)/T)$ we find $\frac{v_p}{T} \to -\infty$. Moreover, as a consequence

$$
\begin{aligned}
&v_p \to -\infty, \quad p\mu_p\nabla\varphi_p \to 0, \quad p\mu_p|\nabla\varphi_p|^2 \to 0, \\
&R = npr_0(1 - \mathrm{e}^{\frac{v_n+v_p}{T}}) \to 0, \quad R(v_n + v_p) = npr_0(1 - \mathrm{e}^{\frac{v_n+v_p}{T}})(v_n + v_p) \to 0.
\end{aligned} \tag{2.1}
$$

For the last convergence one has additionally to verify the convergence $pv_p = N_{p0}\exp((v_p+E_V)/T)v_p \to 0.$ However, this is evident from properties of the exponential funtion $\lim_{x\to-\infty} x\mathrm{e}^x = 0.$

Motivated by the strong n-doping and the negligible p-density ($N_D >> N_A \approx 0$) we assume local charge neutrality. This means that the right-hand side of the Poisson equation fulfils $C-n+p = N_D^+(T)-N_A^-(T)-n+p = 0$ and that in the limit $n = N_D^+(T)$. In addition, physical reasons require that the density of positively charged donors $N_D^+ = N_D^+(T)$ depends on temperature, is increasing, and approaches the total density of donors N_D for high temperatures. A similar behavior holds true for the density of negatively charged acceptors $N_A^- = N_A^-(T)$ (see [18]). Hence, we arrive at characterizing the interaction between the electrochemical potential of the electrons φ_n and the temperature T by the following reduced coupled system,

$$\begin{aligned}
-\nabla\cdot\big(N_D^+(T)\mu_n(T,N_D^+(T))\nabla\varphi_n\big) = 0 \quad &\text{in } \Omega,\\
-\nabla\cdot(\lambda\nabla T) = N_D^+(T)\mu_n(T,N_D^+(T))|\nabla\varphi_n|^2 \quad &\text{in } \Omega,\\
(N_D^+(T)\mu_n(T,N_D^+(T))\nabla\varphi_n)\cdot\nu = 0 \quad \text{on } \Gamma_N, \quad \varphi_n = V_{appl} \quad &\text{on } \Gamma_D,\\
\lambda\nabla T\cdot\nu + \kappa(T-T_a) = 0 \quad &\text{on } \partial\Omega.
\end{aligned} \tag{2.2}$$

In a completely analogous manner, for a strongly p-doped semiconductor region Ω with $N_A >> N_D \approx 0$ we obtain, under the assumption $n \to 0$ whereas the quantities $\nabla\varphi_n$, $\nabla\varphi_p$, ψ, $\nabla\psi$, v_p, p, T and ∇T remain bounded, the following reduced coupled system for the interaction of the electrochemical potential of the holes φ_p and the temperature T,

$$\begin{aligned}
-\nabla\cdot\big(N_A^-(T)\mu_p(T,N_A^-(T))\nabla\varphi_p\big) = 0 \quad &\text{in } \Omega,\\
-\nabla\cdot(\lambda\nabla T) = N_A^-(T)\mu_p(T,N_A^-(T))|\nabla\varphi_p|^2 \quad &\text{in } \Omega,\\
(N_A^-(T)\mu_p(T,N_A^-(T))\nabla\varphi_p)\cdot\nu = 0 \quad \text{on } \Gamma_N, \quad \varphi_p = V_{appl} \quad &\text{on } \Gamma_D,\\
\lambda\nabla T\cdot\nu + \kappa(T-T_a) = 0 \quad &\text{on } \partial\Omega.
\end{aligned} \tag{2.3}$$

The densities of charged donors and acceptors depend continuously on T and are positively bounded from below and above for $T \geq T_a$. Under the assumption that the mobilities $\mu_n,\ \mu_p$ also depend continuously on the temperature and the density, there are solutions (φ_n, T) to (2.2) and (φ_p, T) to (2.3) (see [3, Theorem 2.1]).

In case of (2.2) we reconstruct approximated quantities $(\psi^*, n^*, v_n^*, \varphi_n^*, T^*)$ for the unipolar drift-diffusion system by,

$$T^* := T, \quad n^* := N_D^+(T^*), \quad ,v_n^* := e_n^{-1}(n^*, T^*), \quad \psi^* := \varphi_n + v_n^*.$$

For the case (2.3) we reconstruct the quantities $(\psi^*, p^*, v_p^*, \varphi_p^*, T^*)$ as follows

$$T^* := T, \quad p^* := N_A^-(T^*), \quad ,v_p^* := e_p^{-1}(p^*, T^*), \quad \psi^* := \varphi_p - v_p^*.$$

2.2 Notation and assumptions

In two spatial dimensions, we consider geometric situations as indicated schematically in Fig. 1 and use the following notation: Ω_{D} is the subregion of the device where we consider the full electro-thermal drift-diffusion model, Ω_{n} is the highly n-doped subregion of the device, and Ω_{p} is the highly p-doped subregion of the device. The device region is defined as $\Omega = \mathrm{int}(\overline{\Omega_{\mathrm{n}}} \cup \overline{\Omega_{\mathrm{D}}} \cup \overline{\Omega_{\mathrm{p}}})$, $\Omega_{\mathrm{Dj}} = \mathrm{int}(\overline{\Omega_{\mathrm{D}}} \cup \overline{\Omega_{\mathrm{j}}})$, $\Gamma_{\mathrm{Dj}} := \Gamma_D \cap \overline{\Omega_{\mathrm{j}}}$, $I_{\mathrm{j}} = \mathrm{int}(\overline{\Omega_{\mathrm{D}}} \cap \overline{\Omega_{\mathrm{j}}})$ for $\mathrm{j} = \mathrm{n}, \mathrm{p}$, and $I := I_{\mathrm{n}} \cup I_{\mathrm{p}}$. By ν and ν_{D} we denote the outer unit normals at $\partial\Omega$ and $\partial\Omega_{\mathrm{D}}$, respectively.

We work with the Lebesgue spaces $L^p(\Omega)$ and the Sobolev spaces $W^{1,q}(\Omega)$. Moreover, we make use the following closed subspaces of H^1 functions: $H^1_{\mathrm{Di}}(\Omega_{\mathrm{Di}})$ indicates the closure of C^∞ functions with compact support in $\Omega_{\mathrm{Di}} \cup (\partial\Omega_{\mathrm{Di}} \setminus \Gamma_{\mathrm{Di}})$ with respect to the $H^1(\Omega_{\mathrm{Di}})$ norm, $H^1_I(\Omega_{\mathrm{D}})$ is the closure of C^∞ functions with compact support in $\Omega_{\mathrm{D}} \cup (\partial\Omega_{\mathrm{D}} \setminus I)$ with respect to the $H^1(\Omega_{\mathrm{D}})$ norm. In our estimates, positive constants, which may depend at most on the data of our problem, are denoted by c. In particular, we allow them to change from line to line.

We discuss the stationary hybrid electro-thermal model which we will introduce in Section 2.3 under the following general **Assumptions (A).** In what follows $j = n, p$,

- $\Omega, \Omega_{\mathrm{D}}, \Omega_{\mathrm{Dj}} \in \mathbb{R}^2$ are bounded Lipschitz domains with $\overline{\Omega_{\mathrm{n}}} \cap \overline{\Omega_{\mathrm{p}}} = \emptyset$, $\mathrm{mes}(I_{\mathrm{j}}) > 0$, $\mathrm{mes}(\Gamma_{\mathrm{Dj}}) > 0$ with $\mathrm{dist}(\mathrm{x}, \overline{\Omega_{\mathrm{Dj}}}) \geq$ const. > 0 for all $x \in \Gamma_{\mathrm{Di}},\ \mathrm{i} \neq \mathrm{j}$, and $\widetilde{\Gamma}_{\mathrm{Nj}} := \partial\Omega_{\mathrm{Dj}} \setminus \Gamma_{\mathrm{Dj}}$, $\Omega_{\mathrm{Dj}} \cup \widetilde{\Gamma}_{\mathrm{Nj}}$ are regular in the sense of Gröger [13].

- $\varphi_j^D \in W^{1,\infty}(\Omega_{\mathrm{Dj}})$, $\left\|\varphi_j^D\right\|_{L^\infty(\Omega_{\mathrm{Dj}})} \le K$, $\lambda \in L^\infty(\Omega)$, $0 < \lambda_0 \le \lambda$ a.e. in Ω, $\lambda =$ const in Ω_{D}, $\kappa \in L^\infty_+(\Gamma)$, $\|\kappa\|_{L^1(\Gamma)} > 0$, $T_a =$ const > 0, $\varepsilon =$ const > 0.
- The temperature dependent quantities for Ω_{n} and Ω_{p} fulfil: $\widehat{N}_{n0}$, $\widehat{N}_{p0}$, N_D^+, $N_A^- \in C^1_+(0,\infty)$, $\widehat{E}_C$, $\widehat{E}_V \in C^1(0,\infty)$ and for all $\xi > 0$ there exist $\overline{N}_\xi$, $\underline{N}_\xi$, $\overline{E}_\xi$ such that $|\widehat{E}_C(T)|$, $|\widehat{E}_V(T)| \le \overline{E}_\xi$, $0 < \underline{N}_\xi \le \widehat{N}_{n0}(T), \widehat{N}_{p0}(T), N_D^+(T), N_A^-(T) \le \overline{N}_\xi$ for all $T \in [\xi,\infty)$.
- C, N_{n0}, N_{p0} : $\Omega_{\mathrm{D}} \times (0,\infty) \to \mathbb{R}_+$, E_C, E_V : $\Omega_{\mathrm{D}} \times (0,\infty) \mapsto \mathbb{R}$ are Caratheodory functions which are Lipschitz continuous in the second argument such that for all $\xi > 0$ we have, $0 < \underline{N}_\xi \le N_{j0}(\cdot,T) \le \overline{N}_\xi$, $|E_C(\cdot,T)|$, $|E_V(\cdot,T)| \le \overline{E}_\xi$, $|C(\cdot,T)| \le \overline{C}$ a.e. in Ω_{D} for all $T \in [\xi,\infty)$.
- $r(\cdot,n,p,T) = r_0(\cdot,n,p,T)\,n\,p$, where $r_0(\cdot,n,p,T) : \Omega_{\mathrm{D}} \times (0,\infty)^3 \mapsto \mathbb{R}_+$ is a Caratheodory function with $r_0(\cdot,n,p,T) \le \overline{r}(1+n+p)$ a.e. in Ω_{D} for all $(n,p,T) \in (0,\infty)^3$. Moreover, $|r_0(\cdot,\, n_1,\, p_1,\, T_1) - r_0(\cdot,\, n,\, p,\, T)| \le c(|n_1-n| + |p_1-p| + |T_1-T|)$ a.e. in Ω_{D} and for all (n,p,T), $(n_1,p_1,T_1) \in (0,\infty)^2 \times [T_a,\infty)$.
- $\mu_j : \Omega_{\mathrm{Dj}} \times (0,\infty)^2 \mapsto \mathbb{R}_+$ are Caratheodory functions such that for all $\xi > 0$ there exists $\underline{\mu}_\xi$, $\overline{\mu}_\xi$ with $0 < \underline{\mu}_\xi \le \mu_j(\cdot,T,y) \le \overline{\mu}_\xi$ for all $(T,n,p) \in [\xi,\infty) \times (0,\infty)^2$ a.e. in Ω_{Dj}. $|\mu_j(\cdot,T_1,y_1) - \mu_j(\cdot,T,y)| \le c(|T_1-T| + |y_1-y|)$ a.e. in Ω_{Dj}, and for all T, $T_1 \ge T_a$, for all y, $y_1 \in (0,\infty)$.

Henceforth, we set $\overline{E} := \overline{E}_{T_a}$, $\underline{\mu} := \underline{\mu}_{T_a}$, $\overline{\mu} := \overline{\mu}_{T_a}$, $\underline{N} := \underline{N}_{T_a}$, and $\overline{N} := \overline{N}_{T_a}$. We remark that the assumption on r_0 allows for radiative, Shockley-Read-Hall as well as Auger recombination.

2.3 Hybrid model in case of $\Omega = \Omega_{\mathrm{n}} \cup \Omega_{\mathrm{D}} \cup \Omega_{\mathrm{p}}$

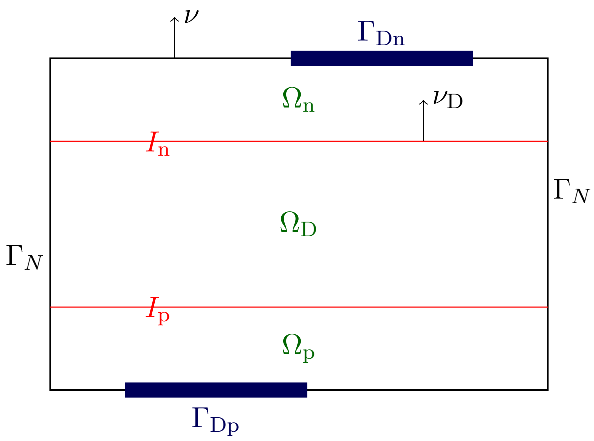

Figure 1: Schematic geometry of the semiconductor device partitioned into the different subregions.

In Ω_{D} we use the quantities R, n, p as they were defined in (1.2). The electro-thermal behavior of the device occupying Ω is now described by the following system of partial differential equations and transfer conditions:

Heat flow equation for T in Ω

$$-\nabla\cdot(\lambda\nabla T) = \begin{cases} N_D^+(T)\mu_n(T,N_D^+(T))|\nabla\varphi_n|^2 & \text{in } \Omega_{\mathrm{n}},\\ n\mu_n(T,n)|\nabla\varphi_n|^2 + p\mu_p(T,p)|\nabla\varphi_p|^2 + R(\varphi_p-\varphi_n) & \text{in } \Omega_{\mathrm{D}},\\ N_A^-(T)\mu_p(T,N_A^-(T))|\nabla\varphi_p|^2 & \text{in } \Omega_{\mathrm{p}},\end{cases} \tag{2.4}$$
$$\lambda\nabla T\cdot\nu + \kappa(T-T_a) = 0 \quad \text{on } \Gamma.$$

Continuity equation for electrons for φ_n in $\Omega_{\rm Dn} := \Omega_{\rm D} \cup \Omega_{\rm n}$

$$\begin{aligned}\nabla\cdot(N_D^+(T)\mu_n(T,N_D^+(T))\nabla\varphi_n) = 0 \quad &\text{in } \Omega_{\rm n},\\ \nabla\cdot(n\mu_n(T,n)\nabla\varphi_n) = -R \quad &\text{in } \Omega_{\rm D},\\ [\![\varphi_n]\!]=0,\ \nu_{\rm D}\cdot(N_D^+(T)\mu_n(T,N_D^+)\nabla\varphi_n) + \nu_{\rm D}\cdot(n\mu_n(T,n)\nabla\varphi_n) = 0 \quad &\text{on } I_{\rm n},\\ \varphi_n = V_{appl} =: \varphi_n^D \quad \text{on } \Gamma_{\rm Dn}, \quad \nabla\varphi_n\cdot\nu = 0 \quad &\text{otherwise.}\end{aligned} \tag{2.5}$$

Continuity equation for holes for φ_p in $\Omega_{\rm Dp} := \Omega_{\rm D} \cup \Omega_{\rm p}$

$$\begin{aligned}-\nabla\cdot(p\mu_p(T,p)\nabla\varphi_p) = -R \quad &\text{in } \Omega_{\rm D},\\ -\nabla\cdot(N_A^-(T)\mu_p(T,N_A^-(T))\nabla\varphi_p) = 0 \quad &\text{in } \Omega_{\rm p},\\ [\![\varphi_p]\!]=0,\ \nu_{\rm D}\cdot(N_A^-(T)\mu_p(T,N_A^-(T))\nabla\varphi_p) + \nu_{\rm D}\cdot(p\mu_p(T,p)\nabla\varphi_p) = 0 \quad &\text{on } I_{\rm p},\\ \varphi_p = V_{appl} =: \varphi_p^D \quad \text{on } \Gamma_{\rm Dp}, \quad \nabla\varphi_p\cdot\nu = 0 \quad &\text{otherwise.}\end{aligned} \tag{2.6}$$

Poisson equation for electrostatic potential ψ in $\Omega_{\rm D}$

$$-\nabla\cdot(\varepsilon\nabla\psi) = C(T) - n + p \quad \text{in } \Omega_{\rm D}. \tag{2.7}$$

If n in $\Omega_{\rm n}$ is assumed to be equal to $N_D^+(T)$ then the chemical potential $v_n = T\ln\frac{N_D^+(T)}{\widehat{N}_{n0}(T)} + \widehat{E}_C(T) =: e_n^{-1}(N_D^+(T);T)$ in $\Omega_{\rm n}$ is not necessarily constant, since the temperature may vary. Here $\widehat{E}_C(T)$, $\widehat{N}_{n0}(T)$ denote the temperature-dependent conduction band-edge and the effective density of states in $\Omega_{\rm n}$ and $e_n^{-1}(\cdot\,;T)$ means the inverse of e_n with respect to the first argument for a fixed temperature T. Because of $\varphi_n = \psi - v_n$, we obtain as boundary condition for ψ on $I_{\rm n}$,

$$\psi|_{I_{\rm n}} = \varphi_n|_{I_{\rm n}} + e_n^{-1}(N_D^+(T);T).$$

In a completely analogous manner, with $\varphi_p = \psi + v_p$ and $v_p = e_p^{-1}(N_A^-(T);T)$ in $\Omega_{\rm p}$ the boundary condition for ψ on $I_{\rm p}$ is,

$$\psi|_{I_{\rm p}} = \varphi_p|_{I_{\rm p}} - e_p^{-1}(N_A^-(T);T).$$

Let $\tau : \Omega_{\rm D} \to [0,1]$ be an arbitrarily fixed $C^1(\overline{\Omega}_{\rm D})$ function such that

$$\tau|_{I_{\rm n}} = 0, \quad \tau|_{I_{\rm p}} = 1, \quad |\nabla\tau| \le \widehat{c}. \tag{2.8}$$

We are looking for ψ fulfilling at the union of interfaces $I := I_{\rm n} \cup I_{\rm p}$ the discussed boundary conditions and express this in the form,

$$\psi \in \tau(\varphi_p - e_p^{-1}(N_A^-(T);T)) + (1-\tau)(\varphi_n + e_n^{-1}(N_D^+(T);T)) + H_I^1(\Omega_{\rm D}).$$

On the remaining part of the boundary $\partial\Omega_{\rm D}\setminus I$, homogeneous Neumann boundary conditions are formulated,

$$\varepsilon\nabla\psi\cdot\nu = 0 \quad \text{on } \partial\Omega_{\rm D}\setminus I.$$

To simplify the above governing equations we introduce the following notation in the entire domain Ω,

$$\chi^1(x) = \begin{cases} 1 \text{ if } x \in \Omega_{\rm Dn} \\ 0 \text{ otherwise}, \end{cases} \qquad \chi^2(x) = \begin{cases} 1 \text{ if } x \in \Omega_{\rm Dp} \\ 0 \text{ otherwise}, \end{cases}$$

$$d_n(n,T) = \chi^1(1-\chi^2)N_D^+(T)\mu_n(T,N_D^+(T)) + \chi^1\chi^2 n\mu_n(T,n), \tag{2.9}$$

$$d_p(p,T) = \chi^2(1-\chi^1)N_A^-(T)\mu_p(T,N_A^-(T)) + \chi^1\chi^2 p\mu_p(T,p), \tag{2.10}$$

$$R_\Omega(n,p,T,\varphi_n,\varphi_p) = \chi^1\chi^2 R(n,p,T,\varphi_n,\varphi_p), \tag{2.11}$$

$$\begin{aligned} h_\Omega(n,p,T,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p) = d_n(n,T)|\nabla\varphi_n|^2 + d_p(p,T)|\nabla\varphi_p|^2 \\ +R_\Omega(n,p,T,\varphi_n,\varphi_p)(\varphi_p-\varphi_n). \end{aligned} \tag{2.12}$$

Using the above notation equations (2.4), (2.5), (2.6), (2.7) and their respective interface and boundary conditions take the following form:

Heat flow equation for T in Ω

$$\begin{aligned} &-\nabla\cdot(\lambda\nabla T) = h_\Omega(n,p,T,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p) && \text{in } \Omega, \\ &\lambda\nabla T\cdot\nu + \kappa(T-T_a) = 0 && \text{on } \Gamma. \end{aligned} \tag{2.13}$$

Continuity equation for electrons in Ω_{Dn}

$$\begin{aligned} \nabla\cdot(d_n(n,T)\nabla\varphi_n) = -R_\Omega(n,p,T,\varphi_n,\varphi_p) \quad & \text{in } \Omega_{\mathrm{Dn}}, \\ [\![\varphi_n]\!] = 0, \quad [\![d_n(n,T)\nabla\varphi_n\cdot\nu_{\mathrm{D}}]\!] = 0 \quad & \text{on } I_{\mathrm{n}}, \\ \varphi_n = \varphi_n^{\mathrm{D}} \text{ on } \Gamma_{\mathrm{Dn}}, \quad \nabla\varphi_n\cdot\nu = 0 \quad & \text{on } \partial\Omega_{\mathrm{Dn}}\backslash\Gamma_{\mathrm{Dn}}. \end{aligned} \tag{2.14}$$

Continuity equation for holes in Ω_{Dp}

$$\begin{aligned} -\nabla\cdot(d_p(p,T)\nabla\varphi_p) = -R_\Omega(n,p,T,\varphi_n,\varphi_p) \quad & \text{in } \Omega_{\mathrm{Dp}}, \\ [\![\varphi_p]\!] = 0, \quad [\![d_p(p,T)\nabla\varphi_p\cdot\nu_{\mathrm{D}}]\!] = 0 \quad & \text{on } I_{\mathrm{p}}, \\ \varphi_p = \varphi_p^{\mathrm{D}} \text{ on } \Gamma_{\mathrm{Dp}}, \quad \nabla\varphi_p\cdot\nu = 0 \quad & \text{on } \partial\Omega_{\mathrm{Dp}}\backslash\Gamma_{\mathrm{Dp}}. \end{aligned} \tag{2.15}$$

Poisson equation for electrostatic potential ψ in Ω_{D}

$$\begin{aligned} -\nabla\cdot(\varepsilon\nabla\psi) = C(T) - n + p \quad & \text{in } \Omega_{\mathrm{D}}, \\ \psi = \tau(\varphi_p - e_p^{-1}(N_A^-;T)) + (1-\tau)(\varphi_n + e_n^{-1}(N_D^+;T)) \quad & \text{on } I, \\ \nabla\psi\cdot\nu = 0 \quad & \text{on } \partial\Omega_{\mathrm{D}}\setminus I. \end{aligned} \tag{2.16}$$

2.4 Concept of solution

With τ as in (2.8), we use the abbreviation,

$$\psi^D(x) := (1-\tau(x))\Big(\varphi_n + T\ln\frac{N_D^+(T)}{\widehat{N}_{n0}(T)} + \widehat{E}_C(T)\Big) + \tau(x)\Big(\varphi_p - T\ln\frac{N_A^-(T)}{\widehat{N}_{p0}(T)} + \widehat{E}_V(T)\Big).$$

Let $s>2$ denote an exponent which will finally be fixed in Theorem 3.1. A weak formulation of our hybrid model is as follows. Find $(\psi,\varphi_n,\varphi_p,T) \in \big[(\psi^D + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}}))\cap L^\infty(\Omega_{\mathrm{D}})\big] \times \big[(\varphi_n^D + H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}}))\cap W^{1,s}(\Omega_{\mathrm{Dn}})\big] \times$

$\big[(\varphi_p^D + H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}}) \cap W^{1,s}(\Omega_{\mathrm{Dp}})\big] \times \{T \in H^1(\Omega) : \ln T \in L^\infty(\Omega)\}$, such that

$$\begin{aligned}
&\int_{\Omega_{\mathrm{D}}} \varepsilon \nabla\psi \cdot \nabla\overline{\psi}\, \mathrm{d}x = \int_{\Omega_{\mathrm{D}}} (C(T) - n + p)\overline{\psi}\, \mathrm{d}x \qquad \forall\, \overline{\psi} \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}}),\\
&\int_{\Omega_{\mathrm{Dn}}} d_n(n,T)\nabla\varphi_n \cdot \nabla\overline{\varphi}_n\, \mathrm{d}x + \int_{\Omega_{\mathrm{Dp}}} d_p(p,T)\nabla\varphi_p \cdot \nabla\overline{\varphi}_p\, \mathrm{d}x\\
&= \int_{\Omega_{\mathrm{D}}} r(n,p,T)\Big(1 - \exp\frac{\varphi_n - \varphi_p}{T}\Big)(\overline{\varphi}_n - \overline{\varphi}_p)\, \mathrm{d}x \quad \forall\, \overline{\varphi}_i \in H^1_{\mathrm{Di}}(\Omega_{\mathrm{Di}}),\ i = n,p, \qquad \text{(P)}\\
&\int_{\Omega} \lambda \nabla T \cdot \nabla \overline{T}\, \mathrm{d}x + \int_{\Gamma} \kappa (T - T_a)\overline{T}\, \mathrm{d}\Gamma\\
&= \int_{\Omega} h_\Omega(n,p,T,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p)\overline{T}\, \mathrm{d}x \quad \forall\, \overline{T} \in H^1(\Omega),
\end{aligned}$$

where $d_n(n,T), d_p(p,T)$, and $h_\Omega(n,p,T,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p)$ are defined in (2.9), (2.10), and (2.12) respectively. We remark that the choice of the definition sets for $(\psi,\varphi_n,\varphi_p,T)$ and Assumptions (A) ensure, $n,p \in L^\infty(\Omega_{\mathrm{D}})$, $\mu_n(T,n)$, $\mu_p(T,p)$, $r(n,p,T) \in L^\infty(\Omega_{\mathrm{D}})$, $N_D^+(T)$, $\mu_n(T,N_D^+(T)) \in L^\infty(\Omega_{\mathrm{n}})$, $N_A^-(T), \mu_p(T,N_A^-(T)) \in L^\infty(\Omega_{\mathrm{p}})$, $d_n(n,T) \in L^\infty(\Omega_{\mathrm{Dn}})$, $d_p(p,T) \in L^\infty(\Omega_{\mathrm{Dp}})$, $h_\Omega(n,p,T,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p) \in L^{s/2}(\Omega)$, and $\psi^D \in H^1(\Omega) \cap L^\infty(\Omega)$.

3 A priori estimates for the hybrid model

If there is no confusion of misunderstanding we leave out the arguments in the functions $\mu_n,\ \mu_p, r_0$. Moreover, we do not explicitly write the temperature dependencies of $N_{i0},\ N_D^+,\ N_A^-,\ E_C, E_V, \widehat{N}_{i0}, \widehat{E}_C$, and $\widehat{E}_V$.

Lemma 3.1 *We suppose Assumption (A). Then $T \geq T_a$ a.e. in Ω for any solution $(\psi,\varphi_n,\varphi_p,T)$ to* (P).

Proof. By Assumption (A) the right hand side of the heat flow equation (2.13) is nonnegative. Thus, the test of the heat flow equation in (P) by $-(T-T_a)^-$ gives

$$\int_\Omega \lambda |\nabla (T-T_a)^-|^2\, \mathrm{d}x + \int_\Gamma \kappa ((T-T_a)^-)^2\, \mathrm{d}\Gamma \leq 0$$

which proves the lemma. □

Lemma 3.2 *We suppose Assumptions (A). Then there exists a constant $c_h > 0$, depending only on the data, such that*

$$\|h_\Omega(n,p,T,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p)\|_{L^1(\Omega)} \leq c_h,\ \|\varphi_n\|_{L^\infty(\Omega_{\mathrm{Dn}})},\ \|\varphi_p\|_{L^\infty(\Omega_{\mathrm{Dp}})} \leq K,$$

where K is defined in Assumptions (A), for any solution $(\psi,\varphi_n,\varphi_p,T)$ to (P).

Proof. 1. Using the test function $((\varphi_n - K)^+, (\varphi_p - K)^+) \in H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}}) \times H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}})$ with K from assumption (A) for the equations for φ_n and φ_p we obtain

$$\begin{aligned}
0 = &\int_{\Omega_{\mathrm{Dn}}} d_n(n,T)|\nabla(\varphi_n - K)^+|^2\, \mathrm{d}x + \int_{\Omega_{\mathrm{Dp}}} d_p(p,T)|\nabla(\varphi_p - K)^+|^2\, \mathrm{d}x\\
&+ \int_{\Omega_{\mathrm{D}}} r(n,p,T)\,\big(\exp\frac{\varphi_n - \varphi_p}{T} - 1\big)\big((\varphi_n - K)^+ - (\varphi_p - K)^+\big)\, \mathrm{d}x.
\end{aligned}$$

Discussing the four different cases $\varphi_n\,(\varphi_p) > K\,(\leq K)$ we find that also the integrand in the second line is always non-negative (note that r_0 is also non-negative). Thus the integrands in all occurring integrals are nonnegative. (If the integral of a nonnegative function is zero then the function itself is zero.) The positivity of $n,\ p,\ \mu_n,\ \mu_p$ in Ω_{D}, of $d_n(n,T)$ in Ω_{Dn} and of $d_p(p,T)$ in Ω_{Dp} guarantee that $\nabla(\varphi_i - K)^+ = 0$ a.e. in Ω_{Di} due to $(\varphi_i - K)^+ \in H^1_{\mathrm{Di}}(\Omega_{\mathrm{Di}})$. This leads to $\varphi_i \le K$ a.e. in Ω_{Di} for $\mathrm{i} = \mathrm{n}, \mathrm{p}$. On the other hand, testing by $(-(\varphi_n + K)^-, -(\varphi_p + K)^-)$ gives the estimates $\varphi_i \ge -K$ a.e. in Ω_{Di}, which together ensure $\|\varphi_i\|_{L^\infty(\Omega_{\mathrm{Di}})} \le K$ for $i = n, p$.

2. We use functions $\tau_{\mathrm{i}} \in C^1(\overline{\Omega_{\mathrm{Di}}})$ with $\tau_{\mathrm{i}}(x) \in [0,1]$, $|\nabla\tau_{\mathrm{i}}(x)| \le \widehat{c}$ in $\overline{\Omega_{\mathrm{Di}}}$, $\tau_{\mathrm{i}}(x) = 1$ for $x \in \Gamma_{D\mathrm{i}}$, $\tau_{\mathrm{i}}(x) = 0$ for $x \in \Omega_{\mathrm{D}}$, $\mathrm{i} = \mathrm{n}, \mathrm{p}$. Note that $\widehat{c} > 0$ depends on the geometry of the problem. We test the continuity equations by $(\varphi_n - \tau_{\mathrm{n}}\varphi_n^D, \varphi_p - \tau_{\mathrm{p}}\varphi_p^D) \in H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}}) \times H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}})$ and obtain,

$$
\begin{aligned}
&\int_\Omega h_\Omega(n,p,T,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p)\,\mathrm{d}x \\
&= \int_{\Omega_{\mathrm{n}}} N_D^+\mu_n\nabla\varphi_n\cdot(\tau_{\mathrm{n}}\nabla\varphi_n^D + \varphi_n\nabla\tau_{\mathrm{n}})\,\mathrm{d}x + \int_{\Omega_{\mathrm{p}}} N_A^-\mu_p\nabla\varphi_p\cdot(\tau_{\mathrm{p}}\nabla\varphi_p^D + \varphi_p\nabla\tau_{\mathrm{p}})\,\mathrm{d}x \\
&\le \int_{\Omega_{\mathrm{n}}} N_D^+\mu_n\Big(\frac{|\nabla\varphi_n|^2}{2} + 2|\nabla\varphi_n^D|^2 + 2K^2\widehat{c}^2\Big)\,\mathrm{d}x + \int_{\Omega_{\mathrm{p}}} N_A^-\mu_p\Big(\frac{|\nabla\varphi_p|^2}{2} + 2|\nabla\varphi_p^D|^2 + 2K^2\widehat{c}^2\Big)\,\mathrm{d}x.
\end{aligned}
$$

Due to the definition of $h_\Omega(n,p,T,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p)$ in (2.12) and the fact that N_D^+, N_A^- and μ_n, μ_p are bounded from above we have

$$
\begin{aligned}
\|h_\Omega(n,p,T,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p)\|_{L^1(\Omega)} \le & 4\overline{N}\overline{\mu}\Big\{\int_{\Omega_{\mathrm{n}}} (|\nabla\varphi_n^D|^2 + K^2\widehat{c}^2)\,\mathrm{d}x \\
&+ \int_{\Omega_{\mathrm{p}}} (|\nabla\varphi_p^D|^2 + K^2\widehat{c}^2)\,\mathrm{d}x\Big\} =: c_h.
\end{aligned} \tag{3.1}
$$

Since $\varphi_i^D \in H^1(\Omega_{\mathrm{Di}})$, $i = n, p$, are given functions, the last assertion follows. □

Lemma 3.3 *We suppose Assumptions (A) then for $q \in [1,2)$, there exist constants $c_q > 0$, and $c_T > 0$, depending only on the data, such that*

$$\|T\|_{W^{1,q}(\Omega)} \le c_q, \quad \|T\|_{L^2(\Gamma)} \le c_T$$

for any solution $(\psi,\varphi_n,\varphi_p,T)$ to (P)*.*

Proof. According to Lemma 3.2 the right hand side of the heat flow equation belongs to $L^1(\Omega)$ and has a L^1 norm bounded by c_h. Using the theory of entropy solutions for elliptic problems with Robin boundary conditions (see e.g. [4, Theorem 3.3]) gives the desired $W^{1,q}(\Omega)$ estimates. The trace inequality in 2D then ensures the $L^2(\Gamma)$ estimate. □

Lemma 3.4 *We suppose Assumptions (A) then there exists a constant $c_{\psi/T} > 0$, depending only on the data, such that,*

$$\|\psi/T\|_{L^\infty(\Omega_{\mathrm{D}})} \le c_{\psi/T}$$

for any solution $(\psi,\varphi_n,\varphi_p,T)$ to (P)*.*

Proof. 1. We introduce the constant $K_1 := \max\big\{\max_T\{\ln\frac{N_D^+(T)}{\widehat{N}_{n0}(T)}\}, \max_T\{\ln\frac{N_A^-(T)}{\widehat{N}_{p0}(T)}\}\big\}$, and use K from Assumptions (A). We note that $(\psi - K - \overline{E} - K_1T)^+ \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ and that for $L > 0$,

$$z_L^{m-1} \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}}) \quad \text{where } z_L := \min(L, (\psi - K - \overline{E} - K_1T)^+), \quad m = 2^k, \quad k \in \mathbb{N},$$

and that these functions extended by zero belong to $H^1(\Omega)$ and can be used as test functions for the heat equation on whole Ω:

$$\begin{aligned}
&\int_\Omega \lambda\nabla T\cdot\nabla z_L^{m-1}\,\mathrm{d}x = \int_{\Omega_\mathrm{D}} \lambda\nabla T\cdot\nabla z_L^{m-1}\,\mathrm{d}x\\
&= \int_{\Omega_\mathrm{D}} \Big(n\mu_n|\nabla\varphi_n|^2 + p\mu_p|\nabla\varphi_p|^2 + R(n,p,T,\varphi_n,\varphi_p)(\varphi_p-\varphi_n)\Big) z_L^{m-1}\,\mathrm{d}x\\
&+ \int_{\Gamma\cap\overline{\Omega}_\mathrm{D}} \kappa(T_a - T) z_L^{m-1}\,\mathrm{d}\Gamma\\
&\geq -c\,\|T\|_{L^2(\Gamma)}\,\big\|z_L^{m-1}\big\|_{L^2(\Gamma\cap\overline{\Omega}_\mathrm{D})}
\end{aligned}$$

since the Joule heat and reaction heat in Ω_D are nonnegative. Using this and the fact that $\varepsilon,\ \lambda = $ const on Ω_D, a test of the Poisson equation by $m\, z_L^{m-1}$ yields with $w_L := z_L^{\frac{m}{2}}$

$$\begin{aligned}
&\int_{\Omega_\mathrm{D}} m(C(T)-n+p) z_L^{m-1}\,\mathrm{d}x\\
&\quad= \int_{\Omega_\mathrm{D}} m\varepsilon\nabla\psi\cdot\nabla z_L^{m-1}\,\mathrm{d}x\\
&\quad= \int_{\Omega_\mathrm{D}} m\varepsilon\nabla(\psi - K - \overline{E} - K_1T + K + \overline{E} + K_1 T)\cdot\nabla z_L^{m-1}\,\mathrm{d}x\\
&\quad= \int_{\Omega_\mathrm{D}} \frac{4(m-1)}{m}\varepsilon|\nabla w_L|^2 + m\varepsilon K_1\nabla T\cdot\nabla z_L^{m-1}\,\mathrm{d}x\\
&\quad\geq 2\varepsilon\int_{\Omega_\mathrm{D}} |\nabla w_L|^2\,\mathrm{d}x - cm\,\|T\|_{L^2(\Gamma)}\,\big\|z_L^{m-1}\big\|_{L^2(\Gamma\cap\overline{\Omega}_\mathrm{D})}\,.
\end{aligned} \tag{3.2}$$

Note that $z_L > 0$ leads to $\psi > 0$, and thus using the lower bound T_a for T from Lemma 3.1 and the L^∞ estimate for φ_p from Lemma 3.2 we derive

$$\begin{aligned}
(C-n+p)z_L^{m-1} &\leq \Big(\overline{C} + N_{p0}\exp\frac{E_V - \psi + \varphi_p}{T}\Big) z_L^{m-1}\\
&\leq \Big(\overline{C} + N_{p0}\exp\frac{E_V + \varphi_p}{T}\Big) z_L^{m-1} \leq c z_L^{m-1}.
\end{aligned} \tag{3.3}$$

Because of Gagliardo-Nirenberg's and trace inequality in 2D we estimate

$$\begin{aligned}
&\big\|z_L^{m-1}\big\|_{L^1(\Omega_\mathrm{D})} \leq \|w_L\|^2_{L^2(\Omega_\mathrm{D})} + c \leq c\,\|w_L\|_{L^1(\Omega_\mathrm{D})}\,\|w_L\|_{H^1(\Omega_\mathrm{D})} + c,\\
&\big\|z_L^{m-1}\big\|_{L^2(\Gamma\cap\overline{\Omega}_\mathrm{D})} \leq \|w_L\|^2_{L^4(\Gamma\cap\overline{\Omega}_\mathrm{D})} + c,\\
&\|w_L\|^2_{L^4(\Gamma\cap\overline{\Omega}_\mathrm{D})} \leq c\,\|w_L\|^{3/2}_{L^6(\Omega_\mathrm{D})}\,\|w_L\|^{1/2}_{H^1(\Omega_\mathrm{D})} \leq c(\|w_L\|^{1/6}_{L^1(\Omega_\mathrm{D})}\,\|w_L\|^{5/6}_{H^1(\Omega_\mathrm{D})})^{3/2}\,\|w_L\|^{1/2}_{H^1(\Omega_\mathrm{D})}\\
&\qquad\qquad\leq c\,\|w_L\|^{1/4}_{L^1(\Omega_\mathrm{D})}\,\|w_L\|^{7/4}_{H^1(\Omega_\mathrm{D})}\,,
\end{aligned}$$

apply Young's inequality, use that mes $\Gamma_I > 0$ and continue the estimate (3.2) by

$$\|w_L\|^2_{H^1(\Omega_\mathrm{D})} \leq cm\,\|T\|_{L^2(\Gamma)} + \frac{1}{4}\,\|w_L\|^2_{H^1(\Omega_\mathrm{D})} + cm^8(\|T\|^8_{L^2(\Gamma)}+1)\,\|w_L\|^2_{L^1(\Omega_\mathrm{D})} + c.$$

From Lemma 3.3 we find

$$\begin{aligned}
\|w_L\|^2_{L^2(\Omega_\mathrm{D})} &\leq cm^8(c_T^8+1)(\|w_L\|^2_{L^1(\Omega_\mathrm{D})} + c_T)\\
&\leq m^8\max\{c(c_T^8+1), c_T\}(\|w_L\|^2_{L^1(\Omega_\mathrm{D})}+1) =: \frac{\widetilde{c}}{2}m^8(\|w_L\|^2_{L^1(\Omega_\mathrm{D})}+1).
\end{aligned}$$

Defining $a_k := 1 + \|z_L\|_{L^{2^k}}^{2^k}$, $k \in \mathbb{N}$, the previous estimate guarantees the recursion

$$\begin{aligned} a_k &\le \widetilde{c}(2^8)^k a_{k-1}^2 \le \widetilde{c}^{1+2}(2^8)^{k+2(k-1)} a_{k-2}^4 \\ &\le \widetilde{c}^{1+2+\dots+2^{k-2}}(2^8)^{k+2(k-1)+\dots+2^{k-2}\cdot 2} a_1^{2^{k-1}} \le \widetilde{c}^{2^k}(2^8)^{2^{k+1}} a_1^{2^k}. \end{aligned} \tag{3.4}$$

Here we used that $\sum_{i=0}^{k-2} 2^i \le 2^k$ and $\sum_{i=0}^{k-2} 2^i(k-i) \le 2^{k+1}$ for $k \ge 2$. To derive the starting estimate for a_1 we set $m = 2$ ($k = 1$) in (3.2) to obtain

$$\|z_L\|_{H^1(\Omega_{\rm D})}^2 \le c_1 \|z_L\|_{L^1(\Omega_{\rm D})} + c_2 \|z_L\|_{L^2(\Gamma\cap\overline{\Omega}_{\rm D})}.$$

Because of embedding, trace and Young's inequality we find

$$\begin{aligned} c_1 \|z_L\|_{L^1(\Omega_{\rm D})} &\le \widehat{c}_1 \|z_L\|_{H^1(\Omega_{\rm D})} \le \frac{1}{4} \|z_L\|_{H^1(\Omega_{\rm D})}^2 + 4\widehat{c}_1^2, \\ c_2 \|z_L\|_{L^2(\Gamma\cap\overline{\Omega}_{\rm D})} &\le \widehat{c}_2 \|z_L\|_{H^1(\Omega_{\rm D})} \le \frac{1}{4} \|z_L\|_{H^1(\Omega_{\rm D})}^2 + 4\widehat{c}_2^2. \end{aligned}$$

This leads to $a_1 = 1 + \|z_L\|_{L^2(\Omega_{\rm D})}^2 \le 1 + \|z_L\|_{H^1(\Omega_{\rm D})}^2 \le c$ which induces together with the recursion formula (3.4) the L^∞ bound for $z_L = \min(L, (\psi - K - \overline{E} - K_1 T)^+)$. Since the estimates do not depend on the value of L, we can pass to the limit $L \to \infty$ and find an upper bound $\overline{c} > 0$ for $\psi - K - \overline{E} - K_1 T$. Therefore, by Lemma 3.1,

$$\frac{\psi}{T} \le \frac{\overline{c} + K + \overline{E}}{T} + K_1 \le \frac{\overline{c} + K + \overline{E}}{T_a} + K_1.$$

2. Similarly we obtain a lower bound for ψ/T by using test functions of the form

$$-m\, \overline{z}_L^{m-1} \in H^1_{\rm I}(\Omega_{\rm D}) \quad \text{with } \overline{z}_L := \min(L, (\psi + K + \overline{E} + K_1 T)^-), \quad m = 2^k, \quad k \in \mathbb{N},$$

where $y^- := \max(0, -y)$. Note that then the second line in (3.2) is rewritten as

$$\begin{aligned} -\int_{\Omega_{\rm D}} & m\varepsilon \nabla(\psi + K + \overline{E} + K_1 T - K - \overline{E} - K_1 T) \cdot \nabla \overline{z}_L^{m-1} \,\mathrm{d}x \\ &= \int_{\Omega_{\rm D}} \tfrac{4(m-1)}{m} \varepsilon |\nabla \overline{z}_L^{\frac{m}{2}}|^2 + m\varepsilon K_1 \nabla T \cdot \nabla \overline{z}_L^{m-1} \,\mathrm{d}x, \end{aligned}$$

where the second expression again can be substituted by the weak formulation of the heat flow equation, tested by $m\, \overline{z}_L^{m-1}$ continued by zero to a function in $H^1(\Omega)$. Moreover, $\overline{z}_L > 0$ leads to $\psi < 0$ such that

$$\begin{aligned} -(C - n + p)\overline{z}_L^{m-1} &\le \Big(\overline{C} + N_{n0} \exp \frac{\psi - \varphi_n - E_C}{T}\Big) \overline{z}_L^{m-1} \\ &\le \Big(\overline{C} + N_{n0} \exp \frac{-\varphi_n - E_C}{T}\Big) \overline{z}_L^{m-1} \le c \overline{z}_L^{m-1}. \end{aligned}$$

Finally we end up with a lower bound $\underline{c} < 0$ for $\psi + K + \overline{E} + K_1 T$. Therefore, by Lemma 3.3,

$$\frac{\psi}{T} \ge \frac{\underline{c} - K - \overline{E}}{T} - K_1 \ge \frac{\underline{c} - K - \overline{E}}{T_a} - K_1. \qquad \square$$

Theorem 3.1 *Under Assumption (A), there are exponents* $s,\ t > 2$ *and constants* $c_{T,t}$, $c_{\varphi,s}$, $c_{T,\infty}$, $c_{\psi,\infty} > 0$ *depending only on the data and the underlying geometry such that*

$$\|\varphi_i\|_{W^{1,s}(\Omega_{\rm Di})} \le c_{\varphi,s},\ i = n,p,\ \|T\|_{W^{1,t}(\Omega)} \le c_{T,t},\ \|T\|_{L^\infty(\Omega)} \le c_{T,\infty},\ \|\psi\|_{L^\infty(\Omega_{\rm D})} \le c_{\psi,\infty},$$

for any solution $(\psi, \varphi_n, \varphi_p, T)$ *to* (P).

Proof. 1. The estimates from Lemma 3.2, Lemma 3.3 and Lemma 3.4 and the bounds for E_C and E_V ensure constants $\underline{c}_d,\ \overline{c}_d > 0$ only depending on the data and the underlying geometry such that

$$\begin{aligned} &\underline{c}_d \le n = N_{n0} \exp \frac{\psi - \varphi_n - E_C}{T},\ p = N_{p0} \exp \frac{E_V - \psi + \varphi_p}{T} \le \overline{c}_d \quad \text{a.e. in } \Omega_{\mathrm{D}}, \\ &\text{where} \quad \underline{c}_d := \underline{N} \exp\Big\{ - \frac{K + \overline{E}}{T_a} - c_{\psi/T}\Big\}, \quad \overline{c}_d := \overline{N} \exp\Big\{ \frac{K + \overline{E}}{T_a} + c_{\psi/T}\Big\}. \end{aligned} \tag{3.5}$$

Using additionally the upper and lower bounds of the mobilities $\mu_n,\ \mu_p$ and N_D^+ and N_A^-, the estimates (3.5), and the resulting upper bound for r_0 and Lemma 3.2 we find that the L^∞ norm of the right hand sides of the continuity equations is bounded by a constant $c_R > 0$. The supposed regularity of $\varphi_n^D,\ \varphi_p^D$ and the regularity result of Gröger [13, Thm. 1] for elliptic problems guarantees an exponent $s > 2$ and an $c_{\varphi,s} > 0$ depending only on the data and the underlying geometry such that $\varphi_n \in W^{1,s}(\Omega_{\mathrm{Dn}})$, $\varphi_p \in W^{1,s}(\Omega_{\mathrm{Dp}})$ and

$$\|\varphi_n\|_{W^{1,s}(\Omega_{\mathrm{Dn}})},\ \|\varphi_p\|_{W^{1,s}(\Omega_{\mathrm{Dp}})} \le c_{\varphi,s}.$$

2. Consequentely, the right-hand side of the heat flow equation (2.13) belongs to $L^{s/2}(\Omega)$ and the $L^{s/2}(\Omega)$ norm is bounded by some constant $c > 0$. Here we used for the reaction heat that $\|\varphi_i\|_{L^\infty(\Omega_{\mathrm{Di}})} \le K$, $i = n, p$. We apply regularity results for second order elliptic equations with non-smooth data in the 2D case. According to [13, Thm. 1] there is a $t^* > 2$ such that the strongly monotone Lipschitz continuous operator $\Lambda:\ H^1(\Omega) \mapsto H^1(\Omega)^*$,

$$\langle \Lambda T, w\rangle := \int_\Omega (\lambda \nabla T \cdot \nabla w + T w)\, \mathrm{d}x, \quad w \in H^1(\Omega),$$

maps $W^{1,\widetilde{t}}(\Omega)$ into and onto $W^{-1,\widetilde{t}}(\Omega)$ for all $\widetilde{t} \in [2, t^*]$. Here, $W^{-1,\widetilde{t}}(\Omega)$ means $W^{1,\widetilde{t}'}(\Omega)^*$ with $\frac{1}{\widetilde{t}} + \frac{1}{\widetilde{t}'} = 1$. Next we define $t \in (2, t^*]$ by

$$t := \begin{cases} t^* & \text{if } \dfrac{s}{s-2} \in \Big[1, \dfrac{2t^*}{t^*-2}\Big] \\ \dfrac{2s}{4-s} & \text{if } \dfrac{s}{s-2} > \dfrac{2t^*}{t^*-2} \end{cases}, \qquad \frac{1}{t} + \frac{1}{t'} = 1.$$

This definition guarantees that $L^{s/2}(\Omega) \hookrightarrow W^{-1,t}(\Omega) = W^{1,t'}(\Omega)^*$. Remark 13 in [13] then ensures $W^{1,t}$-estimates for solutions to problems of the form $\Lambda T = \mathcal{F}(T)$, where $\mathcal{F}$ is any mapping from $W^{1,2}(\Omega)$ into $W^{-1,t}(\Omega)$. For our problem under consideration we use

$$\langle \mathcal{F}(T), w\rangle := \int_\Omega \Big(h_\Omega(n, p, T, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p) + T\Big)\, w\, \mathrm{d}x + \int_\Gamma \kappa(T_a - T)\, w\, \mathrm{d}\Gamma,$$

for all $w \in W^{1,t'}(\Omega)$. Thus, we find a $c_{T,t} > 0$ such that the weak solution T to the heat flow equation belongs to $W^{1,t}(\Omega)$ and $\|T\|_{W^{1,t}(\Omega)} \le c_{T,t}$. The continuous embedding of $W^{1,t}(\Omega)$ in $L^\infty(\Omega)$ ensures $\|T\|_{L^\infty(\Omega)} \le c_{T,\infty}$. Moreover, together with Lemma 3.4 we therefore obtain $\|\psi\|_{L^\infty(\Omega_{\mathrm{D}})} \le c_{\psi,\infty}$, which finishes the proof. ☐

4 Statement of the existence result for the hybrid model

Theorem 4.1 *Under Assumptions (A) there exists a weak solution $(\psi, \varphi_n, \varphi_p, T)$ to* (P).

The proof is done in several steps. First, we regularize the hybrid problem (P) by introducing a regularized problem (P$_M$) with regularization parameter M. Second, for solutions to (P$_M$) we derive a priori estimates and higher integrability properties for the electrostatic potential, quasi Fermi potentials, and the temperature that are independent of M. Lastly, we verify the solvability of the regularized problem using Schauder's fixed point theorem (see Section 5 and 6). We remark that the regularization of the hybrid problem (P) consists of a manipulation of the statistical relation leading to regularized densities which occur in the Poisson equation, the flux terms, reaction coefficient, and the source term of the heat equation. Hence, if one chooses $M > c_{\psi/T}$, with ψ/T from Lemma 3.4 then the manipulation of the statistical relation, of the solutions to the regularized problem, does not become active. Hence, if we verify the solvability of the regularized hybrid problem, the proof of Theorem 4.1 is completed. We further note that the regularization argument is necessary since we are not able to use the Moser iteration scheme directly for the hybrid problem (P) to obtain a priori estimates, computed in Lemma 3.4, also for the expression $\psi/\widetilde{T}$ with $\widetilde{T}$ being the frozen argument, as $\widetilde{T}$ does not satisfy the heat flow equation.

An immediate consequence of Theorem 4.1 is the following corollary.

Corollary 4.1 *We suppose in addition to Assumptions (A) that*

$$\varphi_i^D = \textit{const} \ \text{ in } \Omega_{\mathrm{Di}},\ i = n, p, \text{ and } \varphi_n^D = \varphi_p^D \ \text{ in } \Omega_{\mathrm{D}}, \tag{4.1}$$

then there exists a unique solution to problem (P). *Moreover, this solution is the thermodynamic equilibrium and has the form* $(\psi^*, \varphi_n^*, \varphi_p^*, T^*) = (\psi^*, \varphi_n^D, \varphi_p^D, T_a)$, *where* $\psi^* \in H^1(\Omega_{\mathrm{D}})$ *is the unique solution to the nonlinear Poisson equation in* Ω_{D},

$$-\nabla\cdot(\varepsilon\nabla\psi^*) = C(T_a) - N_{n0}(T_a)\exp\Big(\frac{\psi^* - \varphi_n^D - E_C(T_a)}{T_a}\Big) + N_{p0}(T_a)\exp\Big(\frac{E_V(T_a) - (\psi^* - \varphi_p^D)}{T_a}\Big),$$

with the boundary conditions $\psi^* = \psi^{D*}$ *on* I, $\varepsilon\nabla\psi^*\cdot\nu = 0$ *on* $\partial\Omega_{\mathrm{D}} \setminus I$ *where*

$$\psi^{D*} := (1-\tau)\left(\varphi_n^D + T_a \ln\frac{N_D^+(T_a)}{\widehat{N}_{n0}(T_a)} + \widehat{E}_C(T_a)\right) + \tau\left(\varphi_p^D - T_a\ln\frac{N_A^-(T_a)}{\widehat{N}_{p0}(T_a)} + \widehat{E}_V(T_a)\right).$$

Proof. Assume that the Dirichlet functions φ_i^D in Ω_{Di}, $i = n, p$, satisfy (4.1) and let $(\psi, \varphi_n, \varphi_p, T)$ be an arbitrary solution to (P) as in Theorem 4.1. Using the test function $(\varphi_n - \varphi_n^D, \varphi_p - \varphi_p^D) \in H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}}) \times H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}})$ for the equations for φ_n and φ_p we obtain

$$\begin{aligned} 0 = \int_{\Omega_{\mathrm{Dn}}} d_n(n,T)|\nabla\varphi_n|^2\,\mathrm{d}x + \int_{\Omega_{\mathrm{Dp}}} d_p(p,T)|\nabla\varphi_p|^2\,\mathrm{d}x \\ + \int_{\Omega_{\mathrm{D}}} r(n,p,T)\left(\exp\frac{\varphi_n-\varphi_p}{T} - 1\right)(\varphi_n - \varphi_p)\,\mathrm{d}x. \end{aligned}$$

Hence, the integrands in all occurring integrals are nonnegative. The positivity of d_i in Ω_{Di} for $i = n, p$ guarantees that $\nabla\varphi_i = 0$ a.e. in Ω_{Di}. Together with the prescribed boundary values, we obtain $\varphi_n = \varphi_n^D = \varphi_p^D = \varphi_p$. Therefore, all source terms in the heat flow equation (2.13) vanish. This ensures together with the Robin boundary condition that $T \equiv T_a$. Thus it remains to solve the Poisson equation where n and p on the right hand side are substituted by the statistical relation

$$n = N_{n0}(T_a)\exp\Big(\frac{\psi^* - \varphi_n^D - E_C(T_a)}{T_a}\Big), \quad p = N_{p0}(T_a)\exp\Big(\frac{E_V(T_a) - (\psi^* - \varphi_p^D)}{T_a}\Big),$$

and as Dirichlet function the function ψ^{D*} defined in Corollary 4.1 has to be used. □

5 The regularized problem (P_M)

Let $M > 0$ and $k_M(y) := \min\{\max\{y, -M\}, M\}$. Our problem reads as follows: Find $(\psi, \varphi_n, \varphi_p, T) \in \big[(\psi^D + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})) \cap L^\infty(\Omega_{\mathrm{D}})\big] \times \big[(\varphi_n^D + H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}})) \cap W^{1,s}(\Omega_{\mathrm{Dn}})\big] \times \big[(\varphi_p^D + H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}})) \cap W^{1,s}(\Omega_{\mathrm{Dp}})\big] \times$

$\{T \in H^1(\Omega) : \ln T \in L^\infty(\Omega)\}$ with

$$
\begin{aligned}
&\int_{\Omega_{\mathrm{D}}} \varepsilon \nabla\psi \cdot \nabla\overline{\psi}\,\mathsf{d}x = \int_{\Omega_{\mathrm{D}}} (C(T) - n_M + p_M)\overline{\psi}\,\mathsf{d}x \qquad \forall\overline{\psi} \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}}),\\
&\int_{\Omega_{\mathrm{Dn}}} d_n(n_M, T)\nabla\varphi_n \cdot \nabla\overline{\varphi}_n\,\mathsf{d}x + \int_{\Omega_{\mathrm{Dp}}} d_p(p_M, T)\nabla\varphi_p \cdot \nabla\overline{\varphi}_p\,\mathsf{d}x\\
&= \int_{\Omega_{\mathrm{D}}} r(n_M, p_M, T)\left(1 - \exp\frac{\varphi_n - \varphi_p}{T}\right)(\overline{\varphi}_n - \overline{\varphi}_p)\,\mathsf{d}x \quad \forall\overline{\varphi}_i \in H^1_{\mathrm{Di}}(\Omega_{\mathrm{Di}}),\ i = n, p,\\
&\int_{\Omega} \lambda\nabla T \cdot \nabla\overline{T}\,\mathsf{d}x + \int_{\Gamma} \kappa\,(T - T_a)\,\overline{T}\,\mathsf{d}\Gamma\\
&= \int_{\Omega} h_\Omega(n_M, p_M, T, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p)\overline{T}\,\mathsf{d}x \quad \forall\overline{T} \in H^1(\Omega),
\end{aligned}
\tag{P$_M$}
$$

where the regularized densities n_M and p_M have to be determined pointwise by

$$
n_M = N_{n0}\exp\left(k_M\left(\frac{\psi}{T}\right) - \frac{\varphi_n + E_C}{T}\right), \quad p_M = N_{p0}\exp\left(\frac{E_V + \varphi_p}{T} - k_M\left(\frac{\psi}{T}\right)\right). \tag{5.1}
$$

5.1 A priori estimates for the regularized problem (P_M)

Theorem 5.1 *We suppose Assumption (A). Then each weak solution $(\psi, \varphi_n, \varphi_p, T)$ to the regularized problem (P$_M$) fulfills with the exponents $s, t > 2$ from Theorem 3.1 and the constants T_a, K, c_T, $c_{\psi/T}$, $c_{\varphi,s}$, $c_{T,t}$, $c_{T,\infty}$, and $c_{\psi,\infty}$ from Assumption (A), Lemma 3.2, Lemma 3.3, Lemma 3.4, and Theorem 3.1 the estimates $T \geq T_a$ a.e. in Ω,*

$$
\begin{aligned}
&\|\varphi_i\|_{L^\infty(\Omega_{\mathrm{Di}})} \leq K, \quad \|\varphi_i\|_{W^{1,s}(\Omega_{\mathrm{Di}})} \leq c_{\varphi,s},\ i = n, p, \quad \|\psi/T\|_{L^\infty(\Omega_{\mathrm{D}})} \leq c_{\psi/T},\\
&\|T\|_{L^2(\Gamma)} \leq c_T, \quad \|T\|_{W^{1,t}(\Omega)} \leq c_{T,t}, \quad \|T\|_{L^\infty(\Omega)} \leq c_{T,\infty}, \quad \|\psi\|_{L^\infty(\Omega_{\mathrm{D}})} \leq c_{\psi,\infty}.
\end{aligned}
$$

Proof. We apply the techniques used in Section 3.

1. The estimates of Lemma 3.1 and Lemma 3.2 remain valid with the same constants for solutions to the regularized problem (P$_M$) if one substitutes $h_\Omega(n, p, T, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p)$ by $h_\Omega(n_M, p_M, T, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p)$, see especially (3.1). As a consequence, the estimates of Lemma 3.3 remain also valid with the same constants, especially $\|T\|_{L^2(\Gamma)} \leq c_T$.

2. Next we follow the proof of Lemma 3.4, use that the (regularized) right hand side of the heat equation is nonnegative and apply the estimate for $\|T\|_{L^2(\Gamma)}$. Note that instead of (3.3) we argue now with

$$
\begin{aligned}
(C - n_M + p_M)z_L^{m-1} &\leq \left(\overline{C} + N_{p0}\exp\frac{E_V + \varphi_p}{T} - k_M(\frac{\psi}{T})\right)z_L^{m-1}\\
&\leq \left(\overline{C} + N_{p0}\exp\frac{E_V + \varphi_p}{T}\right)z_L^{m-1} \leq c z_L^{m-1}.
\end{aligned}
$$

Then exactly the same arguments as in the proof of Lemma 3.4 ensure that $\|\psi/T\|_{L^\infty(\Omega_{\mathrm{D}})} \leq c_{\psi/T}$ with $c_{\psi/T}$ from Lemma 3.4.

3. Step 2, $T \geq T_a$, $\|\varphi_i\|_{L^\infty(\Omega_{\mathrm{Di}})} \leq K$ guarantee the estimates for the regularized densities

$$
\underline{c}_d \leq n_M = N_{n0}\exp\left\{k_M\left(\frac{\psi}{T}\right) - \frac{\varphi_n + E_C}{T}\right\},\ p_M = N_{p0}\exp\left\{\frac{E_V + \varphi_p}{T} - k_M\left(\frac{\psi}{T}\right)\right\} \leq \overline{c}_d
$$

a.e. in Ω_{D} (with $\underline{c}_d$, $\overline{c}_d$ defined in (3.5)) not depending on the regularization level M, which enable us to repeat all steps of the proof of Theorem 3.1 with exactly the same constants now for solutions to the regularized problem. □

6 Existence proof for the regularized problem

Theorem 6.1 *Under Assumption (A) there exists a weak solution $(\psi, \varphi_n, \varphi_p, T)$ to the regularized problem* (P_M).

Note that the constants in this section on the solvability of the regularized problem (P_M) are allowed to depend on the regularization level M.

The proof of Theorem 6.1 is based on Schauder's fixed point theorem. First, we shortly introduce the iteration scheme, then we consider relevant subproblems with frozen arguments, and finally we show the continuity of the fixed point map.

6.1 Iteration scheme

We define the non-empty, convex, bounded, closed set

$$\begin{aligned} \mathcal{N} := \Big\{ &(\varphi_n, \varphi_p, T) \in H^1(\Omega_{\mathrm{Dn}}) \times H^1(\Omega_{\mathrm{Dp}}) \times W^{1,t_M}(\Omega) : \\ &\|\varphi_n\|_{H^1(\Omega_{\mathrm{Dn}})}, \|\varphi_p\|_{H^1(\Omega_{\mathrm{Dp}})} \le c_{M,H^1}, \quad \|T\|_{W^{1,t_M}(\Omega)} \le c_{T,t_M}, \\ &-K \le \varphi_n, \varphi_p \le K, \, T \ge T_a \quad \text{a.e. in } \Omega \Big\}, \end{aligned} \tag{6.1}$$

where $c_{M,H^1} > 0$ will be defined in (6.8) and Lemma 6.2, $t_M > 2$ and $c_{T,t_M} > 0$ will be introduced in (6.10) and Lemma 6.3. We construct a fixed point map $\mathcal{Q} : \mathcal{N} \to \mathcal{N}$, $(\varphi_n, \varphi_p, T) = \mathcal{Q}(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$ by the following three steps:

1. For given $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ and τ from Subsection 2.3 we define the $H^1(\Omega_{\mathrm{D}})$ function

$$\widetilde{\psi}^D := (1-\tau)\Big(\widetilde{\varphi}_n + \widetilde{T} \ln \frac{N_D^+(\widetilde{T})}{\widehat{N}_{n0}(\widetilde{T})} + \widehat{E}_C(\widetilde{T})\Big) + \tau\Big(\widetilde{\varphi}_p - \widetilde{T} \ln \frac{N_A^-(\widetilde{T})}{\widehat{N}_{p0}(\widetilde{T})} + \widehat{E}_V(\widetilde{T})\Big) \tag{6.2}$$

and obtain by Lemma 6.1 a unique weak solution $\psi \in \widetilde{\psi}^D + H_I^1(\Omega_{\mathrm{D}})$ to the nonlinear Poisson equation

$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla \psi) &= C(\widetilde{T}) - N_{n0}(\widetilde{T}) \exp\Big(k_M\big(\frac{\psi}{\widetilde{T}}\big) - \frac{\widetilde{\varphi}_n + E_C(\widetilde{T})}{\widetilde{T}}\Big) \\ &\quad + N_{p0}(\widetilde{T}) \exp\Big(\frac{E_V(\widetilde{T}) + \widetilde{\varphi}_p}{\widetilde{T}} - k_M\big(\frac{\psi}{\widetilde{T}}\big)\Big) \quad \text{in } \Omega_{\mathrm{D}}, \\ \psi &= \widetilde{\psi}^D \quad \text{on } I, \quad \varepsilon \nabla \psi \cdot \nu = 0 \quad \text{on } \partial\Omega_{\mathrm{D}} \setminus I. \end{aligned} \tag{6.3}$$

2. We set now

$$\begin{aligned} \widetilde{n}_M &:= N_{n0}(\widetilde{T}) \exp\Big(k_M\big(\frac{\psi}{\widetilde{T}}\big) - \frac{\widetilde{\varphi}_n + E_C(\widetilde{T})}{\widetilde{T}}\Big), \\ \widetilde{p}_M &:= N_{p0}(\widetilde{T}) \exp\Big(\frac{E_V(\widetilde{T}) + \widetilde{\varphi}_p}{\widetilde{T}} - k_M\big(\frac{\psi}{\widetilde{T}}\big)\Big). \end{aligned} \tag{6.4}$$

Our regularization ensures the uniform estimates

$$\underline{c_M} \le \widetilde{n}_M, \widetilde{p}_M \le \overline{c_M}, \tag{6.5}$$

$$0 < c_{Mu} \le d_n(\widetilde{n}_M, \widetilde{T}), d_p(\widetilde{p}_M, \widetilde{T}) \le c_{Mo}. \tag{6.6}$$

Next, we solve the continuity equations for electrons and holes with frozen (regularized) coefficients $d_n(\widetilde{n}_M,\widetilde{T})$, $d_p(\widetilde{p}_M,\widetilde{T})$ and reaction rate coefficient $\widetilde{r} := r(\widetilde{n}_M,\widetilde{p}_M,\widetilde{T})$ for a weak solution (φ_n,φ_p) to

$$\begin{aligned}
&-\nabla\cdot(d_n(\widetilde{n}_M,\widetilde{T})\nabla\varphi_n) = R_\Omega(\widetilde{n}_M,\widetilde{p}_M,\widetilde{T},\varphi_n,\varphi_p) \text{ in } \Omega_{\mathrm{Dn}},\\
&[\![\varphi_n]\!] = 0 \text{ on } I_n, \quad \Big[\!\Big[d_n(\widetilde{n}_M,\widetilde{T})\nabla\varphi_n\cdot\nu_D\Big]\!\Big] = 0 \text{ on } I_n,\\
&\varphi_n = \varphi_n^D \text{ on } \Gamma_{\mathrm{Dn}}, \quad \nabla\varphi_n\cdot\nu = 0 \text{ elsewhere,}\\
&\\
&-\nabla\cdot(d_p(\widetilde{p}_M,\widetilde{T})\nabla\varphi_p) = -R_\Omega(\widetilde{n}_M,\widetilde{p}_M,\widetilde{T},\varphi_n,\varphi_p) \text{ in } \Omega_{\mathrm{Dp}},\\
&[\![\varphi_p]\!] = 0 \text{ on } I_p, \quad \Big[\!\Big[d_p(\widetilde{p}_M,\widetilde{T})\nabla\varphi_p\cdot\nu_D\Big]\!\Big] = 0 \text{ on } I_p,\\
&\varphi_p = \varphi_p^D \text{ on } \Gamma_{\mathrm{Dp}}, \quad \nabla\varphi_p\cdot\nu = 0 \text{ elsewhere.}
\end{aligned} \tag{6.7}$$

By Lemma 6.2 there exists a unique weak solution $(\varphi_n,\varphi_p) \in (\varphi_n^D + H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}})) \times (\varphi_p^D + H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}}))$ to (6.7) that satisfies the following estimates,

$$\|\varphi_i\|_{L^\infty(\Omega_{\mathrm{Di}})} \le K, \|\varphi_i\|_{H^1(\Omega_{\mathrm{Di}})} \le c_{M,H^1}, \|\varphi_i\|_{W^{1,s_M}(\Omega_{\mathrm{Di}})} \le c_{Ms}, \text{ for } i = n,p, \tag{6.8}$$

for some exponent $s_M > 2$. These estimates are uniform with respect to $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$.

3. The above estimates combined with (6.5) and (6.6) ensure that the right hand side of the heat flow equation,

$$\begin{aligned}
-\nabla\cdot(\lambda\nabla T) &= h_\Omega(\widetilde{n}_M,\widetilde{p}_M,\widetilde{T},\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p) && \text{in } \Omega\\
\lambda\nabla T\cdot\nu + \kappa(T - T_a) &= 0 && \text{on } \Gamma
\end{aligned} \tag{6.9}$$

with $h_\Omega(\widetilde{n}_M,\widetilde{p}_M,\widetilde{T},\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p)$ belongs to $L^{s_M/2}(\Omega)$ and has a uniform $L^{s_M/2}$ bound for all possible $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$. According to Lemma 6.3 there exists a unique weak solution $T \in H^1(\Omega)$ to (6.9). For some $t_M > 2$ it fulfils

$$\|T\|_{W^{1,t_M}(\Omega)} \le c_{T,t_M} \quad \text{and} \quad T \ge T_a. \tag{6.10}$$

Therefore, in summary $(\varphi_n,\varphi_p,T) = \mathcal{Q}(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$.

6.2 Solvability and properties of solutions to subproblems

Lemma 6.1 (Poisson equation) *We assume* (A). *Let* $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$ *be arbitrarily given and* $\widetilde{\psi}^D$ *be constructed by* (6.2). *Then there exists a unique weak solution* $\psi \in \widetilde{\psi}^D + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ *to the nonlinear Poisson equation* (6.3). *There is a constant* $c_{\psi,H^1} > 0$ *not depending on the choice of* $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$ *such that*

$$\|\psi\|_{H^1} \le c_{\psi,H^1}.$$

Proof. 1. Due to Assumptions (A), the function $\widetilde{\psi}^D$ representing the Dirichlet boundary conditions belongs to $H^1(\Omega_{\mathrm{D}})$, $\left\|\widetilde{\psi}^D\right\|_{H^1(\Omega_{\mathrm{D}})} \le c$ for all $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$. By the properties of the exponential function, for given $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$ the operator $B_{(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})} : \widetilde{\psi}^D + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}}) \to (H^1_{\mathrm{I}}(\Omega_{\mathrm{D}}))^*$,

$$\begin{aligned}
&\langle B_{(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})}\psi, v\rangle := \int_{\Omega_{\mathrm{D}}} \varepsilon\nabla\psi\cdot\nabla v \,\mathrm{d}x\\
&+\int_{\Omega_{\mathrm{D}}}\Big(N_{n0}(\widetilde{T})\exp\Big(k_M\big(\frac{\psi}{\widetilde{T}}\big)-\frac{\widetilde{\varphi}_n+E_C(\widetilde{T})}{\widetilde{T}}\Big)-N_{p0}(\widetilde{T})\exp\Big(\frac{E_V(\widetilde{T})+\widetilde{\varphi}_p}{\widetilde{T}}-k_M\big(\frac{\psi}{\widetilde{T}}\big)\Big) - C(\widetilde{T})\Big)v \,\mathrm{d}x,
\end{aligned}$$

$v \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$, is strongly monotone, coercive, and hemi–continuous (note that $\|\nabla\cdot\|_{L^2}$ is an equivalent norm on $H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ since $\mathrm{mes}(\mathrm{I}) > 0$). Thus, by the Browder-Minty theorem [7] the problem $B_{(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})}\psi = 0$ has a solution. Since the operator is strongly monotone, the solution $\psi \in \widetilde{\psi}^D + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ to $B_{(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})}\psi = 0$ is unique and gives us the unique weak solution to (6.3).

2. With the test function $\psi - \widetilde{\psi}^D \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ we find

$$\left\|\psi - \widetilde{\psi}^D\right\|^2_{H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})} \le c\left\|\psi - \widetilde{\psi}^D\right\|_{H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})}\left\|\widetilde{\psi}^D\right\|_{H^1(\Omega_{\mathrm{D}})} + c(M)\left\|\psi - \widetilde{\psi}^D\right\|_{L^1(\Omega_{\mathrm{D}})}.$$

Here we used the bounds for $\widetilde{\varphi}_i$, N_{i0}, E_V and E_C, and $\widetilde{T} \ge T_a$. Applying Young's inequality and the fact that $\left\|\widetilde{\psi}^D\right\|_{H^1(\Omega_{\mathrm{D}})} \le c$ we verify that $\|\psi\|_{H^1} \le c_{\psi,H^1}$ independent of the choice of $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$. $\square$

Let $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$ and let ψ be the weak solution to (6.3) and $\widetilde{n}_M$ and $\widetilde{p}_M$ be defined by (6.4). Since E_C, E_V, $\widetilde{\varphi}_n$, and $\widetilde{\varphi}_p$ have upper and lower bounds and $\widetilde{T}$ is bounded from below by T_a we obtain the estimates

$$\begin{aligned} -M - \frac{K+\overline{E}}{T_a} &\le k_M\left(\frac{\psi}{\widetilde{T}}\right) - \frac{\widetilde{\varphi}_n + E_C(\widetilde{T})}{\widetilde{T}} \le M + \frac{K+\overline{E}}{T_a},\\ -M - \frac{K+\overline{E}}{T_a} &\le \frac{E_V(\widetilde{T}) + \widetilde{\varphi}_p}{\widetilde{T}} - k_M\left(\frac{\psi}{\widetilde{T}}\right) \le M + \frac{K+\overline{E}}{T_a}. \end{aligned} \tag{6.11}$$

Since the exponential function is monotonously increasing, this estimate carries over to the corresponding exponentials which leads to the estimates for the regularized densities $\widetilde{n}_M$ and $\widetilde{p}_M$. Exploiting additionally the boundedness of the mobility functions, upper and lower bounds for the ionized dopant densities N_D^+ in Ω_{n} and N_A^- in Ω_{p} we obtain positive constants $c_{Mu},\ c_{Mo}$ such that

$$\begin{aligned} &\underline{c_M} \le \widetilde{n}_M,\ \widetilde{p}_M \le \overline{c_M} \quad \text{in } \Omega_{\mathrm{D}},\\ &0 < c_{Mu} \le \widetilde{d}_{nM} := d_n(\widetilde{n}_M,\widetilde{T}) \le c_{Mo} \quad \text{a.e. in } \Omega_{\mathrm{Dn}},\\ &0 < c_{Mu} \le \widetilde{d}_{pM} := d_p(\widetilde{p}_M,\widetilde{T}) \le c_{Mo} \quad \text{a.e. in } \Omega_{\mathrm{Dp}} \end{aligned} \tag{6.12}$$

uniformly for all $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$.

Lemma 6.2 (Continuity equations) *We assume* (A). *Let $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$ and let ψ be the weak solution to* (6.3) *and $\widetilde{n}_M$ and $\widetilde{p}_M$ be given by* (6.4). *Then there exists a unique weak solution $(\varphi_n,\varphi_p) \in (\varphi_n^D + H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}})) \times (\varphi_p^D + H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}}))$ to* (6.7). *It fulfils*

$$\|\varphi_i\|_{L^\infty(\Omega_{\mathrm{Di}})} \le K, \quad \|\varphi_i\|_{H^1(\Omega_{\mathrm{Di}})} \le c_{M,H^1}, \quad \|\varphi_i\|_{W^{1,s_M}(\Omega_{\mathrm{Di}})} \le c_{Ms}, \quad i = n,p,$$

for some exponent $s_M > 2$. The estimates and s_M are uniform with respect to $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$.

Proof. 1. We define $\rho_S : \mathbb{R}^2 \to [0,1]$ to be a fixed Lipschitz continuous function with

$$\rho_S(y,z) := \begin{cases} 0 & \text{if } \max\{|y|,|z|\} \ge S,\\ 1 & \text{if } \max\{|y|,|z|\} \le \frac{S}{2}. \end{cases}$$

and use the notation $\widetilde{d}_{nM}$ and $\widetilde{d}_{pM}$ from (6.12), and $\widetilde{r}$. Because of (6.12) the operator $A^S_{(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})} : (\varphi_n^D + H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}})) \times (\varphi^D_{\mathrm{Dp}} + H^1_D(\Omega_{\mathrm{Dp}})) \to H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}})^* \times H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}})^*$,

$$A^S_{(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})}(\varphi_n,\varphi_p) = \widehat{A}^S_{(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})}\big((\varphi_n,\varphi_p),(\varphi_n,\varphi_p)\big)$$

with the argument splitting

$$\begin{aligned} &\langle \widehat{A}^S_{(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})}\big((\varphi_n,\varphi_p),(\widehat{\varphi}_n,\widehat{\varphi}_p)\big),(\overline{\varphi}_n,\overline{\varphi}_p)\rangle :=\\ &\sum_{i=n,p}\int_{\Omega_{\mathrm{Di}}} \widetilde{d}_{iM}\nabla\widehat{\varphi}_i\cdot\nabla\overline{\varphi}_i\,\mathrm{d}x + \int_{\Omega_{\mathrm{D}}} \rho_S(\varphi_n,\varphi_p)\,\widetilde{r}\Big(\exp\frac{\varphi_n-\varphi_p}{\widetilde{T}} - 1\Big)(\overline{\varphi}_n - \overline{\varphi}_p)\,\mathrm{d}x, \end{aligned}$$

$\overline{\varphi}_i \in H^1_{\mathrm{Di}}(\Omega_{\mathrm{Di}})$, is an operator of variational type (see [15, p. 182]). Have in mind that the main part (in the arguments $\widehat{\varphi}_n$, $\widehat{\varphi}_p$) is monotone, continuous and bounded and the regularized reaction term is bounded and the mapping $(\varphi_n,\varphi_p) \mapsto \rho_S(\varphi_n,\varphi_p)\big(\exp\{\frac{\varphi_n-\varphi_p}{\widetilde{T}}\}-1\big)$ is Lipschitz continuous. Since the operator $A^S_{(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})}(\varphi_n,\varphi_p)$ additionally is coercive, the equation $A^S_{(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})}(\varphi_n,\varphi_p)=0$ has at least one solution $(\varphi_n^S,\varphi_p^S) \in (\varphi_n^D + H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}})) \times (\varphi_p^D + H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}}))$.

2. Using the test function $((\varphi_n^S-K)^+,(\varphi_p^S-K)^+) \in H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}}) \times H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}})$ for the equation $A^S_{(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})}(\varphi_n^S,\varphi_p^S)=0$ with K from Assumption (A) we obtain

$$
\begin{aligned}
0 = &\sum_{i=n,p}\int_{\Omega_{\mathrm{Di}}} \widetilde{d}_{iM}|\nabla(\varphi_i^S-K)^+|^2\,\mathrm{d}x \\
&+ \int_{\Omega_{\mathrm{D}}} \rho_S(\varphi_n^S,\varphi_p^S)\widetilde{r}\Big(\exp\frac{\varphi_n^S-\varphi_p^S}{\widetilde{T}}-1\Big)\big((\varphi_n^S-K)^+-(\varphi_p^S-K)^+\big)\,\mathrm{d}x.
\end{aligned}
$$

Discussing the four different cases $\varphi_n^S\,(\varphi_p^S) > K\,(\le K)$ we find that the integrand in the last line is always non-negative (note that ρ_S and $\widetilde{r}$ are also non-negative). Thus, (6.12) ensures that $\varphi_i^S \le K$ a.e. in Ω_{Di}, $i=n,p$. On the other hand, testing by $(-(\varphi_n^S+K)^-,-(\varphi_p^S+K)^-)$ gives $\varphi_i^S \ge -K$ a.e. in Ω_{Di}, $i=n,p$. Therefore, if we choose $S \ge 2K$, each solution to $A^S_{(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})}(\varphi_n,\varphi_p)=0$ is a weak solution to (6.7), too. The estimates of Step 2 can be done in exactly the same way but leaving out the factor ρ_S to obtain the upper and lower bounds for all weak solutions (φ_n,φ_p) to (6.7), such that $\|\varphi_i\|_{L^\infty(\Omega_{\mathrm{Di}})} \le K$, $i=n,\,p$.

3. Next, we show that there is at most one weak solution to (6.7). If there would be two different solutions (φ_n,φ_p) and $(\widehat{\varphi}_n,\widehat{\varphi}_p)$, the test function $(\varphi_n-\widehat{\varphi}_n,\varphi_p-\widehat{\varphi}_p) \in H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}}) \times H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}})$ for (6.7) yields

$$
\begin{aligned}
0 = &\sum_{i=n,p}\int_{\Omega_{\mathrm{Di}}} \widetilde{d}_{iM}|\nabla(\varphi_i-\widehat{\varphi}_i)|^2\,\mathrm{d}x \\
&+ \int_{\Omega_{\mathrm{D}}} \widetilde{r}\Big(\exp\frac{\varphi_n-\varphi_p}{\widetilde{T}}-\exp\frac{\widehat{\varphi}_n-\widehat{\varphi}_p}{\widetilde{T}}\Big)\big(\varphi_n-\varphi_p-(\widehat{\varphi}_n-\widehat{\varphi}_p)\big)\,\mathrm{d}x.
\end{aligned}
$$

Because of mes $\Gamma_{\mathrm{Di}} > 0$, (6.12), the monotonicity of the exponential function, and $\widetilde{r} \ge 0$ we obtain $(\varphi_n,\varphi_p) = (\widehat{\varphi}_n,\widehat{\varphi}_p)$.

4. Now we verify the uniform H^1 estimate for the weak solution to (6.7) by testing with $(\varphi_n-\varphi_n^D,\varphi_p-\varphi_p^D) \in H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}}) \times H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}})$, using Hölder's inequality and the fact that $\widetilde{T} \ge T_a$ and $\varphi_i \in [-K,K]$ a.e. in Ω_{Di} from Step 2:

$$
\begin{aligned}
&\sum_{i=n,p}\int_{\Omega_{\mathrm{Di}}} \widetilde{d}_{iM}|\nabla(\varphi_i-\varphi_i^D)|^2\,\mathrm{d}x + \int_{\Omega_{\mathrm{D}}} \widetilde{r}\Big(\exp\frac{\varphi_n-\varphi_p}{\widetilde{T}}-1\Big)\big(\varphi_n-\varphi_p\big)\,\mathrm{d}x \\
&\le \sum_{i=n,p}\int_{\Omega_{\mathrm{Di}}} \frac{\widetilde{d}_{iM}}{2}\big(|\nabla(\varphi_i-\varphi_i^D)|^2+|\nabla\varphi_i^D|^2\big)\,\mathrm{d}x + 2K\overline{r}(1+2\overline{c_M})\overline{c_M}^2\exp\Big\{\frac{2K}{T_a}\Big\}\,\mathrm{mes}(\Omega_{\mathrm{D}}).
\end{aligned}
$$

Exploiting again (6.12), the non-negativity of $\widetilde{r}$, the monotonicity of the exponential function, and that $\varphi_i^D \in H^1(\Omega_{\mathrm{Di}})$ are given functions, and using the constants $\overline{c_M}$ from (6.12), $\overline{r}$, and K from Assumption (A), we end up with the bounds $\|\varphi_i\|_{H^1(\Omega_{\mathrm{Di}})} \le c_{M,H^1}$, $i=n,\,p$, where the constant c_{M,H^1} does not depend on the special choice of $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$.

5. W^{1,s_M} regularity: Note that we supposed that Ω_{Di} together with the Neumann boundary $\widetilde{\Gamma}_{\mathrm{Ni}}$ are regular in the sense of Gröger. Because of (6.12) and uniform estimates for right hand sides resulting from the generation/recombination reaction in Ω_{D} for all $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$ the regularity result of Gröger [13] ensures an exponent $s_M > 2$ such that $\|\varphi_i\|_{W^{1,s_M}(\Omega_{\mathrm{Di}})} \le c_{Ms}$, $i=n,p$. These estimates are again uniform with respect to $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T}) \in \mathcal{N}$. $\square$

Lemma 6.3 (Solution to the heat flow equation) *We assume Assumption* (A). *Let* $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ *and let* ψ *be the weak solution to* (6.3) *and* (φ_n, φ_p) *be the weak solution to* (6.7). *Then there exists a unique weak solution* $T \in H^1(\Omega)$ *to* (6.9). *It fulfils* $T \geq T_a$ *a.e. in* Ω. *Moreover there is an exponent* $t_M > 2$ *and a constant* $c_{T,t_M} > 0$ *such that*

$$\|T\|_{W^{1,t_M}(\Omega)} \leq c_{T,t_M}$$

with $c_{T,t_M} > 0$ *independent of the special choice of* $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$.

Proof. The results of Lemma 6.2, (6.12) and the boundedness of $\widetilde{r}$ ensure a $c_{HM} > 0$ such that

$$\begin{aligned} &\left\| \widetilde{d}_{iM} |\nabla \varphi_i|^2 \right\|_{L^{s_M/2}(\Omega_{\mathrm{Di}})} \leq c_{HM}, \ i = n, p, \\ &\left\| \widetilde{r}\Big(\exp \frac{\varphi_n - \varphi_p}{\widetilde{T}} - 1 \Big)(\varphi_n - \varphi_p) \right\|_{L^{s_M/2}(\Omega_{\mathrm{D}})} \leq c_{HM}. \end{aligned} \tag{6.13}$$

Therefore the right hand side, $h_\Omega(\widetilde{n}_M, \widetilde{p}_M, \widetilde{T}, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p)$, of equation (6.9) has a uniformly bounded $L^{s_M/2}(\Omega)$ norm, $s_M/2 > 1$ for all $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$. Thus, the linear heat equation (6.9) with Robin boundary conditions has exactly one solution $T \in H^1(\Omega)$. We define the exponent $\widehat{s}_M$ which will also be of importance in the proof of Lemma 6.6, Step 3.

$$2 < \widehat{s}_M := \frac{4 s_M}{2 + s_M} < s_M \tag{6.14}$$

and find similar to Step 2 of the proof of Theorem 3.1 by Gröger's regularity result [13] (with $\widehat{s}_M,\ t^*_M,\ t_M$ instead of $s,\ t^*,\ t$) an exponent $t_M > 2$

$$t_M := \begin{cases} t^*_M & \text{if } \dfrac{\widehat{s}_M}{\widehat{s}_M - 2} \in \Big[1, \dfrac{2t^*_M}{t^*_M - 2}\Big] \\ \dfrac{2\widehat{s}_M}{4 - \widehat{s}_M} & \text{if } \dfrac{\widehat{s}_M}{\widehat{s}_M - 2} > \dfrac{2t^*_M}{t^*_M - 2} \end{cases}, \qquad \frac{1}{t_M} + \frac{1}{t'_M} = 1,$$

(depending only on the geometric setting and the data) and a constant $c_{T,t_M} > 0$ such that $\|T\|_{W^{1,t_M}(\Omega)} \leq c_{T,t_M}$ uniformly for all $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$. (Here we used (6.13) and that the definition of t_M guarantees that $L^{s_M/2}(\Omega) \hookrightarrow L^{\widehat{s}_M/2}(\Omega) \hookrightarrow W^{-1,t_M}(\Omega) = W^{1,t'_M}(\Omega)^*$.)

Since the right hand side of the heat equation (6.9) is nonnegative, the test of the equation by $-(T - T_a)^-$ yields the desired estimate $T \geq T_a$ a.e. in Ω. $\square$

6.3 Continuity properties of the fixed point map $\mathcal{Q}$

We prove that the fixed point map $\mathcal{Q} : \mathcal{N} \mapsto \mathcal{N}$ is continuous and completely continuous in two steps. First we verify continuity properties for the solution to the nonlinear Poisson equation with respect to the arguments $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$, see Lemma 6.4, Lemma 6.5. In the second step the continuity properties of $\mathcal{Q}$ itself are demonstrated in Lemma 6.6.

Lemma 6.4 *We assume Assumptions (A). Let* $(\widetilde{\varphi}^l_n, \widetilde{\varphi}^l_p, \widetilde{T}^l),\ (\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ *with* $\widetilde{\varphi}^l_i \rightharpoonup \widetilde{\varphi}_i$ *in* $H^1(\Omega_{\mathrm{Di}})$, $i = n, p$, *and* $\widetilde{T}^l \rightharpoonup \widetilde{T}$ *in* $W^{1,t_M}(\Omega)$. *Then the by* (6.2) *defined boundary value functions* $\widetilde{\psi}^{Dl}$, $\widetilde{\psi}^D$ *fulfil* $\widetilde{\psi}^{Dl} \rightharpoonup \widetilde{\psi}^D$ *in* $H^1(\Omega_{\mathrm{D}})$.

Proof. Note that our assumptions on $N^+_D,\ N^-_A,\ \widehat{N}_{n0},\ \widehat{N}_{p0},\ \widehat{E}_C,\ \widehat{E}_V$, and on the function τ, defined in (2.8), are tailored to guarantee this weak convergence. The parts in (6.2) with $\widetilde{\varphi}_i$ follow directly from $\widetilde{\varphi}^l_i \rightharpoonup \widetilde{\varphi}_i$ in $H^1(\Omega_{\mathrm{Di}}),\ i = n, p$. We demonstrate here exemplarily the weak convergence for the term

$$\tau \widetilde{T}^l \ln \frac{N^+_D(\widetilde{T}^l)}{\widehat{N}_{n0}(\widetilde{T}^l)} \rightharpoonup \tau \widetilde{T} \ln \frac{N^+_D(\widetilde{T})}{\widehat{N}_{n0}(\widetilde{T})} \quad \text{in } H^1(\Omega_{\mathrm{D}}).$$

The compact Sobolev embedding of $W^{1,t_M}(\Omega)$ into $L^\infty(\Omega)$ ensures $\widetilde{T}^l \to \widetilde{T}$ in $L^\infty(\Omega_{\mathrm{D}})$. Moreover, $\widetilde{T}^l \rightharpoonup \widetilde{T}$ in $W^{1,t_M}(\Omega)$ yields that $\nabla\widetilde{T}^l \rightharpoonup \nabla\widetilde{T}$ in $L^2(\Omega_{\mathrm{D}})^2$. Let $v \in H^1(\Omega_{\mathrm{D}})$ be arbitrarily given. Clearly we have

$$\int_{\Omega_{\mathrm{D}}} \tau\Big(\widetilde{T}^l \ln \frac{N_D^+(\widetilde{T}^l)}{\widehat{N}_{n0}(\widetilde{T}^l)} - \widetilde{T}\ln\frac{N_D^+(\widetilde{T})}{\widehat{N}_{n0}(\widetilde{T})}\Big) v \,\mathrm{d}x \to 0.$$

For the part with the gradients we use the following decomposition

$$\int_{\Omega_{\mathrm{D}}} \nabla\Big[\tau\Big(\widetilde{T}^l \ln \frac{N_D^+(\widetilde{T}^l)}{\widehat{N}_{n0}(\widetilde{T}^l)} - \widetilde{T}\ln\frac{N_D^+(\widetilde{T})}{\widehat{N}_{n0}(\widetilde{T})}\Big)\Big]\cdot\nabla v \,\mathrm{d}x = I_1 + I_2 + I_3,$$

where

$$I_1 := \int_{\Omega_{\mathrm{D}}} \Big(\widetilde{T}^l \ln \frac{N_D^+(\widetilde{T}^l)}{\widehat{N}_{n0}(\widetilde{T}^l)} - \widetilde{T}\ln\frac{N_D^+(\widetilde{T})}{\widehat{N}_{n0}(\widetilde{T})}\Big)\nabla\tau\cdot\nabla v \,\mathrm{d}x \to 0$$

due to $\widetilde{T}^l \to \widetilde{T}$ in $L^\infty(\Omega_{\mathrm{D}})$ and $\tau,\ v \in H^1(\Omega_{\mathrm{D}})$.

$$I_2 := \int_{\Omega_{\mathrm{D}}} \tau\Big[\ln \frac{N_D^+(\widetilde{T}^l)}{\widehat{N}_{n0}(\widetilde{T}^l)} - \ln\frac{N_D^+(\widetilde{T})}{\widehat{N}_{n0}(\widetilde{T})} + \widetilde{T}^l\Big(\ln\frac{N_D^+(\widetilde{T}^l)}{\widehat{N}_{n0}(\widetilde{T}^l)}\Big)' - \widetilde{T}\Big(\ln\frac{N_D^+(\widetilde{T})}{\widehat{N}_{n0}(\widetilde{T})}\Big)'\Big]\nabla\widetilde{T}^l\cdot\nabla v \,\mathrm{d}x \to 0$$

because of $\big\|\widetilde{T}^l\big\|_{H^1(\Omega_{\mathrm{D}})} \le c$, $v \in H^1(\Omega_{\mathrm{D}})$, $\widetilde{T}^l \to \widetilde{T}$ in $L^\infty(\Omega_{\mathrm{D}})$, and Lebesgue's theorem.

$$I_3 := \int_{\Omega_{\mathrm{D}}} \nabla(\widetilde{T}^l - \widetilde{T})\cdot\nabla v\,\tau\Big[\ln\frac{N_D^+(\widetilde{T})}{\widehat{N}_{n0}(\widetilde{T})} + \widetilde{T}\Big(\ln\frac{N_D^+(\widetilde{T})}{\widehat{N}_{n0}(\widetilde{T})}\Big)'\Big]\,\mathrm{d}x \to 0$$

since ∇v times τ times the term in the brackets can be used as test function for the weak convergence of $\nabla\widetilde{T}^l \rightharpoonup \nabla\widetilde{T}$ in $L^2(\Omega_{\mathrm{D}})^2$. $\square$

Lemma 6.5 *We assume Assumptions (A). Let $(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l)$, $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ with $\widetilde{\varphi}_i^l \rightharpoonup \widetilde{\varphi}_i$ in $H^1(\Omega_{\mathrm{Di}})$, $i = n, p$, and $\widetilde{T}^l \rightharpoonup \widetilde{T}$ in $W^{1,t_M}(\Omega)$, let ψ^l and ψ denote the corresponding unique weak solutions to* (6.3)*. Then $\psi^l \to \psi$ in $L^r(\Omega_{\mathrm{D}})$ for all $r \in [1,\infty)$.*

Proof. 1. Let ψ be the solution to (6.3) with the boundary function $\widetilde{\psi}^D$ and let $\widehat{\psi}^l \in \widetilde{\psi}^{Dl} + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ be the unique solution to the linear elliptic problem with mixed boundary conditions

$$\begin{aligned} -\nabla\cdot(\varepsilon\nabla\widehat{\psi}^l) &= C(\widetilde{T}) - N_{n0}(\widetilde{T})\exp\Big(k_M\big(\frac{\psi}{\widetilde{T}}\big) - \frac{\widetilde{\varphi}_n + E_C(\widetilde{T})}{\widetilde{T}}\Big) \\ &\quad + N_{p0}(\widetilde{T})\exp\Big(\frac{E_V(\widetilde{T}) + \widetilde{\varphi}_p}{\widetilde{T}} - k_M\big(\frac{\psi}{\widetilde{T}}\big)\Big) \quad \text{in } \Omega_{\mathrm{D}}, \\ \widehat{\psi}^l &= \widetilde{\psi}^{Dl} \quad \text{on } I, \quad \varepsilon\nabla\widehat{\psi}^l\cdot\nu = 0 \quad \text{on } \partial\Omega_{\mathrm{D}}\setminus I. \end{aligned} \tag{6.15}$$

Then $w^l := \psi - \widehat{\psi}^l$ solves the linear elliptic problem with zero right hand side and with mixed boundary conditions with the Dirichlet function $w^{Dl} = \widetilde{\psi}^D - \widetilde{\psi}^{Dl}$. The mapping which associates to the boundary value function w^{Dl} the solution $w^l \in w^{Dl} + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ of the linear elliptic problem is bounded and linear, and therefore continuous. According to [17, Prop. 4.2, p. 159] this operator is also continuous with respect to the weak topology such that $w^{Dl} \rightharpoonup 0$ in $H^1(\Omega_{\mathrm{D}})$ implies $w^l = \psi - \widehat{\psi}^l \rightharpoonup 0$ in $H^1(\Omega_{\mathrm{D}})$ and $\widehat{\psi}^l \to \psi$ in $L^2(\Omega_{\mathrm{D}})$.

2. We test (6.3) for ψ^l and (6.15) for $\widehat{\psi}^l$ by $\psi^l - \widehat{\psi}^l \in H^1_{\mathrm{D}}(\Omega_{\mathrm{D}})$ and obtain

$$\begin{aligned} &c\big\|\psi^l - \widehat{\psi}^l\big\|^2_{H^1(\Omega_{\mathrm{D}})} - \int_{\Omega_{\mathrm{D}}} (C(\widetilde{T}^l) - C(\widetilde{T}))(\psi^l - \widehat{\psi}^l)\,\mathrm{d}x \\ &\le \int_{\Omega_{\mathrm{D}}} \Big(\mathcal{U}(\psi^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) - \mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})\Big)(\psi^l - \widehat{\psi}^l)\,\mathrm{d}x \\ &= \int_{\Omega_{\mathrm{D}}} \Big(\mathcal{U}(\psi^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) - \mathcal{U}(\widehat{\psi}^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) + \mathcal{U}(\widehat{\psi}^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) - \mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})\Big)(\psi^l - \widehat{\psi}^l)\,\mathrm{d}x, \end{aligned}$$

where

$$\mathcal{U}(\psi,\varphi_n,\varphi_p,T):=N_{p0}(T)\exp\Big(\frac{E_V(T)+\varphi_p}{T}-k_M\big(\frac{\psi}{T}\big)\Big)-N_{n0}(T)\exp\Big(k_M\big(\frac{\psi}{T}\big)-\frac{\varphi_n+E_C(T)}{T}\Big).$$

Since the exponential function is monotonous we have

$$(\mathcal{U}(\psi^l,\widetilde{\varphi}_n^l,\widetilde{\varphi}_p^l,\widetilde{T}^l)-\mathcal{U}(\widehat{\psi}^l,\widetilde{\varphi}_n^l,\widetilde{\varphi}_p^l,\widetilde{T}^l))(\psi^l-\widehat{\psi}^l)\le 0.$$

Moreover, using the assumptions on E_C, E_V, N_{n0}, N_{p0} and the fact that the triples $(\widetilde{\varphi}_n^l,\widetilde{\varphi}_p^l,\widetilde{T}^l)$, $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})\in\mathcal{N}$ we estimate

$$|\mathcal{U}(\widehat{\psi}^l,\widetilde{\varphi}_n^l,\widetilde{\varphi}_p^l,\widetilde{T}^l)-\mathcal{U}(\psi,\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})|\le c_M(|\widehat{\psi}^l-\psi|+|\widetilde{\varphi}_n^l-\widetilde{\varphi}_n|+|\widetilde{\varphi}_p^l-\widetilde{\varphi}_p|+|\widetilde{T}^l-\widetilde{T}|).$$

These arguments ensure the estimate,

$$\begin{aligned}\left\|\psi^l-\widehat{\psi}^l\right\|^2_{H^1(\Omega_{\mathrm{D}})}\le c_M\Big(\left\|\widehat{\psi}^l-\psi\right\|_{L^2(\Omega_{\mathrm{D}})}+\left\|\widetilde{\varphi}_n^l-\widetilde{\varphi}_n\right\|_{L^2(\Omega_{\mathrm{D}})}\\ +\left\|\widetilde{\varphi}_p^l-\widetilde{\varphi}_p\right\|_{L^2(\Omega_{\mathrm{D}})}+\left\|\widetilde{T}^l-\widetilde{T}\right\|_{L^2(\Omega_{\mathrm{D}})}\Big)\left\|\psi^l-\widehat{\psi}^l\right\|_{L^2(\Omega_{\mathrm{D}})},\end{aligned}$$

which leads because of Step 1 and $\widetilde{\varphi}_n^l\to\widetilde{\varphi}_n$, $\widetilde{\varphi}_p^l\to\widetilde{\varphi}_p$, $\widetilde{T}^l\to\widetilde{T}$ in $L^2(\Omega_{\mathrm{D}})$ to the convergence $\psi^l-\widehat{\psi}^l\to 0$ in $H^1(\Omega_{\mathrm{D}})$. Therefore, also $\psi^l-\widehat{\psi}^l\rightharpoonup 0$ as $l\to\infty$, which together with $\widehat{\psi}^l\rightharpoonup\psi$ in $H^1(\Omega_{\mathrm{D}})$ from Step 1 ensures $\psi^l\rightharpoonup\psi$ in $H^1(\Omega_{\mathrm{D}})$ and thus, $\psi^l\to\psi$ in $L^r(\Omega_{\mathrm{D}})$ for all $r\in[1,\infty)$ as $l\to\infty$. □

Lemma 6.6 *We assume Assumptions (A). Then the map $\mathcal{Q}:\mathcal{N}\to\mathcal{N}$ is completely continuous.*

Proof. 1. Let $(\widetilde{\varphi}_n^l,\widetilde{\varphi}_p^l,\widetilde{T}^l)$, $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})\in\mathcal{N}$ with $\widetilde{\varphi}_i^l\rightharpoonup\widetilde{\varphi}_i$ in $H^1(\Omega_{\mathrm{Di}})$, $i=n,p$, and $\widetilde{T}^l\rightharpoonup\widetilde{T}$ in $W^{1,t_M}(\Omega)$, let ψ^l and ψ denote the corresponding unique weak solutions to (6.3), and let $\widetilde{n}_M^l$, $\widetilde{n}_M$, $\widetilde{p}_M^l$, $\widetilde{p}_M$ be the corresponding quantities in (6.4). We have to show that $(\varphi_n^l,\varphi_p^l,T^l):=\mathcal{Q}(\widetilde{\varphi}_n^l,\widetilde{\varphi}_p^l,\widetilde{T}^l)\to(\varphi_n,\varphi_p,T):=\mathcal{Q}(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})$ in $H^1(\Omega_{\mathrm{Dn}})\times H^1(\Omega_{\mathrm{Dp}})\times W^{1,t_M}(\Omega)$.

The assumed weak convergences guarantee $\widetilde{\varphi}_i^l\to\widetilde{\varphi}_i$ in $L^r(\Omega_{\mathrm{Di}})$, $i=n,p$, and $\widetilde{T}^l\to\widetilde{T}$ in $L^r(\Omega)$ for all $r\in[1,\infty)$. Lemma 6.5 ensures that also $\psi^l\to\psi$ in $L^r(\Omega_{\mathrm{D}})$, $r\in[1,\infty)$. Therefore the Assumptions (A), (6.11) and the lower bound for the temperatures yield the convergences

$$\begin{aligned}&\widetilde{n}_M^l:=N_{n0}(\widetilde{T}^l)\exp\Big(k_M\big(\frac{\psi^l}{\widetilde{T}^l}\big)-\frac{\widetilde{\varphi}_n^l+E_C(\widetilde{T}^l)}{\widetilde{T}^l}\Big)\to\widetilde{n}_M,\\&\widetilde{p}_M^l:=N_{p0}(\widetilde{T}^l)\exp\Big(\frac{E_V(\widetilde{T}^l)+\widetilde{\varphi}_p^l}{\widetilde{T}^l}-k_M\big(\frac{\psi^l}{\widetilde{T}^l}\big)\Big)\to\widetilde{p}_M,\\&\mu_n(\widetilde{T}^l,\widetilde{n}_M^l)\to\mu_n(\widetilde{T},\widetilde{n}_M),\quad\mu_p(\widetilde{T}^l,\widetilde{p}^l)\to\mu_p(\widetilde{T},\widetilde{p}_M)\quad\text{in } L^r(\Omega_{\mathrm{D}}),\\&N_D^+(\widetilde{T}^l)\to N_D^+(\widetilde{T}),\quad\mu_n(\widetilde{T}^l,N_D^+(\widetilde{T}^l))\to\mu_n(\widetilde{T},N_D^+(\widetilde{T}))\quad\text{in } L^r(\Omega_{\mathrm{n}}),\\&N_A^-(\widetilde{T}^l)\to N_A^-(\widetilde{T}),\quad\mu_p(\widetilde{T}^l,N_A^-(\widetilde{T}^l))\to\mu_p(\widetilde{T},N_A^-(\widetilde{T}))\quad\text{in } L^r(\Omega_{\mathrm{p}}),\quad r\in[1,\infty).\end{aligned}$$

Moreover, our Assumptions (A) additionally ensure the following convergences,

$$\begin{aligned}&\widetilde{d}_{nM}^l:=d_n(\widetilde{n}_M^l,\widetilde{T}^l)\to\widetilde{d}_{nM}\ \text{ in } L^r(\Omega_{\mathrm{Dn}}),\ \widetilde{d}_{pM}^l:=d_p(\widetilde{p}_M^l,\widetilde{T}^l)\to\widetilde{d}_{pM}\ \text{ in } L^r(\Omega_{\mathrm{Dp}}),\\&\widetilde{r}^l:=r(\widetilde{n}_M^l,\widetilde{p}_M^l,\widetilde{T}^l)\to\widetilde{r}\ \text{ in } L^r(\Omega_{\mathrm{D}}),\quad r\in[1,\infty).\end{aligned}\tag{6.16}$$

2. With the test function $(\varphi_n^l-\varphi_n,\varphi_p^l-\varphi_p)\in H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}})\times H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}})$ for (6.7) we obtain

$$\begin{aligned}&\sum_{i=n,p}\int_{\Omega_{\mathrm{Di}}}\big\{\widetilde{d}_{iM}^l\nabla\varphi_i^l-\widetilde{d}_{iM}\nabla\varphi_i\big\}\cdot\nabla(\varphi_i^l-\varphi_i)\,\mathrm{d}x\\&=\int_{\Omega_{\mathrm{D}}}\Big(\widetilde{r}\Big(\exp\frac{\varphi_n-\varphi_p}{\widetilde{T}}-1\Big)-\widetilde{r}^l\Big(\exp\frac{\varphi_n^l-\varphi_p^l}{\widetilde{T}^l}-1\Big)\Big)\Big(\varphi_n^l-\varphi_n-\varphi_p^l+\varphi_p\Big)\,\mathrm{d}x.\end{aligned}\tag{6.17}$$

We use the decomposition

$$\widetilde{d}^l_{iM}\nabla\varphi^l_i = \widetilde{d}^l_{iM}\nabla(\varphi^l_i-\varphi_i)+\widetilde{d}^l_{iM}\nabla\varphi_i\,,$$

$$\begin{aligned}\widetilde{r}^l\exp\frac{\varphi^l_n-\varphi^l_p}{\widetilde{T}^l} &= (\widetilde{r}^l-\widetilde{r})\exp\frac{\varphi^l_n-\varphi^l_p}{\widetilde{T}^l}\\ &\quad+\widetilde{r}\Big[\exp\frac{\varphi^l_n-\varphi^l_p}{\widetilde{T}^l}-\exp\frac{\varphi^l_n-\varphi^l_p}{\widetilde{T}}\Big]+\widetilde{r}\exp\frac{\varphi^l_n-\varphi^l_p}{\widetilde{T}}\end{aligned}$$

and take into account that $\widetilde{T},\,\widetilde{T}^l\ge T_a$ and $\varphi^l_i,\varphi_i\in[-K,K]$ a.e. in $\Omega_{\rm Di}$ by Lemma 6.2 such that $\exp\frac{\varphi^l_n-\varphi^l_p}{\widetilde{T}^l}\le c$. Additionally we exploit that the mapping $(\varphi_n,\varphi_p,T)\mapsto\exp\frac{\varphi_n-\varphi_p}{T}$ is Lipschitz continuous on $[-K,K]^2\times[T_a,\infty)$. Moreover, by Lemma 6.2 we have $\|\varphi_i\|_{W^{1,s_M}(\Omega_{\rm Di})}\le c_{Ms}$, $i=n,p$. We define the exponent $r_M:=\frac{2s_M}{s_M-2}$. In summary, because of (6.12) and mes$(\Gamma_{\rm Di})>0$ it results from (6.17) by Hölder's inequality

$$\begin{aligned}&c\sum_{i=n,p}\Big\|\varphi^l_i-\varphi_i\Big\|^2_{H^1(\Omega_{\rm Di})}+\int_{\Omega_{\rm D}}\widetilde{r}\Big(\exp\frac{\varphi^l_n-\varphi^l_p}{\widetilde{T}}-\exp\frac{\varphi_n-\varphi_p}{\widetilde{T}}\Big)\Big(\varphi^l_n-\varphi_n-\varphi^l_p+\varphi_p\Big)\,\mathrm{d}x\\ &\quad\le c\sum_{i=n,p}\Big\|\nabla(\varphi^l_i-\varphi_i)\Big\|_{L^2(\Omega_{\rm Di})}\Big\|\widetilde{d}^l_{iM}-\widetilde{d}_{iM}\Big\|_{L^{r_M}(\Omega_{\rm Di})}\|\nabla\varphi_i\|_{L^{s_M}(\Omega_{\rm Di})}\\ &\quad\quad+c\sum_{i=n,p}\Big\|\varphi^l_i-\varphi_i\Big\|_{L^2(\Omega_{\rm Di})}\Big(\Big\|\widetilde{r}^l-\widetilde{r}\Big\|_{L^2(\Omega_{\rm D})}+\Big\|\widetilde{T}^l-\widetilde{T}\Big\|_{L^2(\Omega)}\Big).\end{aligned}$$

The integral in the first line is nonnegative. Applying Sobolev's embedding, Young's inequality, the convergences obtained in (6.16) and $\widetilde{T}^l\to\widetilde{T}$ in $L^2(\Omega)$, as well as the bound for $\|\varphi_i\|_{W^{1,s_M}(\Omega_{\rm Di})}$, it follows $\big\|\varphi^l_i-\varphi_i\big\|_{H^1(\Omega_{\rm Di})}\to 0$, $i=n,p$.

3. It remains to show for the corresponding solutions to (6.9) that $T^l\to T\in W^{1,t_M}(\Omega)$. Our construction of $t_M>2$ in Lemma 6.3 ensures the embedding $L^{\widehat{s}_M/2}(\Omega)\hookrightarrow W^{-1,t_M}(\Omega)=W^{1,t'_M}(\Omega)^*$, where $\frac{1}{t_M}+\frac{1}{t'_M}=1$. The result of Gröger [13] for the linear heat equation guarantees the estimate,

$$\Big\|T^l-T\Big\|_{W^{1,t_M}(\Omega)}\le c\Big\|\widetilde{h}^l_\Omega-\widetilde{h}_\Omega\Big\|_{W^{1,t_M'}(\Omega)^*}\le c\Big\|\widetilde{h}^l_\Omega-\widetilde{h}_\Omega\Big\|_{L^{\widehat{s}_M/2}(\Omega)}\tag{6.18}$$

where we defined $\widetilde{h}^l_\Omega:=h_\Omega(\widetilde{n}^l_M,\widetilde{p}^l_M,\widetilde{T}^l,\nabla\varphi^l_n,\nabla\varphi^l_p,\varphi^l_n,\varphi^l_p)$ and, in a similar fashion, we defined $\widetilde{h}_\Omega:=h_\Omega(\widetilde{n}_M,\widetilde{p}_M,\widetilde{T},\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p)$. According to Assumptions (A), the boundedness of the potentials, the lower bound for the temperature, and the convergences of Step 1 we find

$$\widetilde{r}^l\Big(\exp\frac{\varphi^l_n-\varphi^l_p}{\widetilde{T}^l}-1\Big)(\varphi^l_n-\varphi^l_p)\to\widetilde{r}\Big(\exp\frac{\varphi_n-\varphi_p}{\widetilde{T}}-1\Big)(\varphi_n-\varphi_p)\quad\text{in } L^r(\Omega_{\rm D}),\quad r\in[1,\infty).$$

Furthermore, we use the decomposition

$$\widetilde{d}^l_{iM}|\nabla\varphi^l_i|^2-\widetilde{d}_{iM}|\nabla\varphi_i|^2=(\widetilde{d}^l_{iM}-\widetilde{d}_{iM})|\nabla\varphi^l_i|^2+\widetilde{d}_{iM}\big(\nabla\varphi^l_i\cdot\nabla(\varphi^l_i-\varphi_i)+\nabla\varphi_i\cdot\nabla(\varphi^l_i-\varphi_i)\big),$$

$i=n,p$, to continue estimate (6.18) by using Hölder's inequality (note that due to the definition of $\widehat{s}_M$ in (6.14) we have $2/\widehat{s}_M=1/r_M+2/s_M$ for $r_M=2s_M/(s_M-2)$ and $2/\widehat{s}_M=1/s_M+1/2$)

$$\begin{aligned}&\Big\|T^l-T\Big\|_{W^{1,t_M}(\Omega)}\\ &\le\sum_{i=n,p}\Big\{c\Big\|\widetilde{d}^l_{iM}-\widetilde{d}_{iM}\Big\|_{L^{r_M}(\Omega_{\rm Di})}\Big\|\nabla\varphi^l_i\Big\|^2_{L^{s_M}(\Omega_{\rm Di})}\\ &\quad+c\big(\Big\|\nabla\varphi^l_i\Big\|_{L^{s_M}(\Omega_{\rm Di})}+\|\nabla\varphi_i\|_{L^{s_M}(\Omega_{\rm Di})}\big)\Big\|\nabla(\varphi^l_i-\varphi_i)\Big\|_{L^2(\Omega_{\rm Di})}\Big\}\\ &\quad+c\Big\|\widetilde{r}^l\Big(\exp\frac{\varphi^l_n-\varphi^l_p}{\widetilde{T}^l}-1\Big)(\varphi^l_n-\varphi^l_p)-\widetilde{r}\Big(\exp\frac{\varphi_n-\varphi_p}{\widetilde{T}}-1\Big)(\varphi_n-\varphi_p)\Big\|_{L^{\widehat{s}_M/2}(\Omega)},\end{aligned}$$

which proves the strong convergence of $T^l\to T$ in $W^{1,t_M}(\Omega)$ and finishes the proof. □

6.4 Proof of Theorem 6.1

The set $\mathcal{N}$ is nonempty, convex, and closed in $H^1(\Omega_{\mathrm{Dn}}) \times H^1(\Omega_{\mathrm{Dp}}) \times W^{1,t_M}(\Omega)$. Thus, because of Lemma 6.6, Schauder's fixed point theorem ensures the existence of a fixed point $(\varphi_n, \varphi_p, T) \in \mathcal{N}$ of $\mathcal{Q}$. For this fixed point we solve according to Lemma 6.1 the problem $B_{(\varphi_n,\varphi_p,T)}\psi = 0$ and obtain $\psi \in H^1(\Omega_{\mathrm{D}})$. It remains to show that the quadruple $(\psi, \varphi_n, \varphi_p, T)$ lays in the correct spaces in the sense of (P$_M$).

By the definition of $\mathcal{N}$ we find that $T \in \{u \in H^1(\Omega) : \ln u \in L^\infty(\Omega)\}$. Since $(\varphi_n, \varphi_p, T)$ is a fixed point of $\mathcal{Q}$, the regularized continuity equations (middle equation in (P$_M$)) hold true and Step 2 of the proof of Lemma 3.2 done for the hybrid model can be applied with the same constants for the regularized situation if one substitutes h_{D} by h_{DM}, see especially (3.1). Therefore, the estimates of Lemma 2.3, now for the heat equation with the regularized right hand side remain valid with the same constants, especially $\|T\|_{L^2(\Gamma)} \le c_T$.

Since $(\varphi_n, \varphi_p, T)$ is a fixed point of $\mathcal{Q}$, Lemma 6.2 guarantees $\varphi_i \in W^{1,s_M}(\Omega_{\mathrm{Di}}),\ i = n, p$. Moreover, the Poisson equation and the heat equation (first and last equation in (P$_M$)) are simultaneously fulfilled. Therefore we can apply the technique of the proof of Lemma 3.4 (see also Step 2 of the proof of Theorem 5.1) to obtain an L^∞ estimate for ψ/T with exactly the same bound $c_{\psi/T}$. Now we proceed as in Step 3 of the proof of Theorem 5.1 and repeat all steps of the proof of Theorem 3.1 to ensure that $\varphi_i \in W^{1,s}(\Omega_{\mathrm{Di}}),\ i = n, p$.

Thus, $(\psi, \varphi_n, \varphi_p, T)$ is a solution to problem (P$_M$) which proves Theorem 6.1. □

7 Conclusions

We proved existence of a solution of a hybrid model for the electro-thermal behavior of semiconductor heterostructures. The hybrid model couples a drift-diffusion type electro-thermal model with thermistor type models in different subregions of the semiconductor device. For the proof we employed a regularization technique and Schauder's fixed point theorem. Additionally, for boundary data compatible with thermodynamic equilibrium we verified uniqueness as well.

The method of the existence proof of the paper allows also to treat structures with more than one, not directly adjacent, differently strongly n-doped or p-doped regions. Moreover, the technique can also be adapted to the setting of unipolar devices where no Ω_{p} or no Ω_{n} is present. Additionally, since in the unipolar drift-diffusion setting no generation/recombination of electrons and holes takes place, the governing equations become simpler to treat.

References

[1] G. Albinus, H. Gajewski, and R. Hünlich, *Thermodynamic design of energy models of semiconductor devices*, Nonlinearity **15** (2002), 367–383.

[2] U. Bandelow, H. Gajewski, and R. Hünlich, *Thermodynamics-based modelling of edge-emitting quantum well lasers*, Optoelectronic devices: Advanced simulation and analysis (J. Piprek, ed.), Springer, 2005, pp. 63–85.

[3] M. Bulíček, A. Glitzky, and M. Liero, *Systems describing electrothermal effects with $p(x)$-Laplace like structure for discontinuous variable exponents*, SIAM J. Math. Analysis **48** (2016), 3496–3514.

[4] ______, *Thermistor systems of $p(x)$-Laplace-type with discontinuous exponents via entropy solutions*, DCDS-S **10** (2017), 697–713.

[5] A. Fischer, T. Koprucki, K. Gärtner, J. Brückner, B. Lüssem, K. Leo, A. Glitzky, and R. Scholz, *Feel the heat: Nonlinear electrothermal feedback in organic LEDs*, Adv. Funct. Mater. **24** (2014), 3367–3374.

[6] A. Fischer, M. Pfalz, K. Vandewal, M. Liero, A. Glitzky, S. Lenk, and S. Reineke, *Full electrothermal OLED model including nonlinear self-heating effects*, Phys. Rev. Applied **10** (2018), 014023.

[7] H. Gajewski, K. Gröger, and K. Zacharias, *Nichtlineare Operatorgleichungen und Operatordifferentialgleichungen*, Akademie-Verlag, Berlin, 1974.

[8] A. Glitzky and R. Hünlich, *Stationary solutions of two-dimensional heterogeneous energy models with multiple species*, Banach Center Publ. **66** (2004), 135–151.

[9] ______, *Stationary energy models for semiconductor devices with incompletely ionized impurities*, Z. Angew. Math. Mech. **85** (2005), 778–792.

[10] ______, *Stationary solutions to an energy model for semiconductor devices where the equations are defined on different domains*, Math. Nachr. **281** (2008), 1676–1693.

[11] A. Glitzky, M. Liero, and G. Nika, *An existence result for a class of electrothermal drift-diffusion models with Gauss–Fermi statistics for organic semiconductor devices*, WIAS-Preprint 2593, Berlin, 2019.

[12] J. A. Griepentrog, *An application of the implicit function theorem to an energy model of the semiconductor theory*, Z. Angew. Math. Mech. **79** (1999), 43–51.

[13] K. Gröger, *A $W^{1,p}$–estimate for solutions to mixed boundary value problems for second order elliptic differential equations*, Math. Ann. **283** (1989), 679–687.

[14] M. Kantner, *Generalized Scharfetter–Gummel schemes for electro-thermal transport in degenerate semiconductors using the Kelvin formula for the Seebeck coefficient*, WIAS-Preprint 2605, Berlin, 2019.

[15] J. L. Lions, *Quelques méthodes de rèsolution des problémes aux limites non linéaires*, Dunod Gauthier-Villars, Paris, 1969.

[16] A. Mielke, *A gradient structure for reaction-diffusion systems and for energy-drift-diffusion systems*, Nonlinearity **24** (2011), 1329–1346.

[17] T. J. Morrison, *Functional analysis: An introduction to Banach space theory*, J. Wiley & Sons, New York, 2000.

[18] S. M. Sze and Kwok K. Ng, *Physics of semiconductor devices*, John Wiley & Sons Inc., 2007.