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Abstract

We derive and investigate a stationary model for the electrothermal behavior of organic thin-film devices including their electrical and thermal environment. Whereas the electrodes are modeled by Ohm's law, the electronics of the organic device itself is described by a generalized van Roosbroeck system with temperature dependent mobilities and using Gauss–Fermi integrals for the statistical relation. The currents give rise to Joule heat which together with the heat generated by the generation/recombination of electrons and holes in the organic device occur as source terms in the heat flow equation that has to be considered on the whole domain.

The crucial task is to establish that the quantities in the transfer conditions at the interfaces between electrodes and the organic semiconductor device have sufficient regularity. Therefore, we restrict the analytical treatment of the system to two spatial dimensions. We consider layered organic structures, where the physical parameters (total densities of transport states, LUMO and HOMO energies, disorder parameter, basic mobilities, activation energies, relative dielectric permittivity, heat conductivity) are piecewise constant, and we work in a $W^{1,q}$ setting for some $q > 2$. We prove the existence of weak solutions using Schauder's fixed point theorem and a regularity result for strongly coupled systems with nonsmooth data and mixed boundary conditions that is verified by Caccioppoli estimates and a Gehring-type lemma.

1 Introduction

The charge transport in organic semiconductors is realized by hopping processes [15, 28], that are intensified if the temperature is raising meaning that the conductivity is increasing for higher temperatures. On the other hand, the Joule heat due to electrical current leads to a self-heating of the device. This interplay of electronic transport and heat flow results in a complex, nonlinear behavior of organic semiconductor devices. E.g., organic LEDs possess S-shaped current-voltage relations with regions of negative resistance (see [4, 13, 14]). The modeling and simulation of the electrothermal behavior of spatially resolved organic devices is done at different levels (i) simulation based on coupled electrical and thermal networks as performed in [4], or via macroscopic PDE models (ii) using $p(x)$ -Laplace thermistor models, comp. e.g., [18, 17] or (iii) by so called energy-drift-diffusion systems, where a generalized van Roosbroeck system is coupled to the heat equations, see, e.g., [1, 5, 10]. Additional thermoelectric effects (Peltier, Thomson, and Seebeck) are not included in this model. In [16, 23, Sec. II.D] it is argued that in the case of organic semiconductors such effects are negligible as the thermal voltages are small compared to the applied voltage. Moreover, in comparison to classical inorganic semiconductors, adapted statistical relations taking into account the disorder of the organic material and obtained by Gauss-Fermi integrals, specific mobility laws, and a generalized Einstein relation between mobility and diffusivity have to be used.

Experimental findings in [13] impressively demonstrate that the thermal environment enormously influences the electrothermal interplay and the behavior of the device, see also [23, 24, 26]. To study two

different cooling regimes of the device, in one version of the structure, a layer of the poor heat conductor poly(methyl methacrylate) (PMMA) was sandwiched between the substrate and a cooling copper block, see [13, Fig. 3]. For the structure with the additional PMMA layer, the current-voltage relation shows a turnover point at lower current density and voltage. The PMMA functions as a significant vertical heat barrier that prevents heat from leaving the device, the OLED gets a more pronounced temperature increase with respect to the device placed directly onto the copper support and driven with the same supply current. Its electrical conductivity rises more rapidly, which explains its shifted current-voltage curve in [13, Fig. 4]. These non-linear switching effects cannot be ignored also with respect to the long-term operation and stability of OLEDs. Moreover, they are important for the understanding of sudden-death scenarios as investigated in [14].

In the present paper, we study the electrothermal behavior of the organic device together with its thermal environment and follow the energy-drift-diffusion approach. We take into account the Gauss-Fermi integrals (see [21]) for the statistical relation between charge carrier densities and chemical potentials. But instead of the full Extended Gaussian Disorder Model (EGDM) mobility ansatz that contains a temperature, density and electric field strength dependent mobility, see [22], we concentrate in our paper on the temperature dependency of the mobility and model it by an Arrhenius law (this results from a linearization of the pure temperature dependent term in the EGDM mobility). For the analytical treatment of the full EGDM mobility (for a unified domain), see e.g. [10].

1.1 Geometrical setting and model equations

We consider an electrothermal model for an organic thin-film device occupying the domain Ω^{dev} . It is mounted on a glass substrate Ω^{sub} (see Fig. 1), where only heat conduction takes place. The whole domain $\bar{\Omega} = \bar{\Omega}^{\text{dev}} \cup \bar{\Omega}^{\text{sub}}$ is the union of the actual device and the substrate domains. The electrically active region Ω^{dev} consists of M (disjoint) layers Ω^i such that $\bar{\Omega}^{\text{dev}} = \cup_{i=1}^M \bar{\Omega}^i$. The top and bottom layers Ω^M and Ω^1 correspond to well-conducting metal electrodes with various organic layers sandwiched in between, i.e., $\bar{\Omega}^{\text{org}} = \cup_{i=2}^{M-1} \bar{\Omega}^i$ denotes the stack of organic materials. We emphasize that we include the thermal (substrate plus metal electrodes) and electric environment (metal electrodes) of the organic layers into the model frame (in contrast to [10], where only the organic layers are considered). This means, in particular, that we have to take transfer conditions between the subdomains into account.

We assume the following layered geometric structure: The device domain $\Omega^{\text{dev}} = \omega \times (0, h)$, with cross-section ω , satisfies $\Gamma_0 := \omega \times \{0\} \subset \partial\Omega^{\text{sub}}$, i.e., it is mounted directly on top of the glass substrate. Of the M layers of the device Ω^{dev} , each has a thickness $h^i > 0$ such that the total thickness of the device is given by $h = \sum_{i=1}^M h^i$ (see Fig. 1). We put $\hat{h}^0 := 0$ and $\hat{h}^i := \sum_{l=1}^i h^l$, for $i = 1, \dots, M$, to denote the cumulative height of the device and define the subsets corresponding to the layers

$$\Omega^i = \omega \times (\hat{h}^{i-1}, \hat{h}^i) \subset \Omega^{\text{dev}}, \quad \text{for } i = 1, \dots, M.$$

We now introduce the system of coupled equations in the various subdomains:

In the metal electrodes Ω^1 and Ω^M , the charge and heat transport is described by the current and heat equations for the metal Fermi potential φ_m and the temperature T

$$\nabla \cdot \mathbf{j}_m = 0 \quad \text{with} \quad \mathbf{j}_m = -\kappa \nabla \varphi_m, \quad \text{and} \quad -\nabla \cdot (\lambda \nabla T) = \kappa |\nabla \varphi_m|^2 \quad (1.1)$$

with electrical and thermal conductivities κ and λ .

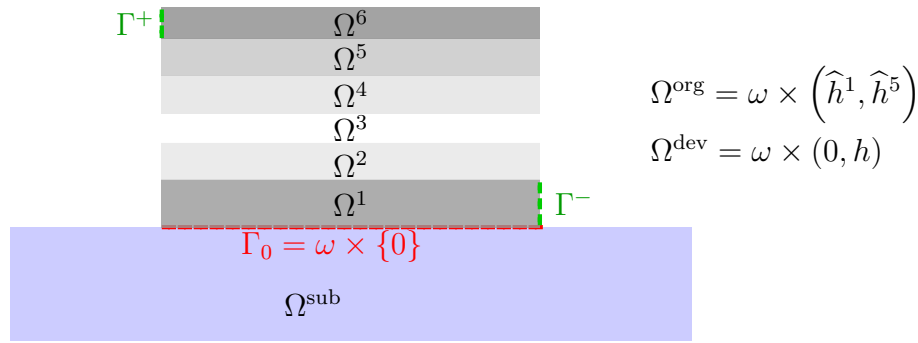


Figure 1: Sketch of the domain Ω consisting of the glass substrate Ω^{sub} and the thin-film device Ω^{dev} . The latter is composed of 6 layers in this picture. The bottom and top layer Ω^1 and Ω^6 represent the electrodes with Dirichlet boundaries Γ^- and Γ^+ (green) for the Fermi potential where the voltage is applied. The device Ω^{dev} is mounted on the surface Γ_0 of the glass substrate Ω^{sub} .

In the organic subdomain Ω^{org} , we assume an electrothermal drift-diffusion system, describing the charge and heat transport. It consists of a generalized van Roosbroeck system (see e.g. [2]), formulated in the quasi-Fermi potentials φ_n, φ_p of electrons and holes and the electrostatic potential ψ , coupled to the heat equation for the temperature T . Hence, we consider in Ω^{org} the system

$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla \psi) &= C - n + p, \\ \nabla \cdot j_n &= R, \quad j_n = -n\mu_n(T)\nabla \varphi_n, \\ -\nabla \cdot j_p &= R, \quad j_p = -p\mu_p(T)\nabla \varphi_p, \quad R = r_0(n, p, T)np \left(1 - \exp \frac{\varphi_n - \varphi_p}{T}\right), \\ -\nabla \cdot (\lambda \nabla T) &= n\mu_n(T)|\nabla \varphi_n|^2 + p\mu_p(T)|\nabla \varphi_p|^2 + R(\varphi_p - \varphi_n). \end{aligned} \quad (1.2)$$

The dielectric permittivity is denoted by ε . The mobilities μ_n and μ_p of electrons and holes in organic materials are increasing with temperature. We model this behavior by an Arrhenius law and assume

$$\mu_j = \mu_{j0}^i B_{j0}^i \exp \left\{ -\frac{a_j^i}{T} \right\} \text{ in } \Omega^i \text{ with positive constants } B_{j0}^i, a_j^i, \mu_{j0}^i > 0,$$

where $i = 2, \dots, M-1, j = n, p$.

The total densities of transport states $N_{n0}^i, N_{p0}^i > 0$, the energy levels E_L^i and E_H^i (related to the so called LUMO and HOMO energies), as well as the disorder parameters σ_n^i , and σ_p^i , for $i = 2, \dots, M-1$, give rise to the statistical relation between the quasi-Fermi potentials φ_n and φ_p and the densities n and p of electrons and holes in the various organic layers, namely

$$n = N_{n0}^i \mathcal{G} \left(\frac{\psi - \varphi_n - E_L^i}{T}, \frac{\sigma_n^i}{T} \right), \quad p = N_{p0}^i \mathcal{G} \left(\frac{E_H^i - \psi + \varphi_p}{T}, \frac{\sigma_p^i}{T} \right) \text{ in } \Omega^i, \quad (1.3)$$

where the function \mathcal{G} is given by the Gauss–Fermi integral, see [21],

$$\mathcal{G}(\eta, z) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp \left(-\frac{\xi^2}{2} \right) \frac{1}{\exp(z\xi - \eta) + 1} d\xi.$$

In the glass substrate Ω^{sub} , we only have to solve the heat equation without any sources

$$-\nabla \cdot (\lambda \nabla T) = 0. \quad (1.4)$$

Having formulated the equations in the various bulk domains, we have to couple them via suitable interface conditions. Moreover, we complement the system by boundary conditions:

On the electrode-organic semiconductor interface, $I := (\overline{\Omega^1} \cap \overline{\Omega^2}) \cup (\overline{\Omega^{M-1}} \cap \overline{\Omega^M})$, we assume that the metal Fermi potential φ_m splits up into the quasi-Fermi potentials φ_n and φ_p of electrons and holes. We suppose that the contact between the electrodes and the organic layers is Ohmic (see e.g. [25, Chap. 6]). Thus, at the interface I we have

$$\varphi_m|_I = \varphi_n|_I = \varphi_p|_I. \quad (1.5a)$$

Moreover, denoting by ν_{org} the outer unit normal vector to the domain Ω^{org} , we assume that the net normal current across the metal-semiconductor interface is continuous

$$j_m \cdot \nu_{\text{org}} = (j_n + j_p) \cdot \nu_{\text{org}}. \quad (1.5b)$$

This equation follows from the flux balance at the metal-semiconductor interface $j_m \cdot \nu_{\text{org}} = (j_n + j_p + j_D) \cdot \nu_{\text{org}}$ (see [27, Chap. 11], where the displacement current density $j_D = -\varepsilon \frac{\partial}{\partial t} \nabla \psi$ does not appear in the stationary setting).

The electrostatic potential ψ satisfies

$$\psi = \varphi_n + V^i(T), \quad i \in \{2, M-1\}, \quad (1.5c)$$

where the (built-in) potentials $V^2(T)$, $V^{M-1}(T)$ solve the local charge neutrality condition separately at the lower and upper interface, i.e.,

$$C - N_{n0}^i \mathcal{G}\left(\frac{V^i - E_L^i}{T}, \frac{\sigma_n^i}{T}\right) + N_{p0}^i \mathcal{G}\left(\frac{E_H^i - V^i}{T}, \frac{\sigma_p^i}{T}\right) = 0, \quad i \in \{2, M-1\}. \quad (1.6)$$

They are determined uniquely provided that the doping at the contact satisfies $C \in (-N_{p0}^i, N_{n0}^i)$ (\mathcal{G} is monotonously increasing in the first argument, see [10, Subsec. 2.1]).

To take relation (1.6) into account and to guarantee sufficient regularity for the Dirichlet boundary condition for the Poisson equation, we will restrict our analysis in this manuscript to the spatially two-dimensional case.

On the outer boundary, $\Gamma := \partial\Omega = \partial(\overline{\Omega^{\text{sub}}} \cup \overline{\Omega^{\text{dev}}})$, we consider Robin boundary conditions for the heat equation, ν denotes the outer unit normal with respect to Ω :

$$\lambda \nabla T \cdot \nu + \beta(T - T_a) = 0 \quad (1.7)$$

with some heat transmission coefficient $\beta > 0$.

On the internal interfaces $\partial(\overline{\Omega^{\text{sub}}} \cap \overline{\Omega^{\text{dev}}})$, $\partial(\overline{\Omega^1} \cap \overline{\Omega^2})$, $\partial(\overline{\Omega^{M-1}} \cap \overline{\Omega^M})$, we suppose the transmission conditions $[\lambda \nabla T \cdot \nu] = 0$ and $[T] = 0$ for the heat flux and the temperature, where $[\cdot]$ denotes the jump across the interface.

The electronic boundary conditions read as follows: On $\Gamma^+ := \gamma^+ \times (\widehat{h}^{M-1}, \widehat{h}^M)$ and $\Gamma^- := \gamma^- \times (0, \widehat{h}^1)$ with $\gamma^+, \gamma^- \subset \partial\omega$ (contacts at electrodes), we prescribe applied voltages

$$\varphi_m = V_{\text{app}}^\pm. \quad (1.8)$$

On the isolated parts of the electrodes $\omega \times \{h\}$, $\omega \times \{0\}$, $(\partial\omega \times (\widehat{h}^{M-1}, \widehat{h}^M)) \setminus \Gamma^+$, and $(\partial\omega \times (0, \widehat{h}^1)) \setminus \Gamma^-$ no flux-boundary conditions $\kappa \nabla \varphi_m \cdot \nu_e = 0$ are supposed. On the isolated parts of organic semiconductor $\partial\omega \times (\widehat{h}^1, \widehat{h}^{M-1})$ also no flux-boundary conditions $n\mu_n \nabla \varphi_n \cdot \nu_{\text{org}} = 0$, $p\mu_p \nabla \varphi_p \cdot \nu_{\text{org}} = 0$, and $\varepsilon \nabla \psi \cdot \nu_{\text{org}} = 0$ are considered. Here, ν_e and ν_{org} denote the outer unit normals of the electrodes and Ω^{org} , respectively.

1.2 Related references

Electrothermal models for organic semiconductor devices on the drift-diffusion level, however, formulated only in the organic subdomain $\Omega = \Omega^{\text{org}}$ and substituting the charge transport in the electrodes by fixed prescribed Dirichlet values in the generalized van Roosbroeck system, are investigated in [10]. Moreover, the temperature dependence in the boundary condition for the electrostatic potential ψ , as it is formulated in (1.5c) and (1.6), is ignored therein, and the Dirichlet data for ψ is a fixed $W^{1,\infty}$ function. A temperature dependent built-in potential following (1.6) for the Dirichlet function in the Poisson equation is only taken into account in the [1, 5], where the numerical simulation of electrothermal behavior of organic devices is carried out. Regularity issues arising from this dependence were not treated.

In [10], we proved for a weak notion of solutions (H^1 setting for potentials and entropy solutions for the heat equation) the solvability of the problem in the spatially three-dimensional case. Note that due to hysteretic effects, uniqueness of the solution cannot be expected.

On a coarser modeling level, $p(x)$ -Laplace thermistor models were considered in [17] for the total current and heat flow. Also here different subdomains for the electric and thermal problems were taken into account. Therein, the whole electrothermal drift-diffusion system (1.2) in the organic layers Ω^{org} is substituted by a $p(x)$ -Laplace thermistor system.

Electrothermal models for inorganic semiconductors where the equations are considered on different domains are studied, e.g., in [8]. There the full coupling including additional thermoelectric effects (Peltier, Thomson, and Seebeck) is taken into account. In difference to our present paper, temperature-independent fixed prescribed Dirichlet functions for the Poisson equation are considered. In this setting for two spatial dimensions, the uniqueness of the stationary solution for data nearly compatible with thermodynamic equilibrium is verified using $W^{1,q}$ regularity ($q > 2$) and the implicit function theorem.

1.3 Structure of the paper

In Section 2, we fix our notation and assumptions, provide analytical properties of the prescribed boundary functions for the Poisson equation, collect needed regularity results for (coupled) elliptic problems with mixed boundary conditions and discontinuous coefficients, and give a weak formulation of the electrothermal model for organic devices including electrical and thermal environment. In Section 3, we formulate and prove our main result (Theorem 3.1), which guarantees the existence of weak solutions. The proof is based on Schauder's fixed point theorem and a regularity result for strongly coupled systems with nonsmooth data and mixed boundary conditions (see Theorem 2.1). The corresponding iteration scheme is introduced in Subsection 3.1 and the required continuity properties of the fixed-point map are validated in Subsection 3.3. The proof of the regularity result in Theorem 2.1 is presented in Section 4 and uses Caccioppoli estimates and a Gehring-type lemma.

2 Notation, assumptions, and weak formulation

2.1 Assumptions and notation

In what follows, we use the (standard) notations for the Lebesgue and Sobolev spaces $L^q(\Omega)$ and $W^{1,q}(\Omega)$, $q \in [1, \infty]$, and write $H^1(\Omega)$ for $q = 2$.

We impose the following **Assumptions (A)** on the geometry and the data:

- (A1) We consider the following layered structure (as indicated in Fig. 1): The full domain $\Omega \subset \mathbb{R}^2$ satisfies $\overline{\Omega} = \overline{\Omega^{\text{sub}}} \cup \overline{\Omega^{\text{dev}}}$ with $\Omega^{\text{sub}} \cap \Omega^{\text{dev}} = \emptyset$ and $\Omega^{\text{sub}} \subset \mathbb{R}^2$ such that $\omega \times \{0\} \subset \partial\Omega^{\text{sub}}$ for $\omega := (0, L)$ and $\Omega^{\text{dev}} := \omega \times (0, \widehat{h}^M)$, $\Omega^{\text{org}} := \omega \times (\widehat{h}^1, \widehat{h}^{M-1})$. Moreover, $\Omega^i := \omega \times (\widehat{h}^{i-1}, \widehat{h}^i)$ denotes the i th layer for $i = 1, \dots, M$. The full boundary is given by $\Gamma := \partial\Omega$, and the contacts by $\Gamma^+ := \gamma^+ \times (\widehat{h}^{M-1}, \widehat{h}^M)$, $\Gamma^- := \gamma^- \times (0, \widehat{h}^1)$ with $\gamma^+, \gamma^- \in \partial\omega$. The metal-semiconductor interface is $I := (\omega \times \{\widehat{h}^1\}) \cup (\omega \times \{\widehat{h}^{M-1}\})$.
- (A2) The Dirichlet function satisfies $\varphi_n^D \in W^{1,\infty}(\Omega^{\text{dev}})$ with $\|\varphi_n^D\|_{L^\infty(\Omega^{\text{dev}})} \leq K$, the electrical conductivities in the metal layers are such that $\kappa = \kappa^i$ in Ω^i with positive constants κ^i for $i = 1$ and $i = M$.
- (A3) The mobilities of electrons and holes are temperature-dependent such that $\mu_j = \mu_{j0}^i B_j^i(T)$ in Ω^i for $i = 2, \dots, M-1$ and $j = n, p$, where $B_j^i(T) = B_{j0}^i \exp\{-\frac{a_j^i}{T}\}$ are of Arrhenius type and B_{j0}^i, a_j^i , and μ_{j0}^i are positive constants.
- (A4) The dielectric permittivity, the effective densities of states, the disorder parameters, the LUMO and HOMO energy levels, and the doping density are piecewise constant with $\varepsilon = \varepsilon^i$, $N_{j0} = N_{j0}^i$, $\sigma_j = \sigma_j^i$, $E_L = E_L^i$, $E_H = E_H^i$, and $C = C^i$ in Ω^i , $i = 2, \dots, M-1$. The constants ε^i , N_{j0}^i , σ_j^i , are positive with $N_{j0}^i \leq \overline{N}$, $j = n, p$, $E_L^i > E_H^i$. We define the energy gap $E_G^i = E_L^i - E_H^i$ and assume that the energy levels satisfy $|E_L^i|, |E_H^i| \leq \overline{E}$, for $i = 2, \dots, M-1$ and the doping profile is such that $C^i \in \left[N_{n0}^i \mathcal{G}\left(\frac{-E_G^i}{T_a}; \frac{\sigma_n^i}{T_a}\right) - \frac{N_{p0}^i}{2}, \frac{N_{n0}^i}{2} - N_{p0}^i \mathcal{G}\left(\frac{-E_G^i}{T_a}; \frac{\sigma_p^i}{T_a}\right) \right]$ for $i = 2$ and for $i = M-1$. Here, $T_a > 0$ is the constant ambient temperature.
- (A5) The recombination rate reads $R = R(n, p, T, \varphi_n, \varphi_p) = r_0(\cdot, n, p, T)np(1 - \exp\frac{\varphi_n - \varphi_p}{T})$, where the reaction rate coefficient $r_0(\cdot, n, p, T) : \Omega^{\text{org}} \times (0, \overline{N})^2 \times (0, \infty) \mapsto \mathbb{R}_+$ is a Caratheodory function and such that $r_0(\cdot, n, p, T) \leq \bar{r}$ a.e. in Ω^{org} for all $(n, p, T) \in (0, \overline{N})^2 \times (0, \infty)$. Moreover, $r_0(x, \cdot, \cdot, \cdot)$ is locally Lipschitz continuous on $(0, \overline{N})^2 \times [T_a, \infty)$ a.e. in Ω^{org} .
- (A6) The heat conductivity satisfies $\lambda \in L^\infty(\Omega)$ such that λ is constant in Ω^i , $i = 1, \dots, M$, and satisfies $\underline{\Lambda}_0 \leq \lambda(x) \leq \overline{\Lambda}_0 < \infty$ a.e. in Ω for constants $\underline{\Lambda}_0, \overline{\Lambda}_0 > 0$. The heat transmission coefficient $\beta \in L_+^\infty(\Gamma)$ satisfies $\int_\Gamma \beta \, d\Gamma > 0$.

For a unified description, we often use $\Omega_n := \Omega^{\text{dev}}$, $\Omega_p := \Omega^{\text{org}}$. With the notation $\Gamma_{Nn} := \partial\Omega_n \setminus \overline{\Gamma^+} \setminus \overline{\Gamma^-}$, $\Gamma_{Dn} := \Gamma^+ \cup \Gamma^-$, and $\Gamma_{Np} := \partial\Omega_p \setminus \overline{I}$, $\Gamma_{Dp} := I$, we introduce the spaces $W_{\Gamma_{Nj}}^{1,q}(\Omega_j)$ as the closure of $\{w \in C^\infty(\mathbb{R}^2) : \text{supp } w \cap \overline{\Gamma_{Dj}} = \emptyset\}$ with respect to the $W^{1,q}(\Omega_j)$ norm, $W_{\Gamma_{Nj}}^{-1,q}(\Omega_j)$ stands for the dual of $W_{\Gamma_{Nj}}^{1,q'}(\Omega_j)$, where $1/q + 1/q' = 1$. Note that $\Omega_j \cup \Gamma_{Nj}$ are regular in the sense of Gröger [12]. Moreover, let χ_j be the characteristic function of Ω_j , $j = n, p$.

The letter c denotes positive constants depending only on the data of the problem, they are allowed to change from line to line. For Banach spaces X, Y , let $\mathcal{L}(X, Y)$ denote the space of linear, bounded operators from X to Y .

2.2 The nonlinear boundary condition for the Poisson equation

In this subsection, we provide regularity properties of the boundary data for the solution ψ of the Poisson equation in (1.5) that are needed for the analysis (see Lemma 2.2 below). We take advantage

of properties of Gauss–Fermi integrals established, e.g., in [10, Subsec. 2.1], and [11, Appendix]. First, we consider arbitrary parameters $-N_{p0} < C < N_{n0}$, $E_L, E_H \in \mathbb{R}$, $\sigma_n, \sigma_p > 0$, and $T > 0$ and discuss properties of the solution to the local charge neutrality condition (1.6). For fixed C , let $V(T)$ denote the unique solution to

$$\mathcal{H}(T, V(T)) = 0, \text{ where } \mathcal{H}(T, v) := N_{n0} \mathcal{G}\left(\frac{v - E_L}{T}; \frac{\sigma_n}{T}\right) - N_{p0} \mathcal{G}\left(\frac{E_H - v}{T}; \frac{\sigma_p}{T}\right) - C.$$

Note that for fixed T and C , the map $\mathcal{H}(T, \cdot) : \mathbb{R} \rightarrow (-N_{p0} - C, N_{n0} - C)$ is strictly monotonously increasing since the function \mathcal{G} is strictly monotonously increasing in the first argument.

We define the energy gap $E_G := E_L - E_H > 0$ and consider doping densities

$$C \in \mathfrak{C}_{\text{dop}} := \left[N_{n0} \mathcal{G}\left(\frac{-E_G}{T_a}; \frac{\sigma_n}{T_a}\right) - \frac{N_{p0}}{2}, \frac{N_{n0}}{2} - N_{p0} \mathcal{G}\left(\frac{-E_G}{T_a}; \frac{\sigma_p}{T_a}\right) \right] \subset \mathbb{R}.$$

Using the implicit function theorem, we obtain the following result, whose proof is postponed to Appendix A.

Lemma 2.1 *We assume $C \in \mathfrak{C}_{\text{dop}}$ and $0 < T_a \leq T$. Let $V(T)$ solve $\mathcal{H}(T, V(T)) = 0$. Then the function $V(T)$ satisfies $E_H \leq V(T) \leq E_L$ for all $T \geq T_a$. Moreover, the derivatives $V'(T)$ and $V''(T)$ are bounded by constants depending on T_a .*

Next, given the solutions for the local charge neutrality, we construct the Dirichlet data for the electrostatic potential ψ in (1.5) as follows: Let $\tau : \overline{\Omega^{\text{org}}} \rightarrow [0, 1]$ be the affine function depending only on the second spatial coordinate x_2 with $\tau(x_1, \widehat{h}^1) = 1$ and $\tau(x_1, \widehat{h}^{M-1}) = 0$. Moreover, let $V^2(T)$ and $V^{M-1}(T)$ denote the function $V(T)$ calculated with respect to the actual doping density C , effective densities of state N_{n0}, N_{p0} , energy levels E_L, E_H , and disorder parameters σ_n, σ_p from Ω^2 and Ω^{M-1} , respectively. Then, we define on Ω^{org}

$$\psi^I = \psi^I(T, \varphi_n) := \varphi_n + \tau V^2(T) + (1 - \tau) V^{M-1}(T). \quad (2.1)$$

Thus, ψ^I is such that $\psi^I = \varphi_n + V^2(T)$ on $\omega \times \{\widehat{h}^1\}$ and $\psi^I = \varphi_n + V^{M-1}(T)$ on $\omega \times \{\widehat{h}^{M-1}\}$.

Lemma 2.2 *We suppose (A4). If $\varphi_n, T \in W^{1,q}(\Omega^{\text{org}})$ for some $q > 1$ and $0 < T_a \leq T$ a.e. in Ω^{org} , then ψ^I defined in (2.1) satisfies also $\psi^I \in W^{1,q}(\Omega^{\text{org}})$. If additionally $\varphi_n \in L^\infty(\Omega^{\text{org}})$, then $\psi^I \in L^\infty(\Omega^{\text{org}})$, too.*

Proof. Since $\nabla V(T) = V'(T) \nabla T$ and $|V'(T)|$ is bounded for temperatures $T \in W^{1,q}(\Omega)$ with $0 < T_a \leq T$ by Lemma 2.1, we obtain $\nabla V(T) \in L^q(\Omega^{\text{org}})$. Together with (A.2), $V(T) \in W^{1,q}(\Omega^{\text{org}})$ follows. If additionally $\varphi_n \in W^{1,q}(\Omega^{\text{org}})$, then $\psi^I(T, \varphi_n) \in W^{1,q}(\Omega^{\text{org}})$, too. Moreover, $\varphi_n \in L^\infty(\Omega^{\text{org}})$ implies by (2.1) and (A.2) that $\psi^I \in L^\infty(\Omega^{\text{org}})$. \square

2.3 Reformulation of the current-flow equations

We establish the weak formulation of the model equations introduced in Subsection 1.1. First, we reformulate the equations: Subtracting the second and third equation in (1.2), i.e., the continuity equations of electron and holes, yields $\nabla \cdot (j_n + j_p) = 0$. Gauss's theorem together with no-flux boundary

conditions for j_n and j_p on $\partial\Omega^{\text{org}} \setminus I$ (recall that $I := (\overline{\Omega^1} \cap \overline{\Omega^2}) \cup (\overline{\Omega^{M-1}} \cap \overline{\Omega^M})$) gives for arbitrary $w \in H^1(\Omega^{\text{dev}})$ the identity

$$0 = \int_{\Omega^{\text{org}}} \nabla \cdot (j_n + j_p) w \, dx = \int_I (j_n + j_p) \cdot \nu_{\text{org}} w \, d\Gamma - \int_{\Omega^{\text{org}}} (j_n + j_p) \cdot \nabla w \, dx. \quad (2.2)$$

To simplify notation and to “save” one variable in our model, we consider the variable φ_n on the whole device domain Ω^{dev} by identifying it in the electrodes with the metal Fermi potential φ_m . Note that the interface condition in (1.5a) justifies to look for $\varphi_n \in H^1(\Omega^{\text{dev}})$, which incorporates that $\varphi_m = \varphi_n$ at I , see also Lemma B.1.

Let $\overline{\varphi}_n \in H_{\Gamma_{N_n}}^1(\Omega^{\text{dev}})$ be arbitrarily given. Exploiting the equation in (1.1) for the charge transport in the electrodes in connection with the boundary and interfacial conditions in (1.5) as well as the identity in (2.2), we find

$$\begin{aligned} 0 &= - \int_{\Omega^1 \cup \Omega^M} \nabla \cdot (\kappa \nabla \varphi_n) \overline{\varphi}_n \, dx = \int_{\Omega^1 \cup \Omega^M} \kappa \nabla \varphi_n \cdot \nabla \overline{\varphi}_n \, dx - \int_I j_m \cdot \nu_{\text{org}} \overline{\varphi}_n \, d\Gamma \\ &= \int_{\Omega^1 \cup \Omega^M} \kappa \nabla \varphi_n \cdot \nabla \overline{\varphi}_n \, dx - \int_I (j_n + j_p) \cdot \nu_{\text{org}} \overline{\varphi}_n \, d\Gamma \\ &= \int_{\Omega^1 \cup \Omega^M} \kappa \nabla \varphi_n \cdot \nabla \overline{\varphi}_n \, dx - \int_{\Omega^{\text{org}}} (j_n + j_p) \cdot \nabla \overline{\varphi}_n \, dx \\ &= \int_{\Omega^1 \cup \Omega^M} \kappa \nabla \varphi_n \cdot \nabla \overline{\varphi}_n \, dx + \int_{\Omega^{\text{org}}} (n\mu_n \nabla \varphi_n + p\mu_p \nabla \varphi_p) \cdot \nabla \overline{\varphi}_n \, dx. \end{aligned}$$

Combining this equation with the weak formulation of the continuity equation for the holes in Ω^{org} and of the Poisson equation, where Dirichlet boundary conditions $\varphi_p = \varphi_n$ and $\psi = \varphi_n + V^i$, $i \in \{2, M-1\}$, have to be taken into account at $I = \Gamma_{Dp}$, we arrive at the weak formulation of the current flow in the organic layers and the electrodes, namely

$$\begin{aligned} &\int_{\Omega^1 \cup \Omega^M} \kappa \nabla \varphi_n \cdot \nabla \overline{\varphi}_n \, dx + \int_{\Omega^{\text{org}}} (n\mu_n \nabla \varphi_n \cdot \nabla \overline{\varphi}_n + p\mu_p \nabla \varphi_p \cdot (\nabla \overline{\varphi}_p + \nabla \overline{\varphi}_n)) \, dx \\ &= \int_{\Omega^{\text{org}}} r_0 n p (\exp \frac{\varphi_n - \varphi_p}{T} - 1) \overline{\varphi}_p \, dx \quad \forall \overline{\varphi}_n \in H_{\Gamma_{N_n}}^1(\Omega^{\text{dev}}), \overline{\varphi}_p \in H_{\Gamma_{N_p}}^1(\Omega^{\text{org}}), \end{aligned} \quad (2.3)$$

$$\int_{\Omega^{\text{org}}} \varepsilon \nabla \psi \cdot \overline{\psi} \, dx = \int_{\Omega^{\text{org}}} (C - n + p) \overline{\psi} \, dx \quad \forall \overline{\psi} \in H_{\Gamma_{N_p}}^1(\Omega^{\text{org}}). \quad (2.4)$$

Remark 2.1 *Let us relate our model to the model in [10], where only the electrothermal drift-diffusion system in the organic domain Ω^{org} is considered and electrodes are only modeled by Dirichlet contacts at I : In this setting we would have $H_{\Gamma_{N_n}}^1(\Omega^{\text{dev}}) = H_{\Gamma_{N_p}}^1(\Omega^{\text{org}})$ such that the test functions $\overline{\varphi}_n \in H_{\Gamma_{N_n}}^1(\Omega^{\text{dev}})$ would also belong to $H_{\Gamma_{N_p}}^1(\Omega^{\text{org}})$. Thus, these test functions could be used also as test function for the continuity equation of holes. Subtracting this relation from our weak formulation (2.3) we obtain the weak formulation in [10]. Indeed, choosing $\overline{\varphi}_n = 0$ in (2.3) gives the usual weak formulation for $\nabla \cdot (p\mu_p \nabla \varphi_p) = R$. While for $\overline{\varphi}_p = 0$, we get the weak formulation for $-\nabla \cdot (n\mu_n \nabla \varphi_n) = \nabla \cdot (p\mu_p \nabla \varphi_p) = R$ in Ω^{org} .*

2.4 Regularity results for elliptic problems with mixed boundary conditions and discontinuous coefficients

Before we state the existence result for the system in (1.1)–(1.8), we start with a theorem ensuring the higher integrability of the gradients of φ_n, φ_p in the coupled current-flow equation in (2.3). For

this purpose, we consider the model **Problem (P_C)** for finding $\varphi_n \in \varphi_n^D + H_{\Gamma_{Nn}}^1(\Omega^{\text{dev}})$, $\varphi_p \in \varphi_n + H_{\Gamma_{Np}}^1(\Omega^{\text{org}})$ such that

$$\begin{aligned} & \int_{\Omega^{\text{dev}}} a_n \nabla \varphi_n \cdot \nabla \bar{\varphi}_n \, dx + \int_{\Omega^{\text{org}}} a_p \nabla \varphi_p \cdot (\nabla \bar{\varphi}_p + \nabla \bar{\varphi}_n) \, dx \\ & = \int_{\Omega^{\text{org}}} f_C \bar{\varphi}_p \, dx \quad \forall \bar{\varphi}_n \in H_{\Gamma_{Nn}}^1(\Omega^{\text{dev}}), \bar{\varphi}_p \in H_{\Gamma_{Np}}^1(\Omega^{\text{org}}), \end{aligned} \quad (\text{P}_C)$$

where the coefficient functions a_n and a_p are related to the conductivities $n\mu_n$, κ^1 , and κ^M as well as $p\mu_p$, respectively, and f_C represents the recombination term R . Note that the Dirichlet value for φ_p on the interface I is given by the solution φ_n , i.e., it is not known a priori.

Theorem 2.1 *We suppose (A1) and (A2). Let $a_n \in L^\infty(\Omega^{\text{dev}})$, $a_p \in L^\infty(\Omega^{\text{org}})$, $f_C \in L^\infty(\Omega^{\text{org}})$ with $a_n, a_p \in [\underline{d}, \bar{d}]$ a.e. (where $\underline{d} > 0$), $|f_C| \leq \bar{f}$. Then there exist $\alpha^* > 1$ and $c_q > 0$ such that for any solution (φ_n, φ_p) to (P_C) we have*

$$\|\varphi_n\|_{W^{1,q}(\Omega^{\text{dev}})} \leq c_q, \quad \|\varphi_p\|_{W^{1,q}(\Omega^{\text{org}})} \leq c_q, \quad q := 2\alpha^*.$$

The constants $q > 2$ and c_q depend only on Ω^{dev} , Ω^{org} , \underline{d} , \bar{d} , \bar{f} , and φ_n^D .

The proof of this theorem is based on Caccioppoli-type estimates, Poincaré-type inequalities, and a Gehring-type lemma. It is postponed to Section 4.

Recall that the quasi-Fermi potential φ_n for electrons is defined on the larger domain $\Omega_n = \Omega^{\text{dev}}$, while the potential φ_p for holes lives on the smaller domain $\Omega_p = \Omega^{\text{org}}$. On the layered structures Ω_n and Ω_p , we define for notational simplicity the conductivity functions

$$\begin{aligned} d_n(\psi, \varphi_n, T) &= \begin{cases} \kappa^1 & \text{in } \Omega^1 \\ \mu_{n0}^i B_n^i(T) N_{n0}^i \mathcal{G}\left(\frac{\psi - \varphi_n - E_L^i}{T}, \frac{\sigma_n^i}{T}\right) & \text{in } \Omega^i, \quad i = 2, \dots, M-1, \\ \kappa^M & \text{in } \Omega^M \end{cases} \\ d_p(\psi, \varphi_p, T) &= \mu_{p0}^i B_p^i(T) N_{p0}^i \mathcal{G}\left(\frac{E_H^i - (\psi - \varphi_p)}{T}, \frac{\sigma_p^i}{T}\right) \quad \text{in } \Omega^i, \quad i = 2, \dots, M-1. \end{aligned} \quad (2.5)$$

For the model introduced in Subsection 1.1, we expect that (i) the temperature is bounded from below by the ambient temperature T_a (heat equation with Robin boundary conditions and nonnegative source terms) and (ii) the quasi Fermi potentials φ_n, φ_p are bounded by the constants K from (A2), see Lemma 3.2 later on.

For a right-hand side $f \in L^\infty(\Omega^{\text{org}})$ with $|f| \leq 3\bar{N}$ and a Dirichlet function $\psi^I \in H^1(\Omega^{\text{org}}) \cap L^\infty(\Omega^{\text{org}})$ with $|\psi^I| \leq K + \bar{E}$, let us consider the Poisson equation for $\psi \in \psi^I + H_{\Gamma_{Np}}^1(\Omega^{\text{org}})$

$$\int_{\Omega^{\text{org}}} \varepsilon \nabla \psi \cdot \nabla \bar{\psi} \, dx = \int_{\Omega^{\text{org}}} f \bar{\psi} \, dx \quad \forall \bar{\psi} \in H_{\Gamma_{Np}}^1(\Omega^{\text{org}}).$$

We denote by $c_{\psi, \infty} > 0$ an $L^\infty(\Omega^{\text{org}})$ bound for the (unique) weak solution ψ (see e.g. [2, Lemma 3.1]). Moreover, for $K^* := K + \bar{E} + c_{\psi, \infty} < \infty$, we define the positive constants

$$\begin{aligned} \underline{d} &:= \min \left\{ \kappa^1, \kappa^M, \min_{j=n,p} \min_{i=2, \dots, M-1} \mu_{j0}^i B_{j0}^i N_{j0}^i \exp \left\{ -\frac{a_j^i}{T_a} \right\} \mathcal{G} \left(-\frac{K^*}{T_a}; \frac{\sigma_j^i}{T_a} \right) \right\}, \\ \bar{d} &:= \max \left\{ \kappa^1, \kappa^M, \max_{j=n,p} \max_{i=2, \dots, M-1} \mu_{j0}^i B_{j0}^i N_{j0}^i \right\}. \end{aligned} \quad (2.6)$$

For arguments φ_j , ψ , and T with $|\varphi_j| \leq K$, $|\psi| \leq c_{\psi, \infty}$, and $T \geq T_a$, we find

$$\underline{d} \leq d_j(\psi, \varphi_j, T) \leq \bar{d}, \quad j = n, p, \quad |r_0 n p (\exp \frac{\varphi_n - \varphi_p}{T} - 1)| \leq c(K, T_a).$$

Thus, we apply Theorem 2.1 with $a_j = d_j(\psi, \varphi_j, T)$, $f_C = r_0 n p (\exp \frac{\varphi_n - \varphi_p}{T} - 1)$ to the current-flow problem in (2.3). **We fix the exponent $q > 2$, given by this theorem, for all our further considerations.**

According to [12, Theorem 1], there is a $t^* > 2$ such that the strongly monotone, Lipschitz continuous operator $\widehat{\mathcal{A}}_\lambda : H^1(\Omega) \mapsto H^1(\Omega)^*$,

$$\langle \widehat{\mathcal{A}}_\lambda T, w \rangle := \int_{\Omega} (\lambda \nabla T \cdot \nabla w + T w) \, dx, \quad w \in H^1(\Omega), \quad (2.7)$$

maps $W^{1, \tilde{t}}(\Omega)$ into and onto $W^{-1, \tilde{t}}(\Omega)$ for all $\tilde{t} \in [2, t^*]$. Next, we define $t \in (2, t^*]$ by

$$t := \begin{cases} t^* & \text{if } \frac{q}{q-2} \in \left[1, \frac{2t^*}{t^*-2}\right] \\ \frac{2q}{4-q} & \text{if } \frac{q}{q-2} > \frac{2t^*}{t^*-2} \end{cases}, \quad \frac{1}{t} + \frac{1}{t'} = 1. \quad (2.8)$$

This definition guarantees that $L^{q/2}(\Omega) \hookrightarrow W^{-1, t}(\Omega)$. Remark 13 in [12] then ensures $W^{1, t}$ -estimates for solutions to problems of the form $\widehat{\mathcal{A}}_\lambda T = \mathcal{F}(T)$, where \mathcal{F} is any mapping from $W^{1, 2}(\Omega)$ into $W^{-1, t}(\Omega)$.

Moreover, we define the exponents \widehat{q} and \widehat{t} (later needed for the fixed point argument)

$$2 < \widehat{q} := \frac{4q}{2+q} < q, \quad \widehat{t} := \begin{cases} t^* & \text{if } \frac{\widehat{q}}{\widehat{q}-2} \in \left[1, \frac{2t^*}{t^*-2}\right] \\ \frac{2\widehat{q}}{4-\widehat{q}} & \text{if } \frac{\widehat{q}}{\widehat{q}-2} > \frac{2t^*}{t^*-2} \end{cases}. \quad (2.9)$$

Additionally, [12, Theorem 1] guarantees the existence of an exponent $s^* > 2$ such that the strongly monotone, Lipschitz continuous operator $\mathcal{A}_\varepsilon : H_{\Gamma_{Np}}^1(\Omega^{\text{org}}) \rightarrow H_{\Gamma_{Np}}^1(\Omega^{\text{org}})^*$,

$$\langle \mathcal{A}_\varepsilon \psi, w \rangle := \int_{\Omega^{\text{org}}} (\varepsilon \nabla \psi \cdot \nabla w + \psi w) \, dx, \quad w \in H_{\Gamma_{Np}}^1(\Omega^{\text{org}}),$$

maps $W^{1, \tilde{s}}(\Omega^{\text{org}})$ into and onto $W^{-1, \tilde{s}}(\Omega^{\text{org}})$ for all $\tilde{s} \in [2, s^*]$. Let $\widehat{\mathcal{A}}_\varepsilon$ denote the corresponding operator on spaces without zero Dirichlet values. Finally, we define the exponent

$$s := \min\{q, s^*, t\}. \quad (2.10)$$

2.5 Weak formulation (P) of the PDE system

In this last subsection, we provide a weak formulation of the whole system given by the equations (1.1)–(1.8): For the exponent $q > 2$ defined in Subsection 2.4, the Dirichlet data ψ^I introduced in (2.1), and the conductivities d_n, d_p set in (2.5) find $\varphi_n \in (\varphi_n^D + H_{\Gamma_{Nn}}^1(\Omega^{\text{dev}})) \cap W^{1, q}(\Omega^{\text{dev}})$, $\varphi_p \in (\varphi_n +$

$H_{\Gamma_{Np}}^1(\Omega^{\text{org}}) \cap W^{1,q}(\Omega^{\text{org}})$, $\psi \in \psi^I(T, \varphi_n) + H_{\Gamma_{Np}}^1(\Omega^{\text{org}})$ and $T \in \{\theta \in H^1(\Omega) : \ln \theta \in L^\infty(\Omega)\}$ such that

$$\begin{aligned} & \int_{\Omega^{\text{dev}}} d_n \nabla \varphi_n \cdot \nabla \bar{\varphi}_n \, dx + \int_{\Omega^{\text{org}}} d_p \nabla \varphi_p \cdot (\nabla \bar{\varphi}_p + \nabla \bar{\varphi}_n) \, dx \\ &= \int_{\Omega^{\text{org}}} r_0 n p (\exp \frac{\varphi_n - \varphi_p}{T} - 1) \bar{\varphi}_p \, dx \quad \forall \bar{\varphi}_j \in H_{\Gamma_{Nj}}^1(\Omega_j), \end{aligned} \quad (2.11)$$

$$\int_{\Omega^{\text{org}}} \varepsilon \nabla \psi \cdot \nabla \bar{\psi} \, dx = \int_{\Omega^{\text{org}}} (C - n + p) \bar{\psi} \, dx \quad \forall \bar{\psi} \in H_{\Gamma_{Np}}^1(\Omega^{\text{org}}), \quad (2.12)$$

$$\begin{aligned} & \int_{\Omega} \lambda \nabla T \cdot \nabla \bar{T} \, dx + \int_{\Gamma} \beta (T - T_a) \bar{T} \, d\Gamma = \int_{\Omega^{\text{dev}}} d_n |\nabla \varphi_n|^2 \bar{T} \, dx \\ & + \int_{\Omega^{\text{org}}} \left(d_p |\nabla \varphi_p|^2 \bar{T} + r_0 n p (1 - \exp \frac{\varphi_n - \varphi_p}{T}) (\varphi_p - \varphi_n) \bar{T} \right) dx \quad \forall \bar{T} \in H^1(\Omega). \end{aligned} \quad (2.13)$$

The system (2.11) – (2.13) is called **Problem (P)**. The splitting of φ_n , φ_p , ψ in a function with homogeneous Dirichlet values and the inhomogeneous Dirichlet function is also to be understood in the $W^{1,q}$ setting.

Remark 2.2 *i) Due to the choice of $q > 2$, we have $\varphi_j \in L^\infty(\Omega_j)$. Since also $\ln T \in L^\infty(\Omega)$, the generation-recombination rate in the continuity equations and the reaction heat term in the right-hand side of the heat equation (2.13) are well-defined.*

ii) Since φ_n , φ_p belong to $W^{1,q}$, also the Joule heat terms in the right-hand side of (2.13) are well-defined and the sum of all heat sources belongs to $L^{q/2}(\Omega)$. Our choice of q and $t > 2$ in (2.8) ensures that $L^{q/2} \hookrightarrow (W^{1,t'})^$, and thus the $W^{1,t}$ isomorphism setting allows us to treat the heat equation with quadratic gradient terms and reaction heat.*

iii) Moreover, the Dirichlet function $\psi^I = \psi^I(T, \varphi_n)$ belongs to $W^{1,s}(\Omega^{\text{org}})$, see Lemma 2.2. Therefore, also $\hat{\mathcal{A}}_\varepsilon \psi^I \in W_{\Gamma_{Np}}^{-1,s}(\Omega^{\text{org}})$ for $s > 2$ from (2.10).

3 Solvability of Problem (P)

In this section, we formulate and prove our main result, Theorem 3.1, that concerns the solvability of Problem (P). We start with preliminary results concerning the equilibrium solution and a priori estimates for solutions to Problem (P).

Lemma 3.1 *We assume (A). If $\varphi_n^D = \text{const}$ in Ω^{dev} , then Problem (P) has the unique (equilibrium) solution $(\varphi_n^D, \varphi_p^D, \psi^*, T_a)$, where ψ^* is the unique weak solution to the nonlinear Poisson equation*

$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla \psi^*) &= C - N_{n0} \mathcal{G} \left(\frac{\psi^* - \varphi_n^D - E_L}{T_a}; \frac{\sigma_n}{T_a} \right) + N_{p0} \mathcal{G} \left(\frac{E_H + \varphi_n^D - \psi^*}{T_a}; \frac{\sigma_p}{T_a} \right) \quad \text{in } \Omega^{\text{org}}, \\ \psi^* &= \psi^I(T_a, \varphi_n^D) \quad \text{on } I, \quad \varepsilon \nabla \psi^* \cdot \nu = 0 \quad \text{on } \partial \Omega^{\text{org}} \setminus I. \end{aligned}$$

Proof. We use the test function $(\varphi_n - \varphi_n^D, \varphi_p - \varphi_n) \in H_{\Gamma_{Nn}}^1(\Omega^{\text{dev}}) \times H_{\Gamma_{Np}}^1(\Omega^{\text{org}})$ for (2.11). Since $\varphi_n^D = \text{const}$, we obtain

$$\int_{\Omega^{\text{dev}}} d_n |\nabla \varphi_n|^2 \, dx + \int_{\Omega^{\text{org}}} \left(d_p |\nabla \varphi_p|^2 + r_0 n p (\exp \frac{\varphi_n - \varphi_p}{T} - 1) (\varphi_n - \varphi_p) \right) dx = 0.$$

Due to the monotonicity of the exponential function this yields $\varphi_n = \varphi_p = \text{const} = \varphi_n^D$. Since all source terms in the heat equation (2.13) are zero, it follows from (2.13) that $T \equiv T_a$. Finally, using these observations in the statistical relation for n and p , it is clear that ψ^* solves the nonlinear Poisson equation as stated in the assertion. \square

Lemma 3.2 *We assume (A). Let the constants K and T_a be as in (A2) and (A6). Then, for any solution $(\varphi_n, \varphi_p, \psi, T)$ to Problem (P), we have for $j = n, p$ the estimates*

$$|\varphi_j| \leq K \text{ a.e. in } \Omega_j, \quad |\psi| \leq c_{\psi, \infty} \text{ a.e. in } \Omega^{\text{org}}, \quad T \geq T_a \text{ a.e. in } \Omega, \quad \|\varphi_j\|_{H^1(\Omega_j)} \leq c.$$

Proof. Step 1. We test (2.11) by $((\varphi_n - K)^+, (\varphi_p - K)^+ - (\varphi_n - K)^+) \in H_{\Gamma_{Nn}}^1(\Omega_n) \times H_{\Gamma_{Np}}^1(\Omega_p)$ such that

$$\sum_{j=n,p} \int_{\Omega_j} d_j |\nabla(\varphi_j - K)^+|^2 dx + \int_{\Omega^{\text{org}}} r_0 np (\exp \frac{\varphi_n - \varphi_p}{T} - 1) ((\varphi_n - K)^+ - (\varphi_p - K)^+) dx = 0.$$

Discussing the four different cases $\varphi_n(\varphi_p) > K (\leq K)$, we find that the integrand in the reaction term is always nonnegative. This ensures that $\varphi_j \leq K$ a.e. in Ω_j . On the other hand, testing with $(-(\varphi_n + K)^-, -(\varphi_p + K)^- + (\varphi_n + K)^-) \in H_{\Gamma_{Nn}}^1(\Omega_n) \times H_{\Gamma_{Np}}^1(\Omega_p)$ gives the estimates $\varphi_j \geq -K$ a.e. in Ω_j , $j = n, p$. Since $|C - n + p| \leq 3\bar{N}$ and $|\psi^I| \leq K + \bar{E}$ a.e. on Ω^{org} it is guaranteed that $\|\psi\|_{L^\infty(\Omega^{\text{org}})} \leq c_{\psi, \infty}$ as in the arguments of Subsection 2.4 and [2, Lemma 3.1]. Testing the heat equation (2.13) with $(T - T_a)^-$ yields $T \geq T_a$ a.e. in Ω due to the nonnegativity of the heat sources.

Step 2. Testing the continuity equations by $(\varphi_n - \varphi_n^D, \varphi_p - \varphi_n) \in H_{\Gamma_{Nn}}^1(\Omega_n) \times H_{\Gamma_{Np}}^1(\Omega_p)$ and using Hölder's and Young's inequality gives

$$\begin{aligned} & \int_{\Omega_n} d_n |\nabla \varphi_n|^2 + \int_{\Omega_p} (d_p |\nabla \varphi_p|^2 + r_0 np (\exp \frac{\varphi_n - \varphi_p}{T} - 1) (\varphi_n - \varphi_p)) dx \\ & \leq \int_{\Omega_n} \frac{1}{2} d_n (|\nabla \varphi_n|^2 + |\nabla \varphi_n^D|^2) dx + \int_{\Omega_p} \frac{1}{2} d_p (|\nabla \varphi_p|^2 + |\nabla \varphi_n^D|^2) dx. \end{aligned}$$

Using $d_j \in [\underline{d}, \bar{d}]$ a.e. in Ω_j , the nonnegativity of $r_0 np$, the monotonicity of the exponential function, that $\varphi_n^D \in H^1(\Omega_n)$ is a fixed function, and the L^∞ estimates for φ_j from Step 1, we obtain the estimates $\|\varphi_j\|_{H^1(\Omega_j)} \leq c_{H^1}$, $j = n, p$. \square

Theorem 3.1 (Main result) *Under Assumptions (A) there exists a solution $(\varphi_n, \varphi_p, \psi, T)$ to Problem (P). For the exponents q from Subsection 2.4, s and t defined in (2.10) and (2.8), respectively, there are positive constants c_j, c_s, c_t, T_u such that all solutions to (P) satisfy the estimates*

$$\|\varphi_j\|_{W^q(\Omega_j)} \leq c_j, \quad j = n, p, \quad \|\psi\|_{W^{1,s}(\Omega^{\text{org}})} \leq c_s, \quad \|T\|_{W^{1,t}(\Omega)} \leq c_t, \quad T_u \geq T \geq T_a \text{ a.e. in } \Omega.$$

Remark 3.1 *The uniqueness of solutions cannot be expected. Due to self-heating, S-shaped current-voltage relations with regions of negative differential resistance are observed for OLEDs in experiments and in simulations (see [4, 5, 1]). This means that for certain applied voltages multiple solutions exist with different temperature distributions. Even tristability phenomena could be detected, where for certain applied voltages multiple solutions exist with different temperature distributions as well as for certain currents in the IV characteristic different voltages are possible, see [14].*

Our existence proof uses Schauder's fixed point theorem. First, we introduce the iteration scheme that defines the fixed-point map, then we study subproblems with frozen arguments, next we verify continuity properties of the fixed-point map, and finally we prove the solvability of Problem (P).

3.1 Iteration scheme

We define our fixed-point map on the non-empty, bounded, closed, convex set

$$\mathcal{N} := \left\{ (\varphi_n, \varphi_p, T) \in H^1(\Omega_n) \times H^1(\Omega_p) \times W^{1,\hat{t}}(\Omega) : \|\varphi_j\|_{W^{1,q}(\Omega_j)} \leq c_j, \right. \\ \left. \|T\|_{W^{1,\hat{t}}(\Omega)} \leq c_{\hat{t},T}, |\varphi_j| \leq K \text{ a.e. in } \Omega_j, j = n, p, T \geq T_a \text{ a.e. in } \Omega \right\}, \quad (3.1)$$

where the constants K and T_a are from Assumption (A), $c_n, c_p > 0$ will be defined in (3.8) of Lemma 3.4; the exponent \hat{t} is given in (2.9) and $c_{\hat{t},T} > 0$ will be introduced in Equation (3.10) of Lemma 3.5. For a more compact notation, we use the auxiliary function

$$\mathcal{U}(\psi, \varphi_n, \varphi_p, T) := N_{p0} \mathcal{G}\left(\frac{E_H - (\psi - \varphi_p)}{T}; \frac{\sigma_p}{T}\right) - N_{n0} \mathcal{G}\left(\frac{\psi - \varphi_n - E_L}{T}; \frac{\sigma_n}{T}\right). \quad (3.2)$$

Our fixed-point map $\mathcal{Q} : \mathcal{N} \rightarrow \mathcal{N}$, $(\varphi_n, \varphi_p, T) = \mathcal{Q}(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})$ is defined via the following three steps:

Step 1. For given $(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) \in \mathcal{N}$ and for the functions τ , $V^2(\tilde{T})$, and $V^{M-1}(\tilde{T})$ introduced in Subsection 2.2, we define the $H^1(\Omega^{\text{org}})$ function

$$\tilde{\psi}^I(x) := \psi^I(\tilde{T}(x), \tilde{\varphi}_n(x)), \quad |\tilde{\psi}^I| \leq K_\psi \text{ a.e. in } \Omega^{\text{org}} \quad (3.3)$$

with ψ^I given in (2.1) (see also Lemma 2.2). By Lemma 3.3 there is a unique weak solution $\psi \in \tilde{\psi}^I + H_{\Gamma_{Np}}^1(\Omega^{\text{org}})$ to the nonlinear Poisson equation

$$-\nabla \cdot (\varepsilon \nabla \psi) = C + \mathcal{U}(\psi, \tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) \text{ in } \Omega^{\text{org}}, \\ \psi = \tilde{\psi}^I \text{ on } I, \quad \varepsilon \nabla \psi \cdot \nu = 0 \text{ on } \partial\Omega^{\text{org}} \setminus I. \quad (3.4)$$

Step 2. With ψ from Step 1, satisfying $\|\psi\|_{L^\infty(\Omega^{\text{org}})} \leq c_{\psi,\infty}$ (see Lemma 3.3 below), we introduce the quantities

$$\tilde{n} := N_{n0} \mathcal{G}\left(\frac{\psi - \tilde{\varphi}_n - E_L}{\tilde{T}}; \frac{\sigma_n}{\tilde{T}}\right), \quad \tilde{p} := N_{p0} \mathcal{G}\left(\frac{E_H + \tilde{\varphi}_p - \psi}{\tilde{T}}; \frac{\sigma_p}{\tilde{T}}\right). \quad (3.5)$$

Together with the definition of the set \mathcal{N} and properties of the Gauss–Fermi integral, we verify that $d_j(\psi, \tilde{\varphi}_j, \tilde{T}) \in [\underline{d}, \bar{d}]$ a.e. in Ω_j , $j = n, p$, where $\underline{d}, \bar{d} > 0$ are defined in (2.6). With frozen coefficients $d_j(\psi, \tilde{\varphi}_j, \tilde{T})$ and frozen reaction rate coefficient $\tilde{r} := r_0(\tilde{n}, \tilde{p}, \tilde{T})\tilde{n}\tilde{p}$, we solve the problem

$$\int_{\Omega^{\text{dev}}} d_n(\psi, \tilde{\varphi}_n, \tilde{T}) \nabla \varphi_n \cdot \nabla \bar{\varphi}_n \, dx + \int_{\Omega^{\text{org}}} d_p(\psi, \tilde{\varphi}_p, \tilde{T}) \nabla \varphi_p \cdot (\nabla \bar{\varphi}_p + \nabla \bar{\varphi}_n) \, dx \\ = \int_{\Omega^{\text{org}}} \tilde{r} (\exp \frac{\varphi_n - \varphi_p}{\tilde{T}} - 1) \bar{\varphi}_p \, dx \quad \forall \bar{\varphi}_j \in H_{\Gamma_{Nj}}^1(\Omega_j). \quad (3.6)$$

According to Lemma 3.4 below, we obtain a unique weak solution $(\varphi_n, \varphi_p) \in (\varphi_n^D + W_{\Gamma_{Nn}}^{1,q}(\Omega_n)) \times (\varphi_n + W_{\Gamma_{Np}}^{1,q}(\Omega_p))$ to (3.6). The pair fulfills $\|\varphi_j\|_{L^\infty(\Omega_j)} \leq K$ and $\|\varphi_j\|_{W^{1,q}(\Omega_j)} \leq c_j$, $j = n, p$.

Step 3. Together with the L^∞ bounds for $\tilde{d}_n := d_n(\psi, \tilde{\varphi}_n, \tilde{T})$ and $\tilde{d}_p := d_p(\psi, \tilde{\varphi}_p, \tilde{T})$, these estimates ensure that the right-hand side $\tilde{h} = \tilde{h}(\tilde{n}, \tilde{p}, \tilde{T}, \nabla \varphi_n, \nabla \varphi_p, \varphi_n, \varphi_p) := \tilde{d}_n |\nabla \varphi_n|^2 \chi_n + \tilde{d}_p |\nabla \varphi_p|^2 \chi_p + \tilde{r} (\exp \frac{\varphi_n - \varphi_p}{\tilde{T}} - 1) (\varphi_n - \varphi_p) \chi_p$ of the heat equation,

$$-\nabla \cdot (\lambda \nabla T) = \tilde{h} \quad \text{in } \Omega, \\ \lambda \nabla T \cdot \nu + \beta(T - T_a) = 0 \quad \text{on } \Gamma \quad (3.7)$$

has a uniform $L^{q/2}$ bound for all possible $(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) \in \mathcal{N}$. Lemma 3.5 below ensures a unique weak solution $T \in W^{1,\tilde{t}}(\Omega)$ to (3.7), it satisfies $\|T\|_{W^{1,\tilde{t}}(\Omega)} \leq c_{\tilde{t},T}$ and $T \geq T_a$, which in summary confirms that $\mathcal{Q}(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) := (\varphi_n, \varphi_p, T) \in \mathcal{N}$.

Clearly, a fixed point $(\varphi_n, \varphi_p, T)$ of this map with associated electrostatic potential ψ is a solution to the original problem (P) from Subsection 2.5.

3.2 Solvability of subproblems and estimates for their solutions

Lemma 3.3 (Poisson equation) *We assume (A). Let $(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) \in \mathcal{N}$ be arbitrarily given and $\tilde{\psi}^I$ be defined by (3.3). Then there exists a unique weak solution $\psi \in \tilde{\psi}^I + H_{\Gamma_{Np}}^1(\Omega^{\text{org}})$ to the nonlinear Poisson equation (3.4). Moreover, $\|\psi\|_{L^\infty(\Omega^{\text{org}})} \leq c_{\psi,\infty}$.*

Proof. Since $\tilde{\psi}^I \in H^1(\Omega^{\text{org}})$, analogously to [2, Lemma 3.1] (here without any gate contact) one obtains a unique solution $\psi \in \tilde{\psi}^I + H_{\Gamma_{Np}}^1(\Omega^{\text{org}})$ of the nonlinear Poisson equation (3.4) as well as a uniform H^1 bound of the solution. Since $|C + \mathcal{U}(\psi, \tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})| \leq 3\bar{N}$ and $|\psi^I| \leq K + \bar{E}$ a.e. on Ω^{org} it is guaranteed that $\|\psi\|_{L^\infty(\Omega^{\text{org}})} \leq c_{\psi,\infty}$. \square

Lemma 3.4 (Continuity equations) *We assume (A). Let $(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) \in \mathcal{N}$ be arbitrarily given and $\psi \in \tilde{\psi}^I + H_{\Gamma_{Np}}^1(\Omega^{\text{org}})$ the unique weak solution to the nonlinear Poisson equation (3.4). Then there exists a unique weak solution $(\varphi_n, \varphi_p) \in (\varphi_n^D + W_{\Gamma_{Nn}}^{1,q}(\Omega_n)) \times (\varphi_n + W_{\Gamma_{Np}}^{1,q}(\Omega_p))$ to (3.6). It satisfies the following estimates that are uniform with respect to $(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) \in \mathcal{N}$,*

$$\begin{aligned} \|\varphi_j\|_{L^\infty(\Omega_j)} &\leq K, \quad \|\varphi_j\|_{W^{1,q}(\Omega_j)} \leq c_j, \quad j = n, p, \\ \left\| r_0(\cdot, \tilde{n}, \tilde{p}, \tilde{T}) \tilde{n} \tilde{p} \left(\exp \frac{\varphi_n - \varphi_p}{\tilde{T}} - 1 \right) (\varphi_n - \varphi_p) \right\|_{L^\infty(\Omega_p)} &\leq c_r. \end{aligned} \quad (3.8)$$

Proof. First, we verify the solvability of the problem in an H^1 setting, show its uniqueness, and then we derive the higher integrability and estimates for the solution to (3.6).

1. *Existence.* For $\ell > 0$ let $\rho_\ell : \mathbb{R}^2 \rightarrow [0, 1]$ be a fixed Lipschitz continuous function with

$$\rho_\ell(y, z) := \begin{cases} 0 & \text{if } \max\{|y|, |z|\} \geq \ell, \\ 1 & \text{if } \max\{|y|, |z|\} \leq \frac{\ell}{2}. \end{cases}$$

For fixed $(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) \in \mathcal{N}$, the operator $B_{(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})}^\ell : H_{\Gamma_{Nn}}^1(\Omega_n) \times H_{\Gamma_{Np}}^1(\Omega_p) \rightarrow H_{\Gamma_{Nn}}^1(\Omega_n)^* \times H_{\Gamma_{Np}}^1(\Omega_p)^*$, with the argument splitting in $(\varphi_n^0, \varphi_p^0)$ for the reaction part and $(\hat{\varphi}_n^0, \hat{\varphi}_p^0)$ for the main part

$$\begin{aligned} B_{(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})}^\ell(\varphi_n^0, \varphi_p^0) &= \hat{B}_{(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})}^\ell((\varphi_n^0, \varphi_p^0), (\varphi_n^0, \varphi_p^0)), \\ \left\langle \hat{B}_{(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})}^\ell((\varphi_n^0, \varphi_p^0), (\hat{\varphi}_n^0, \hat{\varphi}_p^0)), (\bar{\varphi}_n^0, \bar{\varphi}_p^0) \right\rangle &:= \int_{\Omega_n} \tilde{d}_n \nabla(\hat{\varphi}_n^0 + \varphi_n^D) \cdot \nabla \bar{\varphi}_n^0 \, dx \\ &+ \int_{\Omega_p} \tilde{d}_p \nabla(\hat{\varphi}_p^0 + \hat{\varphi}_n^0 + \varphi_n^D) \cdot \nabla(\bar{\varphi}_p^0 + \bar{\varphi}_n^0) \, dx \\ &+ \int_{\Omega_p} \rho_\ell(\varphi_n^0 + \varphi_n^D, \varphi_p^0 + \varphi_n^0 + \varphi_n^D) \tilde{r} \left(1 - \exp \frac{-\varphi_p^0}{\tilde{T}} \right) \bar{\varphi}_p^0 \, dx, \end{aligned}$$

$\bar{\varphi}_j^0 \in H_{\Gamma_{Nj}}^1(\Omega_j)$, is an operator of variational type (see [19, p. 182]). Have in mind that the main part (in the arguments $\bar{\varphi}_n^0, \bar{\varphi}_p^0$) is bounded, continuous, and monotone. Furthermore, the regularized reaction term is bounded and the map

$$(\varphi_n^0, \varphi_p^0) \mapsto \rho_\ell(\varphi_n^0 + \varphi_n^D, \varphi_p^0 + \varphi_n^0 + \varphi_n^D) \tilde{r}\left(1 - \exp\frac{-\varphi_p^0}{\tilde{T}}\right)$$

is Lipschitz continuous. Since the operator $B_{(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})}^\ell$ is coercive, the problem $B_{(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})}^\ell(\varphi_n^0, \varphi_p^0) = 0$ has at least one solution $(\varphi_n^{0\ell}, \varphi_p^{0\ell}) \in H_{\Gamma_{Nn}}^1(\Omega_n) \times H_{\Gamma_{Np}}^1(\Omega_p)$. Thus, $(\varphi_n^\ell, \varphi_p^\ell) := (\varphi_n^{0\ell} + \varphi_n^D, \varphi_p^{0\ell} + \varphi_n^{0\ell} + \varphi_n^D) \in (\varphi_n^D + H_{\Gamma_{Nn}}^1(\Omega_n)) \times (\varphi_n^\ell + H_{\Gamma_{Np}}^1(\Omega_p))$ solves

$$\begin{aligned} & \int_{\Omega^{\text{dev}}} d_n(\psi, \tilde{\varphi}_n, \tilde{T}) \nabla \varphi_n^\ell \cdot \nabla \bar{\varphi}_n \, dx + \int_{\Omega^{\text{org}}} d_p(\psi, \tilde{\varphi}_p, \tilde{T}) \nabla \varphi_p^\ell \cdot (\nabla \bar{\varphi}_p + \nabla \bar{\varphi}_n) \, dx \\ & = \int_{\Omega^{\text{org}}} \rho_\ell(\varphi_n^\ell, \varphi_p^\ell) \tilde{r}\left(\exp\frac{\varphi_n^\ell - \varphi_p^\ell}{\tilde{T}} - 1\right) \bar{\varphi}_p \, dx \quad \forall \bar{\varphi}_j \in H_{\Gamma_{Nj}}^1(\Omega_j). \end{aligned} \quad (3.9)$$

Arguing as in the first step of the proof of Lemma 3.2, we find $\|\varphi_j^\ell\|_{L^\infty(\Omega_j)} \leq K, j = n, p$. Therefore, if we choose $\ell \geq 2K$, each solution to $B_{(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})}^\ell(\varphi_n^0, \varphi_p^0) = 0$ leads via $(\varphi_n, \varphi_p) := (\varphi_n^0 + \varphi_n^D, \varphi_p^0 + \varphi_n^0 + \varphi_n^D) \in (\varphi_n^D + H_{\Gamma_{Nn}}^1(\Omega_n)) \times (\varphi_n + H_{\Gamma_{Np}}^1(\Omega_p))$ to a weak solution to (3.6), as well. Again, as in the proof of Lemma 3.2, we obtain $\|\varphi_j\|_{L^\infty(\Omega_j)} \leq K, j = n, p$.

2. Uniqueness. To verify the uniqueness of the weak solution to (3.6), we assume there would be two solutions $\varphi_n^i \in \varphi_n^D + H_{\Gamma_{Nn}}^1(\Omega_n), \varphi_p^i \in \varphi_n^i + H_{\Gamma_{Np}}^1(\Omega_p), i = 1, 2$. By testing (3.6) for these two solutions with $(\varphi_n^1 - \varphi_n^2, \varphi_p^1 - \varphi_n^1 - \varphi_p^2 + \varphi_n^2) \in H_{\Gamma_{Nn}}^1(\Omega_n) \times H_{\Gamma_{Np}}^1(\Omega_p)$ we find

$$\begin{aligned} & \int_{\Omega_n} \tilde{d}_n |\nabla(\varphi_n^1 - \varphi_n^2)|^2 \, dx + \int_{\Omega_p} \tilde{d}_p \nabla(\varphi_p^1 - \varphi_p^2) \cdot \nabla(\varphi_p^1 - \varphi_n^1 - \varphi_p^2 + \varphi_n^2 + \varphi_n^1 - \varphi_n^2) \, dx \\ & = \int_{\Omega_p} \tilde{r}\left(\exp\frac{\varphi_n^1 - \varphi_p^1}{\tilde{T}} - \exp\frac{\varphi_n^2 - \varphi_p^2}{\tilde{T}}\right) (\varphi_p^1 - \varphi_n^1 - \varphi_p^2 + \varphi_n^2) \, dx. \end{aligned}$$

Therefore the monotonicity of the exponential function ensures the uniqueness result.

3. Higher integrability. With the same arguments as in Step 2 of the proof of Lemma 3.2, we establish a uniform H^1 -estimate for the weak solution to (3.6). Again, taking advantage of $a_j := \tilde{d}_j = d_j(\psi, \tilde{\varphi}_j, \tilde{T}) \in [\underline{d}, \bar{d}]$ a.e. in $\Omega_j, \|\tilde{r}\left(\exp\frac{\varphi_n - \varphi_p}{\tilde{T}} - 1\right)\|_{L^\infty(\Omega_p)} \leq c(K, T_a)$, and $\varphi_n^D \in W^{1,\infty}(\Omega_n)$, we apply the regularity result of Theorem 2.1 to problem (3.6) and obtain $\|\varphi_j\|_{W^{1,q}(\Omega_j)} \leq c_j, j = n, p$. Moreover, the L^∞ estimates of φ_n, φ_p guarantee the last estimate in (3.8). \square

Lemma 3.5 (Heat equation) *We assume (A). Let $(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) \in \mathcal{N}$ be arbitrarily given, let $\psi \in \tilde{\psi}^I + H_{\Gamma_{Np}}^1(\Omega^{\text{org}})$ be the unique weak solution to the nonlinear Poisson equation (3.4) and let $(\varphi_n, \varphi_p) \in (\varphi_n^D + W_{\Gamma_{Nn}}^{1,q}(\Omega_n)) \times (\varphi_n + W_{\Gamma_{Np}}^{1,q}(\Omega_p))$ be the unique solution to (3.6). Then there exists a unique weak solution $T \in W^{1,\hat{t}}(\Omega)$ to (3.7). Uniformly for all $(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) \in \mathcal{N}$, it satisfies*

$$\|T\|_{W^{1,\hat{t}}(\Omega)} \leq c_{\hat{t},T}, \quad \|T\|_{W^{1,t}(\Omega)} \leq c_{t,T}, \quad \text{and} \quad T \geq T_a \text{ a.e. in } \Omega. \quad (3.10)$$

Proof. By Lemma 3.4, the reaction heat $\tilde{r}\left(\exp\frac{\varphi_n - \varphi_p}{\tilde{T}} - 1\right)(\varphi_n - \varphi_p)$ as well as the Joule heat terms $\tilde{d}_n |\nabla \varphi_n|^2, \tilde{d}_p |\nabla \varphi_p|^2$ have bounded norms in $L^\infty(\Omega_p)$ and $L^{q/2}(\Omega_n), L^{q/2}(\Omega_p)$, respectively. By

(A6) and since $q > 2$, there is a unique weak solution T to the (linear) heat equation (3.7) with Robin boundary conditions in the $H^1(\Omega)$ setting. It satisfies

$$\begin{aligned} \|T\|_{H^1(\Omega)} &\leq c \left(\bar{d} \|\nabla \varphi_n\|_{L^{q/2}(\Omega_n)}^2 + \bar{d} \|\nabla \varphi_p\|_{L^{q/2}(\Omega_p)}^2 + T_a \|\beta\|_{L^\infty(\Gamma)} \right) \\ &\quad + \left\| \tilde{r} \left(\exp \frac{\varphi_n - \varphi_p}{\tilde{T}} - 1 \right) (\varphi_n - \varphi_p) \right\|_{L^\infty(\Omega_p)} \leq c. \end{aligned}$$

We denote $\tilde{h} := \tilde{d}_n |\nabla \varphi_n|^2 \chi_n + \tilde{d}_p |\nabla \varphi_p|^2 \chi_p + \tilde{r} \left(\exp \frac{\varphi_n - \varphi_p}{\tilde{T}} - 1 \right) (\varphi_n - \varphi_p) \chi_p$. For t from (2.8) the operator $\hat{\mathcal{A}}_\lambda : W^{1,t}(\Omega) \rightarrow W^{1,t}(\Omega)^*$ (defined via (2.7)) is a topological isomorphism. Thus, we obtain $T \in W^{1,t}(\Omega)$ and the estimate

$$\begin{aligned} \|T\|_{W^{1,t}(\Omega)} &\leq c \|\hat{\mathcal{A}}_\lambda^{-1}\|_{\mathcal{L}(W^{1,t}(\Omega)^*, W^{1,t}(\Omega))} \left(\|\tilde{h} + T\|_{W^{1,t}(\Omega)^*} + \|\beta\|_{L^\infty(\Gamma)} (\|T\|_{L^t(\Gamma)} + T_a) \right) \\ &\leq c \left(\|\nabla \varphi_n\|_{L^{q/2}(\Omega_n)}^2 + \|\nabla \varphi_p\|_{L^{q/2}(\Omega_p)}^2 + \|T\|_{H^1(\Omega)} + 1 \right) \\ &\quad + \left\| \tilde{r} \left(\exp \frac{\varphi_n - \varphi_p}{\tilde{T}} - 1 \right) (\varphi_n - \varphi_p) \right\|_{L^\infty(\Omega_p)} \leq c_{t,T}. \end{aligned}$$

And also $\|T\|_{W^{1,\hat{t}}(\Omega)} \leq c_{\hat{t},T}$ follows. The test by $(T - T_a)^-$ yields $T \geq T_a$ a.e. in Ω . \square

3.3 Complete continuity of the fixed-point map \mathcal{Q}

Here, we prove the complete continuity of the fixed-point map $\mathcal{Q} : \mathcal{N} \rightarrow \mathcal{N}$, which directly implies the continuity of \mathcal{Q} . This proof is done in several steps: Let $\tilde{\varphi}_j^l \rightarrow \tilde{\varphi}_j$ in $H^1(\Omega_j)$, $j = n, p$, and $\tilde{T}^l \rightarrow \tilde{T}$ in $W^{1,\hat{t}}(\Omega)$ for $l \rightarrow \infty$. We denote $(\varphi_n^l, \varphi_p^l, T^l) = \mathcal{Q}(\tilde{\varphi}_n^l, \tilde{\varphi}_p^l, \tilde{T}^l)$ and $(\varphi_n, \varphi_p, T) = \mathcal{Q}(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})$ and establish the following results: First, we verify for the Dirichlet functions for the Poisson equations (see (3.3)) that $\tilde{\psi}^{ll} \rightarrow \tilde{\psi}^I$ in $H^1(\Omega^{\text{org}})$ (first part of Lemma 3.6). Then, we prove $\psi^l \rightarrow \psi$ in $H^1(\Omega^{\text{org}})$ for solutions to (3.4) (second part of Lemma 3.6). Next, in Step 1 of the proof of Lemma 3.7, we derive that solutions $(\varphi_n^l, \varphi_p^l)$ to (3.6) converge strongly to (φ_n, φ_p) in $H^1(\Omega_n) \times H^1(\Omega_p)$. Finally, in Step 2 of this proof it is shown that solutions T^l to (3.7) converge strongly to T in $W^{1,\hat{t}}(\Omega)$. We conclude that $\mathcal{Q}(\tilde{\varphi}_n^l, \tilde{\varphi}_p^l, \tilde{T}^l)$ converges strongly to $\mathcal{Q}(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})$ as $l \rightarrow \infty$.

Lemma 3.6 *We assume (A). Let $(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}), (\tilde{\varphi}_n^l, \tilde{\varphi}_p^l, \tilde{T}^l) \in \mathcal{N}$ for all l and $(\tilde{\varphi}_n^l, \tilde{\varphi}_p^l, \tilde{T}^l) \rightarrow (\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})$ in $H^1(\Omega_n) \times H^1(\Omega_p) \times W^{1,\hat{t}}(\Omega)$.*

i) Then $\tilde{\psi}^{ll} \rightarrow \tilde{\psi}^I$ in $H^1(\Omega^{\text{org}})$ for the Dirichlet functions constructed in (3.3).

ii) Let ψ^l and ψ denote the unique weak solutions to (3.4) corresponding to the Dirichlet functions $\tilde{\psi}^{ll}$ and $\tilde{\psi}^I$, respectively. Then $\psi^l \rightarrow \psi$ in $H^1(\Omega^{\text{org}})$ and thus also $\psi^l \rightarrow \psi$ in $L^r(\Omega^{\text{org}})$ for all $r \in [1, \infty)$.

Proof. Step 1. We consider a sequence $(\tilde{\varphi}_n^l, \tilde{\varphi}_p^l, \tilde{T}^l) \rightarrow (\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})$ in $H^1(\Omega_n) \times H^1(\Omega_p) \times W^{1,\hat{t}}(\Omega)$. Recall that $\tilde{\psi}^{ll}$ is defined via

$$\tilde{\psi}^{ll} = \psi^I(\tilde{T}^l, \tilde{\varphi}_n^l) = \tilde{\varphi}_n^l + \tau V^2(\tilde{T}^l) + (1-\tau)V^{M-1}(\tilde{T}^l).$$

The weak convergence of the first term on the right-hand side follows directly from $\tilde{\varphi}_n^l \rightarrow \tilde{\varphi}_n$ in $H^1(\Omega_n)$. For the properties of the function τ , see Subsection 2.2. The difficult part is to prove the convergences of $V^2(\tilde{T}^l)$ and $V^{M-1}(\tilde{T}^l)$. Since $(\tilde{\varphi}_n^l, \tilde{\varphi}_p^l, \tilde{T}^l), (\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) \in \mathcal{N}$, we have uniform

L^∞ bounds for $\tilde{\varphi}_j^l, \tilde{\varphi}_j, j = n, p$, as well as uniform lower bounds $\tilde{T}^l, \tilde{T} \geq T_a > 0$. The results of Lemma 2.1 ensure the needed continuity and differentiability properties of the map $T \mapsto V^i(T)$. We show the weak convergence for the terms $\tau V^i(\tilde{T}^l) \rightharpoonup \tau V^i(\tilde{T})$ in $H^1(\Omega^{\text{org}})$, $i = 2, M-1$: The compact Sobolev embedding of $W^{1,\tilde{t}}(\Omega)$ into $L^\infty(\Omega)$ ensures $\tilde{T}^l \rightarrow \tilde{T}$ in $L^2(\Omega)$ and $L^\infty(\Omega)$. Moreover, $\tilde{T}^l \rightharpoonup \tilde{T}$ in $W^{1,\tilde{t}}(\Omega)$ yields that $\nabla \tilde{T}^l \rightharpoonup \nabla \tilde{T}$ in $L^{\tilde{t}}(\Omega^{\text{org}})^2$. Let $v \in H^1(\Omega^{\text{org}})$ be arbitrarily given. Due to the continuous differentiability of the map $T \mapsto V^i(T)$ and boundedness of the derivative (see Lemma 2.1) we have

$$\int_{\Omega^{\text{org}}} \tau \left(V^i(\tilde{T}^l) - V^i(\tilde{T}) \right) v \, dx \leq c \|v\|_{L^2} \|\tilde{T}^l - \tilde{T}\|_{L^2} \sup_{\theta \geq T_a} \left| (V^i)'(\theta) \right| \rightarrow 0.$$

For the convergence of the gradients, we use the following decomposition

$$\int_{\Omega^{\text{org}}} \nabla \left[\tau \left(V^i(\tilde{T}^l) - V^i(\tilde{T}) \right) \right] \cdot \nabla v \, dx = I_1 + I_2 + I_3,$$

where

$$\begin{aligned} |I_1| &:= \left| \int_{\Omega^{\text{org}}} \left(V^i(\tilde{T}^l) - V^i(\tilde{T}) \right) \nabla \tau \cdot \nabla v \, dx \right| \\ &\leq c \|v\|_{H^1(\Omega^{\text{org}})} \|\tilde{T}^l - \tilde{T}\|_{L^2(\Omega^{\text{org}})} \sup_{\theta \geq T_a} \left| (V^i)'(\theta) \right| \rightarrow 0, \\ |I_2| &:= \left| \int_{\Omega^{\text{org}}} \tau \left[(V^i)'(\tilde{T}^l) - (V^i)'(\tilde{T}) \right] \nabla \tilde{T}^l \cdot \nabla v \, dx \right| \\ &\leq c \|v\|_{H^1(\Omega^{\text{org}})} \|\tilde{T}^l\|_{H^1(\Omega^{\text{org}})} \|\tilde{T}^l - \tilde{T}\|_{L^\infty(\Omega^{\text{org}})} \sup_{\theta \geq T_a} \left| (V^i)''(\theta) \right| \rightarrow 0 \end{aligned}$$

where we have used that $\|\tilde{T}^l\|_{H^1(\Omega)} \leq c$, $v \in H^1(\Omega^{\text{org}})$, $\tilde{T}^l \rightarrow \tilde{T}$ in $L^\infty(\Omega)$, and that $(V^i)''(\theta)$ is bounded. Moreover, since $\tau (V^i)'(\tilde{T}) \nabla v \in L^2(\Omega^{\text{org}})^2$ can be used as test function for the weak convergence $\nabla \tilde{T}^l \rightharpoonup \nabla \tilde{T}$ in $L^{\tilde{t}}(\Omega^{\text{org}})^2$, we obtain

$$I_3 := \int_{\Omega_D} \nabla(\tilde{T}^l - \tilde{T}) \cdot \nabla v \tau (V^i)'(\tilde{T}) \, dx \rightarrow 0.$$

We conclude that $\tilde{\psi}^{II} \rightharpoonup \tilde{\psi}^I$ in $H^1(\Omega^{\text{org}})$.

Step 2. Let ψ be the solution to (3.4) corresponding to the boundary function $\tilde{\psi}^I$ and let $\hat{\psi}^l \in \tilde{\psi}^{II} + H^1_I(\Omega^{\text{org}})$ be the unique solutions to the linear elliptic problems

$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla \hat{\psi}^l) &= C + \mathcal{U}(\psi, \tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) \quad \text{in } \Omega^{\text{org}}, \\ \hat{\psi}^l &= \tilde{\psi}^{II} \quad \text{on } I, \quad \varepsilon \nabla \hat{\psi}^l \cdot \nu = 0 \quad \text{on } \partial\Omega^{\text{org}} \setminus I. \end{aligned} \tag{3.11}$$

(Note the right-hand side $C + \mathcal{U}(\psi, \tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})$ instead of $C + \mathcal{U}(\psi, \tilde{\varphi}_n^l, \tilde{\varphi}_p^l, \tilde{T}^l)$, where \mathcal{U} is defined in (3.2).)

Since the sequence $\tilde{\psi}^{II}$ is uniformly bounded in $H^1(\Omega^{\text{org}})$ and $C + \mathcal{U}(\psi, \tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T})$ is bounded in $L^\infty(\Omega^{\text{org}})$, the functions $\hat{\psi}^l$ are uniformly bounded in $H^1(\Omega^{\text{org}})$. Moreover, $w^l := \psi - \hat{\psi}^l$ is the solution to the linear elliptic problem with zero right-hand side and mixed boundary conditions with Dirichlet function $w^{II} = \tilde{\psi}^I - \tilde{\psi}^{II}$. The solution operator that maps the boundary value function w^{II} to the solution $w^l \in W^{II} + H^1_{\Gamma_{Np}}(\Omega^{\text{org}})$ of the linear elliptic problem is bounded and linear, and therefore

continuous. According to [20, Prop. 4.2, p. 159] this operator is also continuous with respect to the weak topology, meaning that $w^l \rightharpoonup 0$ in $H^1(\Omega^{\text{org}})$ implies $w^l = \psi - \widehat{\psi}^l \rightharpoonup 0$ in $H^1(\Omega^{\text{org}})$.

Step 3. Using the test function $\psi^l - \widehat{\psi}^l \in H_{\Gamma_{Np}}^1(\Omega^{\text{org}})$ for problem (3.4) with solution ψ^l for the right-hand side $C + \mathcal{U}(\psi^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l)$ and for problem (3.11) with solution $\widehat{\psi}^l$ for the right-hand side $C + \mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$, it follows

$$\begin{aligned} c\|\psi^l - \widehat{\psi}^l\|_{H^1(\Omega^{\text{org}})}^2 &\leq \int_{\Omega^{\text{org}}} (\mathcal{U}(\psi^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) - \mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}))(\psi^l - \widehat{\psi}^l) \, dx \\ &= \int_{\Omega^{\text{org}}} (\mathcal{U}(\psi^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) - \mathcal{U}(\widehat{\psi}^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) + \mathcal{U}(\widehat{\psi}^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) - \mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}))(\psi^l - \widehat{\psi}^l) \, dx. \end{aligned}$$

The monotonicity of $\eta \rightarrow \mathcal{G}(\eta, z)$ gives $(\mathcal{U}(\psi^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) - \mathcal{U}(\widehat{\psi}^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l))(\psi^l - \widehat{\psi}^l) \leq 0$. Since $(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l), (\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ (uniform lower and upper bounds T_a and T_u for the temperatures are available) and the sequence $\widehat{\psi}^l$ is uniformly bounded, we have continuous and bounded derivatives $\frac{\partial \mathcal{G}}{\partial \eta}, \frac{\partial \mathcal{G}}{\partial z}$ in the considered arguments (see [10, Subsec. 2.1]). The latter guarantees that

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

In summary we obtain

$$\|\psi^l - \widehat{\psi}^l\|_{H^1(\Omega^{\text{org}})} \leq c(\|\widehat{\psi}^l - \psi\|_{L^2(\Omega^{\text{org}})} + \|\widetilde{\varphi}_n^l - \widetilde{\varphi}_n\|_{L^2(\Omega^{\text{org}})} + \|\widetilde{\varphi}_p^l - \widetilde{\varphi}_p\|_{L^2(\Omega^{\text{org}})} + \|\widetilde{T}^l - \widetilde{T}\|_{L^2(\Omega^{\text{org}})})$$

which tends to zero because of Step 2 and $\widetilde{\varphi}_n^l \rightarrow \widetilde{\varphi}_n, \widetilde{\varphi}_p^l \rightarrow \widetilde{\varphi}_p, \widetilde{T}^l \rightarrow \widetilde{T}$ in $L^2(\Omega^{\text{org}})$.

Step 4. Together with $\widehat{\psi}^l \rightharpoonup \psi$ in $H^1(\Omega^{\text{org}})$ from Step 2, we conclude that $\psi^l \rightharpoonup \psi$ in $H^1(\Omega^{\text{org}})$ and thus also $\psi^l \rightarrow \psi$ in $L^r(\Omega^{\text{org}})$ for all $r \in [1, \infty)$ as $l \rightarrow \infty$. \square

Lemma 3.7 *Under Assumption (A), the map $\mathcal{Q} : \mathcal{N} \rightarrow \mathcal{N}$, defined in Subsection 3.1, is completely continuous.*

Proof. We consider $(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l), (\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$, where $\widetilde{\varphi}_j^l \rightharpoonup \widetilde{\varphi}_j$ in $W^{1,q}(\Omega_j)$, $j = n, p$, and $\widetilde{T}^l \rightharpoonup \widetilde{T}$ in $W^{1,\hat{t}}(\Omega)$ and show the strong convergence $(\varphi_n^l, \varphi_p^l, T^l) := \mathcal{Q}(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) \rightarrow (\varphi_n, \varphi_p, T) := \mathcal{Q}(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$ in $H^1(\Omega_n) \times H^1(\Omega_p) \times W^{1,\hat{t}}(\Omega)$.

Step 1. We first verify the strong convergence $\varphi_j^l \rightarrow \varphi_j$ in $H^1(\Omega_j)$, $j = n, p$. The assumed weak convergences imply the strong convergences $\widetilde{\varphi}_j^l \rightarrow \widetilde{\varphi}_j$ in $L^\pi(\Omega_j)$, $j = n, p$, and $\widetilde{T}^l \rightarrow \widetilde{T}$ in $L^\pi(\Omega)$ for any $\pi \in [1, \infty)$. Moreover, Lemma 3.6 guarantees for the corresponding unique weak solutions to (3.4) that also $\psi^l \rightarrow \psi$ in $L^\pi(\Omega^{\text{org}})$ for all $\pi \in [1, \infty)$. We fix now $\pi := \frac{2q}{q-2} > 2$.

The Lipschitz continuity of the functions d_j and r for bounded arguments with a positive lower bound for the temperature leads to the convergences

$$\begin{aligned} \widetilde{d}_j^l &:= d_j(\psi^l, \widetilde{\varphi}_j^l, \widetilde{T}^l) \rightarrow \widetilde{d}_j := d_j(\psi, \widetilde{\varphi}_j, \widetilde{T}) \quad \text{in } L^\pi(\Omega_j), \quad j = n, p, \\ \widetilde{r}^l &:= r(\widetilde{n}^l, \widetilde{p}^l, \widetilde{T}^l) \rightarrow \widetilde{r} := r(\widetilde{n}, \widetilde{p}, \widetilde{T}) \quad \text{in } L^\pi(\Omega_p). \end{aligned} \tag{3.12}$$

We test the equations (3.6) for (φ_n, φ_p) and $(\varphi_n^l, \varphi_p^l)$ (same Dirichlet function φ_n^D) by $(\varphi_n - \varphi_n^l, \varphi_p - \varphi_n - \varphi_p^l + \varphi_n^l) \in H_{\Gamma_{Nn}}^1(\Omega_n) \times H_{\Gamma_{Np}}^1(\Omega_p)$. Let us note that

$$(i) \quad (\widetilde{d}_n \nabla \varphi_n - \widetilde{d}_n^l \nabla \varphi_n^l) \cdot \nabla (\varphi_n - \varphi_n^l) = \widetilde{d}_n |\nabla (\varphi_n - \varphi_n^l)|^2 + (\widetilde{d}_n - \widetilde{d}_n^l) \nabla \varphi_n^l \cdot \nabla (\varphi_n - \varphi_n^l),$$

$$\begin{aligned}
\text{(ii)} \quad & (\tilde{d}_p \nabla \varphi_p - \tilde{d}_p^l \nabla \varphi_p^l) \cdot \nabla (\varphi_p - \varphi_n - \varphi_p^l + \varphi_n^l + \varphi_n - \varphi_n^l) \\
& = \tilde{d}_p |\nabla (\varphi_p - \varphi_p^l)|^2 + (\tilde{d}_p - \tilde{d}_p^l) \nabla \varphi_p^l \cdot \nabla (\varphi_p - \varphi_p^l), \\
\text{(iii)} \quad & (\tilde{r} (\exp \frac{\varphi_n - \varphi_p}{T} - 1) - \tilde{r}^l (\exp \frac{\varphi_n^l - \varphi_p^l}{T^l} - 1)) (\varphi_p - \varphi_n - \varphi_p^l + \varphi_n^l) \\
& = (\tilde{r} - \tilde{r}^l) (\exp \frac{\varphi_n^l - \varphi_p^l}{T^l} - 1) (\varphi_p - \varphi_n - \varphi_p^l + \varphi_n^l) \\
& + \tilde{r} (\exp \frac{\varphi_n - \varphi_p}{T} - \exp \frac{\varphi_n^l - \varphi_p^l}{T^l}) (\varphi_p - \varphi_n - \varphi_p^l + \varphi_n^l).
\end{aligned}$$

Moreover, we take into account that the last term on the right-hand side of (iii) is non-positive due to the monotonicity of the exponential function. Since $\bar{d} \geq \tilde{d}_j$, $\tilde{d}_j^l \geq \underline{d}$ the identities in (i), (ii), and (iii) yield after testing

$$\begin{aligned}
\sum_{j=n,p} \|\nabla (\varphi_j - \varphi_j^l)\|_{L^2(\Omega_j)}^2 &\leq c \sum_{j=n,p} \|\tilde{d}_j - \tilde{d}_j^l\|_{L^\pi(\Omega_j)} \|\varphi_j^l\|_{W^{1,q}(\Omega_j)} \|\nabla (\varphi_j - \varphi_j^l)\|_{L^2(\Omega_j)} \\
&+ c \|\tilde{r} - \tilde{r}^l\|_{L^2(\Omega_p)} \sum_{j=n,p} \|\varphi_j - \varphi_j^l\|_{L^2(\Omega_j)}.
\end{aligned}$$

Therefore Sobolev's embedding and Young's inequality ensure

$$\sum_{j=n,p} \|\varphi_j - \varphi_j^l\|_{H^1(\Omega_j)}^2 \leq c \left(\sum_{j=n,p} \|\tilde{d}_j - \tilde{d}_j^l\|_{L^\pi(\Omega_j)}^2 \|\varphi_j^l\|_{W^{1,q}(\Omega_j)}^2 + \|\tilde{r} - \tilde{r}^l\|_{L^2(\Omega_p)}^2 \right) \rightarrow 0,$$

where we have also used $\|\varphi_j^l\|_{W^{1,q}(\Omega_j)} \leq c_j$ and the convergence in (3.12).

Step 2. It remains to verify that $T^l \rightarrow T$ in $W^{1,\hat{t}}(\Omega)$ for the corresponding solutions to the heat equations (3.7). According to Lemma 3.5, we have $\|T^l\|_{W^{1,\hat{t}}} \leq c_{\hat{t},T}$ for all l . First, we show that all weakly convergent subsequences of $\{T^l\}$ in $W^{1,\hat{t}}(\Omega)$ converge weakly to T . Then, we have $T^l \rightarrow T$ in $W^{1,\hat{t}}(\Omega)$ for the entire sequence ([6, Lemma 5.4]).

Indeed, let us take some subsequence $\{T^{l_k}\}$ and some $T^* \in W^{1,\hat{t}}(\Omega)$ such that $T^{l_k} \rightharpoonup T^*$ in $W^{1,\hat{t}}(\Omega)$. We verify that $T^* = T$. We consider a further non-re-labeled subsequence, where especially $\varphi_j^{l_k} \rightarrow \varphi_j$ in $H^1(\Omega_j)$, $\varphi_j^{l_k} \rightarrow \varphi_j$ a.e. in Ω_j , $\tilde{T}^{l_k} \rightarrow \tilde{T}$ a.e. in Ω , $\psi^{l_k} \rightarrow \psi$ a.e. in Ω^{org} , $j = n, p$. Our construction of $q, \hat{q}, t, \hat{t} > 2$ in Subsection 2.4 ensures the embedding $L^{\hat{q}/2}(\Omega) \hookrightarrow W^{1,\hat{t}}(\Omega)^*$. The result of Gröger [12] for the linear heat equation guarantees the estimate,

$$\|T^{l_k} - T\|_{W^{1,\hat{t}}(\Omega)} \leq c \|\tilde{h}^{l_k} - \tilde{h}\|_{W^{1,\hat{t}}(\Omega)^*} + \theta^{l_k} \leq c \|\tilde{h}^{l_k} - \tilde{h}\|_{L^{\hat{q}/2}(\Omega)} + \theta^{l_k} \quad (3.13)$$

with the right-hand sides

$$\tilde{h}^{l_k} := h(\tilde{n}^{l_k}, \tilde{p}^{l_k}, \tilde{T}^{l_k}, \nabla \varphi_n^{l_k}, \nabla \varphi_p^{l_k}, \varphi_n^{l_k}, \varphi_p^{l_k}), \quad \tilde{h} := h(\tilde{n}, \tilde{p}, \tilde{T}, \nabla \varphi_n, \nabla \varphi_p, \varphi_n, \varphi_p),$$

and $\theta^{l_k} \rightarrow 0$ for $T^{l_k} \rightarrow T$ in $H^1(\Omega)$. We have to show $\|\tilde{h}^{l_k} - \tilde{h}\|_{L^{\hat{q}/2}(\Omega)} \rightarrow 0$. Since

$$\begin{aligned}
& \left| \tilde{d}_j^{l_k} |\nabla \varphi_j^{l_k}|^2 - \tilde{d}_j |\nabla \varphi_j|^2 \right| \\
& \leq \tilde{d}_j^{l_k} |\nabla (\varphi_j^{l_k} - \varphi_j)| |\nabla \varphi_j^{l_k}| + \tilde{d}_j^{l_k} |\nabla \varphi_j| |\nabla (\varphi_j^{l_k} - \varphi_j)| + |\tilde{d}_j^{l_k} - \tilde{d}_j| |\nabla \varphi_j|^2
\end{aligned}$$

we find with (2.9)

$$\begin{aligned}
& \|\tilde{d}_j^{l_k} |\nabla \varphi_j^{l_k}|^2 - \tilde{d}_j |\nabla \varphi_j|^2\|_{L^{\hat{q}/2}(\Omega_j)}^{\hat{q}/2} \\
& \leq c \int_{\Omega_j} \left(|\nabla (\varphi_j^{l_k} - \varphi_j)|^{\hat{q}/2} |\nabla \varphi_j^{l_k}|^{\hat{q}/2} + |\nabla \varphi_j|^{\hat{q}/2} |\nabla (\varphi_j^{l_k} - \varphi_j)|^{\hat{q}/2} + |\tilde{d}_j^{l_k} - \tilde{d}_j|^{\hat{q}/2} |\nabla \varphi_j|^{\hat{q}} \right) dx \\
& \leq c \|\varphi_j^{l_k} - \varphi_j\|_{H^1(\Omega_j)}^{\hat{q}/2} \left(\|\varphi_j^{l_k}\|_{W^{1,q}(\Omega_j)}^{\hat{q}/2} + \|\varphi_j\|_{W^{1,q}(\Omega_j)}^{\hat{q}/2} \right) + c \int_{\Omega_j} |\tilde{d}_j^{l_k} - \tilde{d}_j|^{\hat{q}/2} |\nabla \varphi_j|^{\hat{q}} dx.
\end{aligned}$$

Using the a.e. convergence $\tilde{d}_j^{l_k} \rightarrow \tilde{d}_j$ and the integrable majorant $c|\nabla\varphi_j|^{\hat{q}}$, Lebesgue's dominated convergence theorem gives the convergence to zero of the last integral. Since $\|\varphi_j^{l_k} - \varphi_j\|_{H^1(\Omega_j)} \rightarrow 0$ and $\|\varphi_j^{l_k}\|_{W^{1,q}(\Omega_j)}, \|\varphi_j\|_{W^{1,q}(\Omega_j)} \leq c_j$ the right-hand side tends to zero for the considered subsubsequence. Moreover, exploiting

$$\tilde{r}^{l_k} \rightarrow \tilde{r} \text{ and } \exp \frac{\varphi_n^{l_k} - \varphi_p^{l_k}}{\tilde{T}^{l_k}} \rightarrow \exp \frac{\varphi_n - \varphi_p}{\tilde{T}} \text{ a.e. in } \Omega^{\text{org}},$$

and the integrable majorant $(4K\tilde{r}\bar{N}^2 \exp \frac{2K}{T_a})^{\hat{q}/2}$ Lebesgue's dominated convergence theorem gives for this subsequence

$$\int_{\Omega^{\text{org}}} \left| \tilde{r}^{l_k} \left(\exp \frac{\varphi_n^{l_k} - \varphi_p^{l_k}}{\tilde{T}^{l_k}} - 1 \right) (\varphi_n^{l_k} - \varphi_p^{l_k}) - \tilde{r} \left(\exp \frac{\varphi_n - \varphi_p}{\tilde{T}} - 1 \right) (\varphi_n - \varphi_p) \right|^{\hat{q}/2} dx \rightarrow 0.$$

Thus, we conclude $\|\tilde{h}^{l_k} - \tilde{h}\|_{L^{\hat{q}/2}(\Omega)} \rightarrow 0$. Therefore, by testing the heat equations for T^{l_k} and T (with corresponding right-hand sides) with $T^{l_k} - T$, we obtain $\|T^{l_k} - T\|_{H^1(\Omega)} \rightarrow 0$. Moreover, due to (3.13) this ensures $T^{l_k} \rightarrow T$ in $W^{1,\hat{t}}(\Omega)$. According to [12], the solution to (3.7) with right-hand side \tilde{h} is unique, and it follows that $T^{l_k} \rightarrow T^* = T$ in $W^{1,\hat{t}}(\Omega)$, for this subsequence. Since we verified for arbitrary weakly convergent subsequences $T^{l_k} \rightharpoonup T^*$ in $W^{1,\hat{t}}(\Omega)$ that $T^* = T$, we obtain the weak convergence of the entire sequence $T^l \rightharpoonup T$ in $W^{1,\hat{t}}(\Omega)$.

Summarizing, at least for one subsequence $\{T^{l_k}\}$, we proved $T^{l_k} \rightarrow T$ in $W^{1,\hat{t}}(\Omega)$, and for the entire sequence we know $T^l \rightharpoonup T$ in $W^{1,\hat{t}}(\Omega)$. The arguments of Step 3 and the uniqueness of the weak limit ensure that every strongly converging subsequence converges to T . If there would be any subsequence $\{T^{l_n}\}$ that does not contain any converging subsequence then there would be a $\delta > 0$ such that $\|T^{l_n} - T\|_{W^{1,\hat{t}}(\Omega)} \geq \delta$ for all l_n . Following again the arguments of Step 2, we lead this to a contradiction using the convergences a.e. for a corresponding non-relabelled subsequence. At the end, the entire sequence T^l must strongly converge to T in $W^{1,\hat{t}}(\Omega)$, which completes the proof. \square

3.4 Proof of Theorem 3.1

Proof. Step 1. Since the set \mathcal{N} is nonempty, convex, and closed in $H^1(\Omega^{\text{dev}}) \times H^1(\Omega^{\text{org}}) \times W^{1,\hat{t}}(\Omega)$, Lemma 3.7, and Schauder's fixed point theorem ensure the existence of a fixed point $(\varphi_n, \varphi_p, T) \in \mathcal{N}$ of \mathcal{Q} . In particular, we have $\varphi_j \in W^{1,q}(\Omega_j)$, $j = n, p$, $T \geq T_a$ and $\ln T \in L^\infty(\Omega)$. For $(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) = (\varphi_n, \varphi_p, T)$, we define the Dirichlet function $\tilde{\psi}^I$ according to (3.3) and solve uniquely the nonlinear Poisson equation (3.4) (see Lemma 3.3) to obtain the electrostatic potential $\psi \in \tilde{\psi}^I + H_{\Gamma_{Np}}^1(\Omega^{\text{org}})$. Then $(\varphi_n, \varphi_p, \psi, T)$ is a solution to (P).

Step 2. The norm estimates for φ_j , stated in Theorem 3.1, follow directly from Theorem 2.1 for $a_j = d_j(\psi, \varphi_j, T)$, $j = n, p$. Setting $(\tilde{\varphi}_n, \tilde{\varphi}_p, \tilde{T}) = (\varphi_n, \varphi_p, T)$, the $W^{1,t}(\Omega)$ estimate for T is derived in the proof of Lemma 3.5, the L^∞ estimate then follows from the continuous embedding of $W^{1,t}(\Omega)$ in $L^\infty(\Omega)$. Since Lemma 3.3 provides $\|\psi\|_{L^\infty(\Omega^{\text{org}})} \leq c_{\psi,\infty}$, it only remains to verify the $W^{1,s}$ estimate for ψ . Lemma 3.4 and Lemma 3.5 together with Lemma 2.2 ensure that the boundary function for the Poisson equation ψ^I is bounded in $W^{1,s}(\Omega^{\text{org}})$. Additionally, we have $\|C - n + p\|_{L^\infty} \leq 3\bar{N}$. Since \mathcal{A}_ε for s from (2.10) is a topological isomorphism we find

$$\begin{aligned} \|\psi\|_{W^{1,s}(\Omega^{\text{org}})} &\leq \|\psi^I\|_{W^{1,s}(\Omega^{\text{org}})} + \|\mathcal{A}_\varepsilon^{-1}\|_{\mathcal{L}(W_{\Gamma_{Np}}^{-1,s}(\Omega^{\text{org}}), W_{\Gamma_{Np}}^{1,s}(\Omega^{\text{org}}))} \times \\ &\times \left(\|C - n + p + \psi - \psi^I\|_{W_T^{-1,s}(\Omega^{\text{org}})} + c\|\hat{\mathcal{A}}_\varepsilon\|_{\mathcal{L}(W^{1,s}(\Omega^{\text{org}}), W^{1,s'}(\Omega^{\text{org}})^*)} \|\psi^I\|_{W^{1,s}(\Omega^{\text{org}})} \right) \\ &\leq c(\|C - n + p\|_{L^\infty(\Omega^{\text{org}})} + c_{\psi,\infty} + \|\psi^I\|_{W^{1,s}(\Omega^{\text{org}})}) \leq c. \end{aligned}$$

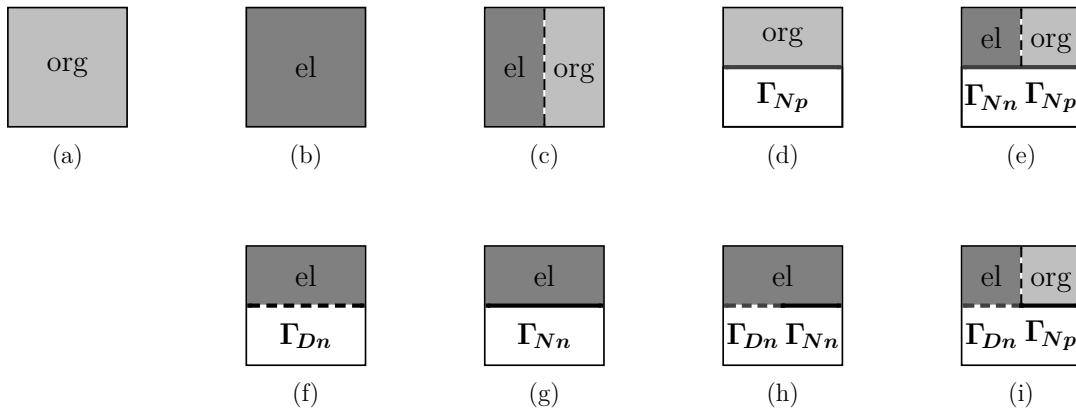


Figure 2: Model sets $C_1(0)$ with different materials (electrode/organics) and different boundary conditions. Dashed lines indicate Dirichlet boundary conditions.

This estimate finishes the proof.

4 Proof of the regularity result in Theorem 2.1

To prove the higher integrability of $\nabla\varphi_n$ and $\nabla\varphi_p$ for solutions to Problem (P_C) , we proceed in several steps: First, we localize the problem to squares, where we distinguish between the different situations depicted in Fig. 2 (a) – (i). Then, we derive Caccioppoli-type inequalities near the boundary (Lemma 4.1) and use reflection arguments to extend the estimates from half squares to full squares (Lemma 4.2). The Caccioppoli-type inequalities for interior squares are derived similarly and hence only briefly discussed (Lemma 4.3). Finally, we establish the higher integrability of the gradients by applying a Gehring-type lemma (Subsection 4.5).

We highlight that from now on, the letters r, s, t refer to arbitrary real numbers that are not related to the reaction rate coefficient and the exponents in the previous sections.

4.1 Localization

We denote by $C_1(0) \subset \mathbb{R}^2$ the unit square centered at 0 with side length 2 and by $C_1^+(0)$ its upper half. For $x^0 \in \partial\Omega^{\text{dev}}$ let $\Phi_{x^0} : U_{x^0} \cap \Omega^{\text{dev}} \rightarrow C_1^+(0)$ and for $x^0 \in \Omega^{\text{dev}}$ let $\Phi_{x^0} : U_{x^0} \cap \Omega^{\text{dev}} \rightarrow C_1(0)$ be bi-Lipschitz transformations with $\Phi_{x^0}(x) = y$, which exist due to (A1). Let

$$\overline{\Omega^{\text{dev}}} \subset \bigcup_{i=1}^{L_S} \Phi_{x_i^0}^{-1}(C_{\frac{1}{24}}(0)) \cup \bigcup_{i=L_S+1}^L \Phi_{x_i^0}^{-1}(C_{\frac{1}{24}}(0))$$

be a finite open covering of $\overline{\Omega^{\text{dev}}}$. If $x^0 \in \partial\Omega^{\text{dev}}$ is such that $\Gamma_{Dn} \cap U_{x^0} \neq \emptyset$, we denote $\widehat{\Gamma}_{Dn} = \Phi_{x^0}(\Gamma_{Dn} \cap U_{x^0})$ the localized part of the Dirichlet boundary Γ_{Dn} . We find constants $0 < \underline{\gamma} \leq \overline{\gamma} < \infty$ such that for $\gamma_i(y) := |\det D\Phi_{x_i^0}^{-1}(y)|$ it holds $\gamma_i \in L^\infty(C_1(0))$ and $\underline{\gamma} \leq \gamma_i(y) \leq \overline{\gamma}$ almost everywhere. For the center points $x_i^0, i = 1, \dots, L$, we introduce

$$\begin{aligned} v_n &:= \varphi_n \circ \Phi_{x_i^0}^{-1}, & v_p &:= \varphi_p \circ \Phi_{x_i^0}^{-1}, & v_n^D &:= \varphi_n^D \circ \Phi_{x_i^0}^{-1}, & \bar{v}_j &:= \bar{\varphi}_j \circ \Phi_{x_i^0}^{-1}, \\ \widehat{a}_j(y) &:= a_j(\Phi_{x_i^0}^{-1}(y)), & \widehat{f}_C(y) &:= f_C(\Phi_{x_i^0}^{-1}(y)), & \widehat{\chi}_{\text{org}}(y) &:= \chi_{\text{org}}(\Phi_{x_i^0}^{-1}(y)) \end{aligned}$$

and neglect the dependency on x_i^0 of the transformation $\Phi_{x_i^0}$.

In the following, we concentrate on the covering of the boundary. For $i = 1, \dots, L$, we have $x_i^0 \in \partial\Omega^{\text{dev}}$. Let x^0 be one of them. According to the transformation formula, we obtain for the solution to problem (P_C) and for test functions $\bar{\varphi}_j \in H_{\Gamma_{D_j}}^1(\Omega_j)$ with support in $U_{x^0} \cap (\Omega_j \cup \Gamma_{N_j})$, $j = n, p$, that

$$\begin{aligned} 0 &= \int_{U_{x^0} \cap \Omega_n} a_n \nabla \varphi_n \cdot \nabla \bar{\varphi}_n \, dx + \int_{U_{x^0} \cap \Omega_p} \{a_p \nabla \varphi_p \cdot \nabla (\bar{\varphi}_n + \bar{\varphi}_p) - f_C \bar{\varphi}_p\} \, dx \\ &= \int_{C_1^+(0)} \left\{ a_n(\Phi^{-1}(y)) \nabla_x \varphi_n(\Phi^{-1}(y)) \cdot \nabla_x \bar{\varphi}_n(\Phi^{-1}(y)) \right. \\ &\quad + \chi_{\text{org}}(\Phi^{-1}(y)) \left\{ a_p(\Phi^{-1}(y)) \nabla_x \varphi_p(\Phi^{-1}(y)) \cdot \nabla_x (\bar{\varphi}_n(\Phi^{-1}(y)) + \bar{\varphi}_p(\Phi^{-1}(y))) \right. \\ &\quad \left. \left. - f_C(\Phi^{-1}(y)) \bar{\varphi}_p(\Phi^{-1}(y)) \right\} \right\} |\det D\Phi^{-1}(y)| \, dy \end{aligned}$$

which, for $H(y) = D\Phi|_{\Phi^{-1}(y)}$, gives us the “localized” relation

$$\begin{aligned} 0 &= \int_{C_1^+(0)} \left\{ \hat{a}_n(\nabla_y v_n H) \cdot (\nabla_y \bar{v}_n H) \right. \\ &\quad \left. + \hat{\chi}_{\text{org}}(\hat{a}_p(\nabla_y v_p H) \cdot (\nabla_y \bar{v}_n H + \nabla_y \bar{v}_p H) - \hat{f}_C \bar{v}_p) \right\} \gamma \, dy. \end{aligned} \quad (4.1)$$

Here and later we leave out the argument y . Note that $0 < \underline{d}\gamma \leq \hat{a}_n \gamma \leq \bar{d}\gamma$ a.e. in $C_1^+(0)$, $0 < \underline{d}\gamma \leq \hat{a}_p \gamma \leq \bar{d}\gamma$ a.e. in $C_1^+(0) \cap \text{supp} \hat{\chi}_{\text{org}}$. Moreover, we introduce the notation

$$\begin{aligned} \underline{\epsilon} &:= \min_{i=1, \dots, L} \left\{ \epsilon : \epsilon \text{ is the smallest eigenvalue of } D\Phi_{x_i^0}^T D\Phi_{x_i^0} \text{ on } U_{x_i^0} \cap \Omega^{\text{dev}} \right\}, \\ \bar{\epsilon} &:= \max_{i=1, \dots, L} \left\{ \epsilon_n : \epsilon_n \text{ is the maximal norm of } D\Phi_{x_i^0}^T D\Phi_{x_i^0} \text{ on } U_{x_i^0} \cap \Omega^{\text{dev}} \right\}. \end{aligned}$$

We have to study the different model cases for $C_1(0)$ depicted in Fig. 2. The interesting situations are the ones at the boundary, i.e., where $x^0 \in \partial\Omega^{\text{dev}}$. The “interior” cases (a), (b) and (c) with $x^0 \in \Omega^{\text{dev}}$ follow by similar arguments, hence, they are only briefly discussed.

4.2 Caccioppoli-type inequalities near the boundary

We consider further squares $C_s(y^0)$ with smaller side length $0 < 2s < 2$ and centers y^0 . For a given $y^0 \in C_{1/4}^+(0)$ and $0 < r < \frac{1}{4}$ we have $C_{3r}(y^0) \subset C_1(0)$. We often abbreviate $C_r(y^0)$ with C_r and $C_r^+(y^0) := \{y \in C_r(y^0) : y_2 > 0\}$ with C_r^+ , respectively. For a given y^0 , we denote by $C_{r_{\text{org}}}^+$ (resp. $C_{3r_{\text{org}}}^+$) the part of $C_r^+(y^0)$ (resp. $C_{3r}^+(y^0)$), which belongs to the organic region, $m_{r_{\text{org}}}^+(v)$ (resp. $m_{3r_{\text{org}}}^+(v)$) stands for the mean value of a function v on $C_{r_{\text{org}}}^+$ (resp. $C_{3r_{\text{org}}}^+$). A corresponding notion is used for the electrode region $C_{r_{\text{el}}}^+$.

Note that the geometric structure of the sets $C_r \subset C_1(0)$ and $C_r^+ \subset C_1^+(0)$ is not necessarily the same as for their parents C_1 and C_1^+ , i.e., if C_1 or C_1^+ corresponds to one of the model cases in Fig. 2, the smaller sets are in general different (except for cases (a) and (b) in Fig. 2). The new resulting cases for C_r^+ are collected in Tables 1 and 2.

Lemma 4.1 *Let the assumptions of Theorem 2.1 be satisfied. We suppose that $x^0 \in \partial\Omega^{\text{dev}}$ and that $\Phi_{x^0} : U_{x^0} \cap \Omega^{\text{dev}} \rightarrow C_1^+(0)$ is the corresponding bi-Lipschitzian map leading to one of the Cases*

(d)–(i) in Fig. 2. Let (φ_n, φ_p) be a solution to (P_C) and $v_j = \varphi_j \circ \Phi_{x_0}^{-1}$ the corresponding localized part of φ_j , $v_{n0} = \varphi_n \circ \Phi_{x_0}^{-1} - \varphi_n^D \circ \Phi_{x_0}^{-1}$, $v_{p0} = \varphi_p \circ \Phi_{x_0}^{-1} - \varphi_n \circ \Phi_{x_0}^{-1}$. Let $y^0 \in C_{1/4}^+(0)$ and $0 < r < \frac{1}{4}$. Then there exists a constant $\tilde{c}_1 > 0$ independent of y^0 and r such that

$$\begin{aligned} & \int_{C_{\frac{r}{2}}^+} \{ |\nabla v_{n0}|^2 + \widehat{\chi}_{\text{org}} |\nabla v_{p0}|^2 \} dy \\ & \leq \tilde{c}_1 \int_{C_{3r}^+} (|\nabla v_n^D|^2 + \widehat{\chi}_{\text{org}}) dy + \frac{\tilde{c}_1}{r^2} \left(\int_{C_{3r}^+} |\nabla v_{n0}| dy \right)^2 + \frac{\tilde{c}_1}{r^2} \left(\int_{C_{3r \text{ org}}^+} |\nabla v_{p0}| dy \right)^2. \end{aligned} \quad (4.2)$$

Proof. We fix an arbitrary $y^0 \in C_{1/4}^+(0)$ and consider $0 < r < \frac{1}{4}$. Moreover, we take t and s such that $\frac{r}{2} \leq t < s \leq r$. We work with cut-off functions $\xi \in C^1(\mathbb{R}^2; [0, 1])$ fulfilling

$$\xi|_{C_t} = 1, \quad \xi|_{\mathbb{R}^2 \setminus C_s} = 0, \quad |\nabla \xi| \leq \frac{\theta}{s-t}, \quad (4.3)$$

where $\theta \geq 1$ does not depend on t and s . For $v_{n0} = v_n - v_n^D$, $v_{p0} = v_p - v_n$ we have

$$\nabla(v_{j0}\xi) = \xi \nabla v_{j0} + v_{j0} \nabla \xi, \quad |\nabla v_n| \leq |\nabla v_{n0}| + |\nabla v_n^D|, \quad |\nabla v_p| \leq |\nabla v_{p0}| + |\nabla v_{n0}| + |\nabla v_n^D|. \quad (4.4)$$

Depending on the position of $C_r^+(y_0)$, we consider different test functions for the localized current-flow equation (4.1). In particular, we choose $\bar{v}_n = (v_{n0} - k_n)\xi$, $\bar{v}_p = (v_p - v_n - k_p)\xi$, where $k_j \in \mathbb{R}$ are constants to be fixed, see Tab. 1 and Tab. 2. Assuming that (\bar{v}_n, \bar{v}_p) is an admissible test function we can use it to test (4.1) to obtain with (4.4)

$$\begin{aligned} & \int_{C_s^+} \left\{ \widehat{a}_n \nabla v_n H \cdot \left[\xi \nabla (v_n - v_n^D) + (v_n - v_n^D - k_n) \nabla \xi \right] H \right. \\ & \quad + \widehat{\chi}_{\text{org}} \widehat{a}_p \nabla v_p H \cdot \left[\xi \nabla (v_p - v_n^D) + (v_p - v_n - k_p + v_n - v_n^D - k_n) \nabla \xi \right] H \\ & \quad \left. - \widehat{\chi}_{\text{org}} \xi \widehat{f}_C (v_p - v_n - k_p) \right\} \gamma dy = 0. \end{aligned} \quad (4.5)$$

Applying again (4.4), we continue by

$$\begin{aligned} & \int_{C_s^+} \xi \{ \widehat{a}_n |\nabla v_n H|^2 + \widehat{\chi}_{\text{org}} \widehat{a}_p |\nabla v_p H|^2 \} \gamma dy \\ & \leq \int_{C_s^+} \left\{ \xi \widehat{a}_n |\nabla v_n H| |\nabla v_n^D H| + \widehat{\chi}_{\text{org}} \xi \widehat{a}_p |\nabla v_p H| |\nabla v_n^D H| \right. \\ & \quad + \widehat{a}_n |\nabla v_n H| |v_{n0} - k_n| |\nabla \xi H| + \widehat{\chi}_{\text{org}} \widehat{a}_p |\nabla v_p H| (|v_{p0} - k_p| + |v_{n0} - k_n|) |\nabla \xi H| \\ & \quad \left. + \widehat{\chi}_{\text{org}} \xi |\widehat{f}_C| |v_{p0} - k_p| \right\} \gamma dy \\ & \leq \int_{C_s^+} \left\{ \xi \widehat{a}_n (|\nabla v_{n0} H| + |\nabla v_n^D H|) |\nabla v_n^D H| \right. \\ & \quad + \widehat{\chi}_{\text{org}} \xi \widehat{a}_p (|\nabla v_{p0} H| + |\nabla v_{n0} H| + |\nabla v_n^D H|) |\nabla v_n^D H| \\ & \quad + \widehat{a}_n |\nabla v_n H| |v_{n0} - k_n| |\nabla \xi H| + \widehat{\chi}_{\text{org}} \widehat{a}_p |\nabla v_p H| (|v_{p0} - k_p| + |v_{n0} - k_n|) |\nabla \xi H| \\ & \quad \left. + \widehat{\chi}_{\text{org}} \xi |\widehat{f}_C| |v_{p0} - k_p| \right\} \gamma dy. \end{aligned}$$

Using that

$$|\nabla v_{n0} H|^2 + \widehat{\chi}_{\text{org}} |\nabla v_{p0} H|^2 \leq 2 \left(2 |\nabla v_n H|^2 + \widehat{\chi}_{\text{org}} |\nabla v_p H|^2 + |\nabla v_n^D H|^2 \right),$$

no	situation	k_n	PF on	PS on	ra	Dir	k_p	PF on	PS on	ra	Dir
1	$C_r^+ = C_{rel}^+$	m_r^+	-	C_r^+	$2r \times r$	-	0	-	-	-	-
2	$ C_{rel}^+ , C_{org}^+ > 0$	m_r^+	-	C_r^+	$2r \times r$	-	0	$C_{3r\ org}^+$	-	$2r \times 3r$	$3r$
3	$C_r^+ = C_{r\ org}^+$ $\overline{C_r^+} \cap \widehat{\Gamma}_{Dp} = \emptyset$	m_r^+	-	C_r^+	$2r \times r$	-	$m_{r\ org}^+$	-	$C_{r\ org}^+$	$2r \times r$	-
4	$C_r^+ = C_{r\ org}^+$ $\overline{C_r^+} \cap \widehat{\Gamma}_{Dp} \neq \emptyset$	m_r^+	-	C_r^+	$2r \times r$	-	0	$C_{r\ org}^+$	-	$2r \times r$	r

Table 1: Parameters like constants k_j and the domains for the application of Poincaré-Friedrichs (PF) or Poincaré-Sobolev (PS) inequality Lemma B.2 and Lemma B.3 in the Case A. Here, 'ra' indicates the side lengths of a rectangle fully included in the domains for 'PF' or 'PS', respectively. 'Dir' gives the minimal length of the involved Dirichlet boundary for 'PF'.

the definition of $\underline{\epsilon}$ and $\bar{\epsilon}$ and taking into account the bounds for $\gamma, \widehat{a}_n, \widehat{a}_p, \widehat{f}_C$, (4.3), and applying Young's inequality, we find a constant $c_1 > 0$ such that

$$\begin{aligned}
& c_1 \int_{C_s^+} \xi \{ |\nabla v_{n0}|^2 + \widehat{\chi}_{org} |\nabla v_{p0}|^2 \} \, dy \\
& \leq \int_{C_s^+} c \{ \xi (|\nabla v_{n0}| + |\nabla v_n^D|) |\nabla v_n^D| + \widehat{\chi}_{org} \xi (|\nabla v_{p0}| + |\nabla v_{n0}| + |\nabla v_n^D|) |\nabla v_n^D| \\
& \quad + |\nabla v_n| |v_{n0} - k_n| \frac{1}{s-t} + \widehat{\chi}_{org} |\nabla v_p| (|v_{p0} - k_p| + |v_{n0} - k_n|) \frac{1}{s-t} \\
& \quad + \widehat{\chi}_{org} \xi |v_{p0} - k_p| \} \, dy \\
& \leq \int_{C_s^+} \left\{ \frac{c_1}{4} \xi \{ |\nabla v_{n0}|^2 + \widehat{\chi}_{org} |\nabla v_{p0}|^2 \} + c \xi |\nabla v_n^D|^2 + c \xi \widehat{\chi}_{org} |v_{p0} - k_p| \right. \\
& \quad + \frac{c_1}{8} |\nabla v_{n0}|^2 + c |\nabla v_n^D|^2 + c \left(\frac{v_{n0} - k_n}{s-t} \right)^2 \\
& \quad \left. + \widehat{\chi}_{org} \left(\frac{c_1}{8} |\nabla v_{p0}|^2 + \frac{c_1}{8} |\nabla v_{n0}|^2 + c |\nabla v_n^D|^2 + c \left(\frac{v_{p0} - k_p}{s-t} \right)^2 + c \left(\frac{v_{n0} - k_n}{s-t} \right)^2 \right) \right\} \, dy.
\end{aligned}$$

We exploit that $\xi=1$ in C_t^+ and $\xi \leq 1$, we restrict to the smaller domain C_t^+ in the left-hand side, use $s-t \in (0, 1)$ and $|v_{p0} - k_p| \leq 1 + (|v_{p0} - k_p|/(s-t))^2$ for the reaction term and arrive finally at

$$\begin{aligned}
& \int_{C_t^+} (|\nabla v_{n0}|^2 + \widehat{\chi}_{org} |\nabla v_{p0}|^2) \, dy \\
& \leq \int_{C_s^+} \left\{ \frac{1}{2} (|\nabla v_{n0}|^2 + \widehat{\chi}_{org} |\nabla v_{p0}|^2) + c (|\nabla v_n^D|^2 + \widehat{\chi}_{org}) \right\} \, dy \\
& \quad + \left(\frac{1}{s-t} \right)^2 \int_{C_s^+} c \left\{ (v_{n0} - k_n)^2 + \widehat{\chi}_{org} (v_{p0} - k_p)^2 \right\} \, dy.
\end{aligned} \tag{4.6}$$

Case A: Let $\overline{C_r^+} \cap \widehat{\Gamma}_{Dn} = \emptyset$. In dependence of C_r^+ , we choose the constants k_j and the domains for the application of Poincaré-Friedrichs (PF) or Poincaré-Sobolev (PS) inequality Lemma B.2 and Lemma B.3 as given in Tab. 1.

We estimate the last two terms in the right-hand side of (4.6) (without the factor $(s-t)^{-2}$) and follow for all cases in Tab. 1 the rules:

no	situation	k_n	PF on	PS on	ra	Dir	k_p	PF on	PS on	ra	Dir
5	$C_r^+ = C_{r\text{el}}^+$	0	C_{3r}^+	-	$6r \times 3r$	$2r$	0	-	-	-	-
6	$ C_{r\text{el}}^+ , C_{r\text{org}}^+ > 0$	0	C_{3r}^+	-	$6r \times 3r$	$2r$	0	$C_{3r\text{org}}^+$	-	$2r \times 3r$	$3r$
7	$C_r^+ = C_{r\text{org}}^+$ $\overline{C_r^+} \cap \widehat{\Gamma}_{Dp} \neq \emptyset$	0	C_{3r}^+	-	$6r \times 3r$	$2r$	0	$C_{r\text{org}}^+$	-	$2r \times r$	r

Table 2: Parameters like constants k_j and the domains for the application of Poincaré-Friedrichs (PF) or Poincaré-Sobolev (PS) inequality Lemma B.2 and Lemma B.3 in the Case B. Here, 'ra' indicates the side lengths of a rectangle fully included in the domains for 'PF' or 'PS', respectively. 'Dir' gives the minimal length of the involved Dirichlet boundary for 'PF'.

- use k_n and k_p as given in Tab. 1
- enlarge the integration domain for these terms (without factor $(s-t)^{-2}$) to the domain for Poincaré-Friedrichs (PF) or Poincaré-Sobolev (PS) inequality, respectively
- apply PF and PS inequality Lemma B.2 and Lemma B.3 with a uniform constant (geometry information in 'ra' and 'Dir' in Tab. 1 ensure this), $\max\{C_{\text{PS}}, C_{\text{PF}}\}$ is finite
- enlarge the integration domains to C_{3r}^+ and $C_{3r\text{org}}^+$, respectively.

Exemplarily, for the situation 2, we obtain

$$\begin{aligned}
& \int_{C_s^+} (|v_{n0} - m_r^+(v_{n0})|^2 + \widehat{\chi}_{\text{org}} |v_{p0}|^2) \mathbf{d}y \leq \int_{C_r^+} |v_{n0} - m_r^+(v_{n0})|^2 \mathbf{d}y + \int_{C_{3r\text{org}}^+} |v_{p0}|^2 \mathbf{d}y \\
& \leq C_{\text{PS}} \left(\int_{C_r^+} |\nabla v_{n0}| \mathbf{d}y \right)^2 + C_{\text{PF}} \left(\int_{C_{3r\text{org}}^+} |\nabla v_{p0}| \mathbf{d}y \right)^2 \\
& \leq C_{\text{PS}} \left(\int_{C_{3r}^+} |\nabla v_{n0}| \mathbf{d}y \right)^2 + C_{\text{PF}} \left(\int_{C_{3r\text{org}}^+} |\nabla v_{p0}| \mathbf{d}y \right)^2.
\end{aligned}$$

Case B: Let $\overline{C_r^+} \cap \widehat{\Gamma}_{Dn} \neq \emptyset$. Here we have to distinguish the three situations occurring in Tab. 2. Note that in the case $C_r^+ = C_{r\text{org}}^+$ with $\overline{C_r^+} \cap \widehat{\Gamma}_{Dn} \neq \emptyset$ it follows automatically $\overline{C_r^+} \cap \widehat{\Gamma}_{Dp} \neq \emptyset$. Have in mind that situation 5 has to manage also the change of Dirichlet and Neumann boundary conditions as indicated in Fig. 2 (h). We choose the parameters as given in Tab. 2 and follow exactly the rules in the items fixed in Case A.

In all the situations 1 - 7 we end up with the estimate

$$\begin{aligned}
& \int_{C_t^+} (|\nabla v_{n0}|^2 + \widehat{\chi}_{\text{org}} |\nabla v_{p0}|^2) \mathbf{d}y \leq \int_{C_s^+} \frac{1}{2} (|\nabla v_{n0}|^2 + \widehat{\chi}_{\text{org}} |\nabla v_{p0}|^2) \mathbf{d}y \\
& + c \int_{C_{3r}^+} (|\nabla v_n^D|^2 + \widehat{\chi}_{\text{org}}) \mathbf{d}y + \frac{c}{(s-t)^2} \left\{ \left(\int_{C_{3r}^+} |\nabla v_{n0}| \mathbf{d}y \right)^2 + \left(\int_{C_{3r\text{org}}^+} |\nabla v_{p0}| \mathbf{d}y \right)^2 \right\}.
\end{aligned}$$

Setting $R = r$, $\rho = \frac{r}{2}$, $\mu = 2$, $\iota = \frac{1}{2}$, and

$$Z(t) = \int_{C_t^+} (|\nabla v_{n0}|^2 + \widehat{\chi}_{\text{org}} |\nabla v_{p0}|^2) \mathbf{d}y, \quad Y = c \int_{C_{3r}^+} (|\nabla v_n^D|^2 + \widehat{\chi}_{\text{org}}) \mathbf{d}y,$$

$$W = \left(\int_{C_{3r}^+} |\nabla v_{n0}| \, dy \right)^2 + \left(\int_{C_{3r \text{ org}}^+} |\nabla v_{p0}| \, dy \right)^2,$$

we apply Lemma B.4 to obtain the claimed estimate in (4.2) of Lemma 4.1. \square

4.3 Reflection

To extend the estimates from Lemma 4.1 to full squares $C_{r/2}(y^0)$ and $C_{3r}(y^0)$, respectively, we expand functions v_j from $C_1^+(0)$ to $C_1^-(0)$ by reflection at $\{y \in \mathbb{R}^2 : y_2 = 0\}$. Defining

$$\tilde{v}_j(y) := \begin{cases} v_j(y_1, y_2), & \text{if } y \in C_1^+(0), \\ v_j(y_1, -y_2), & \text{if } y \in C_1^-(0), \end{cases} \quad (4.7)$$

and extending the Dirichlet function v_n^D and $\hat{\chi}_{\text{org}}$ in the same way to \tilde{v}_n^D and $\tilde{\chi}_{\text{org}}$ gives $\tilde{v}_j \in W^{1,2}(C_1(0))$ for $v_j \in W^{1,2}(C_1^+(0))$. We work with $\tilde{v}_{n0} = \tilde{v}_n - \tilde{v}_n^D$ and $\tilde{v}_{p0} = \tilde{v}_p - \tilde{v}_n$.

Lemma 4.2 *Let the assumptions of Lemma 4.1 be satisfied, and let $y^0 \in C_{1/4}(0)$ and $0 < r < \frac{1}{4}$. Then there exists a constant $\tilde{c}_2 > 0$ independent of y^0, r such that*

$$\begin{aligned} & \int_{C_{\frac{r}{2}}} \{|\nabla \tilde{v}_{n0}|^2 + \tilde{\chi}_{\text{org}} |\nabla \tilde{v}_{p0}|^2\} \, dy \\ & \leq \tilde{c}_2 \int_{C_{3r}} (|\tilde{v}_n^D|^2 + \tilde{\chi}_{\text{org}}) \, dy + \frac{\tilde{c}_2}{r^2} \left(\int_{C_{3r}} |\nabla \tilde{v}_{n0}| \, dy \right)^2 + \frac{\tilde{c}_2}{r^2} \left(\int_{C_{3r \text{ org}}} |\nabla \tilde{v}_{p0}| \, dy \right)^2. \end{aligned} \quad (4.8)$$

Proof. We follow the ideas in [3] and discuss separately the following two cases.

Case A: $C_{3r}(y^0) \cap \{y \in \mathbb{R}^2 : y_2 = 0\} \neq \emptyset$:

i) In case of $y_2^0 > 0$ we use the estimate

$$\int_{C_{\frac{r}{2}}(y^0)} \{|\nabla \tilde{v}_{n0}|^2 + \tilde{\chi}_{\text{org}} |\nabla \tilde{v}_{p0}|^2\} \, dy \leq 2 \int_{C_{\frac{r}{2}}^+(y^0)} \{|\nabla v_{n0}|^2 + \hat{\chi}_{\text{org}} |\nabla v_{p0}|^2\} \, dy,$$

apply Lemma 4.1 and enlarge the integration domains from $C_{3r}^+(y^0)$ to $C_{3r}(y^0)$, from $C_{3r \text{ org}}^+(y^0)$ to $C_{3r \text{ org}}(y^0)$ and change the integrands to the corresponding prolonged quantities to verify the desired estimate of Lemma 4.2.

ii) If $y_2^0 < 0$ we find for $\bar{y}^0 = (y_1^0, -y_2^0)$ that

$$\begin{aligned} \int_{C_{\frac{r}{2}}(y^0)} \{|\nabla \tilde{v}_{n0}|^2 + \tilde{\chi}_{\text{org}} |\nabla \tilde{v}_{p0}|^2\} \, dy &= \int_{C_{\frac{r}{2}}(\bar{y}^0)} \{|\nabla \tilde{v}_{n0}|^2 + \tilde{\chi}_{\text{org}} |\nabla \tilde{v}_{p0}|^2\} \, dy \\ &\leq 2 \int_{C_{\frac{r}{2}}^+(\bar{y}^0)} \{|\nabla v_{n0}|^2 + \hat{\chi}_{\text{org}} |\nabla v_{p0}|^2\} \, dy. \end{aligned}$$

Next we exploit Lemma 4.1 and with estimates of the type

$$\int_{C_{3r}^+(\bar{y}^0)} |w|^\beta \, dy \leq \int_{C_{3r}(\bar{y}^0)} |\tilde{w}|^\beta \, dy = \int_{C_{3r}(y^0)} |\tilde{w}|^\beta \, dy$$

for functions $w = \nabla v_{n0}, \hat{\chi}_{\text{org}} \nabla v_{p0}, \nabla v_n^D$ and $\beta = 1, 2$, we arrive at the desired result.

Case B: $C_{3r}(y^0) \cap \{y \in \mathbb{R}^2 : y_2 = 0\} = \emptyset$:

i) If $y_2^0 > 0$ then $C_{r/2}^+(y^0) = C_{r/2}(y^0)$ and $C_{3r}^+(y^0) = C_{3r}(y^0)$ and $\tilde{v}_{j0} = v_{j0}$. Therefore we can directly apply the result of Lemma 4.1.

ii) In case of $y_2^0 < 0$ we find for $\bar{y}^0 = (y_1^0, -y_2^0)$ that $C_{r/2}(\bar{y}^0), C_{3r}(\bar{y}^0) \subset \{y \in \mathbb{R}^2 : y_2 > 0\}$ which ensures

$$\begin{aligned} \int_{C_{\frac{r}{2}}(\bar{y}^0)} \{|\nabla \tilde{v}_{n0}|^2 + \tilde{\chi}_{\text{org}} |\nabla \tilde{v}_{p0}|^2\} dy &= \int_{C_{\frac{r}{2}}(\bar{y}^0)} \{|\nabla \tilde{v}_{n0}|^2 + \tilde{\chi}_{\text{org}} |\nabla \tilde{v}_{p0}|^2\} dy \\ &= \int_{C_{\frac{r}{2}}(\bar{y}^0)} \{|\nabla v_{n0}|^2 + \hat{\chi}_{\text{org}} |\nabla v_{p0}|^2\} dy. \end{aligned}$$

Thus, again Lemma 4.1 and arguments as in Case A ii) give the desired estimate. This finishes the proof. \square

4.4 Caccioppoli-type inequalities for interior squares

Lemma 4.3 *Let the assumptions of Theorem 2.1 be satisfied. We suppose that $x^0 \in \Omega^{\text{dev}}$ and that $\Phi_{x^0} : U_{x^0} \cap \Omega^{\text{dev}} \rightarrow C_1(0)$ is the corresponding bi-Lipschitzian map producing the Cases (a), (b) or (c) of Fig. 2. Let (φ_n, φ_p) be a solution to (\mathbf{P}_C) and $v_j = \varphi_j \circ \Phi_{x^0}^{-1}$ the corresponding localized part of φ_j , $v_{n0} = \varphi_n \circ \Phi_{x^0}^{-1} - \varphi_n^D \circ \Phi_{x^0}^{-1}$, $v_{p0} = \varphi_p - v_n$. Let $y^0 \in C_{1/4}(0)$ and $0 < r < \frac{1}{4}$. Then there exists $\tilde{c}_3 > 0$ independent of y^0 and r such that*

$$\begin{aligned} &\int_{C_{\frac{r}{2}}} \{|\nabla v_{n0}|^2 + \hat{\chi}_{\text{org}} |\nabla v_{p0}|^2\} dy \\ &\leq \tilde{c}_3 \int_{C_{3r}} (|v_n^D|^2 + \hat{\chi}_{\text{org}}) dy + \frac{\tilde{c}_3}{r^2} \left(\int_{C_{3r}} |\nabla v_{n0}| dy \right)^2 + \frac{\tilde{c}_3}{r^2} \left(\int_{C_{3r \text{ org}}} |\nabla v_{p0}| dy \right)^2. \end{aligned} \quad (4.9)$$

Proof. We work with the cut-off functions introduced in (4.3) and orient ourself by the procedure for the Cases 1 – 4 of Tab. 1. We use $v_{n0} - m_r(v_{n0})$ (for all cases) but v_{p0} in Cases 2 and 4, and $v_{p0} - m_{r \text{ org}}(v_{p0})$ in Case 3. We can follow all the arguments in the proof of Lemma 4.1, substituting the sets $C_t^+(y^0), C_s^+(y^0), C_{r/2}^+(y^0), C_r^+(y^0), C_{3r}^+(y^0), C_{r \text{ org}}^+(y^0), C_{3r \text{ org}}^+(y^0)$, and $C_1^+(0)$ by the corresponding sets $C_t(y^0), C_s(y^0), C_{r/2}(y^0), C_r(y^0), C_{3r}(y^0), C_{r \text{ org}}(y^0), C_{3r \text{ org}}(y^0)$, and $C_1(0)$. Having in mind that the uniform bound for the Poincaré-Sobolev constant in Lemma B.3 covers also this situation, we obtain the result. \square

4.5 Higher integrability of the gradient

Our aim is to apply the Giaquinta-Modica Theorem B.1 to establish the higher integrability of the gradients of φ_n and φ_p stated in Theorem 2.1. If $x^0 \in \partial\Omega^{\text{dev}}$ let $\tilde{v}_j, \tilde{v}_{j0}$ be given as in (4.7), while for $x^0 \in \Omega^{\text{dev}}$ we set $\tilde{v}_j = v_j, \tilde{v}_{j0} = v_{j0}$. We introduce the functions

$$g(y) := |\nabla \tilde{v}_{n0}(y)|^2 + \tilde{\chi}_{\text{org}}(y) |\nabla \tilde{v}_{p0}(y)|^2, \quad h(y) := c(|\nabla \tilde{v}_n^D(y)|^2 + \tilde{\chi}_{\text{org}}(y)). \quad (4.10)$$

With this, the left hand side in (4.8) and (4.9) can be written as $r^2 \int_{C_{r/2}} g dy$. Moreover, we have for the last two terms in (4.8) and (4.9)

$$\frac{1}{r^4} \left(\int_{C_{3r}} |\nabla \tilde{v}_{n0}| dy \right)^2, \quad \frac{1}{r^4} \left(\int_{C_{3r \text{ org}}} |\nabla \tilde{v}_{p0}| dy \right)^2 \leq \frac{1}{r^4} \left(\int_{C_{3r}} g^{\frac{1}{2}} dy \right)^2 \leq c \left(\int_{C_{3r}} g^{\frac{1}{2}} dy \right)^2.$$

Thus, in summary our estimates in (4.8) and (4.9) and the definition of g and h in (4.10) ensure the uniform estimate

$$\int_{C_{r/2}} g \, dy \leq c \left\{ \left(\int_{C_{3r}} g^{\frac{1}{2}} \, dy \right)^2 + \int_{C_{3r}} h(y) \, dy \right\} \quad \forall y^0 \in C_{\frac{1}{4}}(0), \forall r \in (0, \frac{1}{4}). \quad (4.11)$$

We apply the Giaquinta-Modica Theorem B.1, where we set $Q_R := C_{1/4}(0)$ and $a := 1/2$ and take g and h as in (4.10). Since $\varphi_n^D \in W^{1,\infty}(\Omega^{\text{dev}})$, there is some $b > 1$ such that $h \in L^b(C_{1/4}(0))$. Then, (4.11) guarantees the assumptions of Theorem B.1 for all $Q \subset \tilde{Q} \subset Q_R$, where \tilde{Q} has six times the diameter of Q . Thus, Theorem B.1 yields an exponent $\alpha^* > 1$ and a constant $c > 0$ such that $g = |\nabla \tilde{v}_{n0}|^2 + \tilde{\chi}_{\text{org}} |\nabla \tilde{v}_{p0}|^2 \in L^{\alpha^*}(C_{1/24}(0))$ and

$$\int_{C_{\frac{1}{24}}(0)} g(y)^{\alpha^*} \, dy \leq c \left\{ \left(\int_{C_{\frac{1}{4}}(0)} g(y) \, dy \right)^{\alpha^*} + \int_{C_{\frac{1}{4}}(0)} h(y)^{\alpha^*} \, dy \right\}.$$

Therefore we obtain the estimate

$$\begin{aligned} & \int_{C_{\frac{1}{24}}(0)} (|\nabla \tilde{v}_{n0}|^2 + \tilde{\chi}_{\text{org}} |\nabla \tilde{v}_{p0}|^2)^{\alpha^*} \, dy \\ & \leq c \left\{ \left(\int_{C_{\frac{1}{4}}(0)} (|\nabla \tilde{v}_{n0}|^2 + \tilde{\chi}_{\text{org}} |\nabla \tilde{v}_{p0}|^2) \, dy \right)^{\alpha^*} + \int_{C_{\frac{1}{4}}(0)} (|\nabla \tilde{v}_n^D|^2 + \tilde{\chi}_{\text{org}})^{\alpha^*} \, dy \right\}. \end{aligned}$$

If $x^0 \in \partial\Omega^{\text{dev}}$, restriction to the upper half square and back transformation by means of $\Phi_{x^0}^{-1}$ (or only back transformation by means of $\Phi_{x^0}^{-1}$ if $x^0 \in \Omega^{\text{dev}}$) leads to

$$\begin{aligned} & \int_{\Phi_{x^0}^{-1}(C_{\frac{1}{24}}) \cap \Omega^{\text{dev}}} (|\nabla \varphi_{n0}|^{2\alpha^*} + \chi_{\text{org}} |\nabla \varphi_{p0}|^{2\alpha^*}) \, dx \\ & \leq c \left\{ \left(\int_{\Phi_{x^0}^{-1}(C_{\frac{1}{4}}) \cap \Omega^{\text{dev}}} (|\nabla \varphi_{n0}|^2 + \chi_{\text{org}} |\nabla \varphi_{p0}|^2) \, dx \right)^{\alpha^*} + \int_{\Phi_{x^0}^{-1}(C_{\frac{1}{4}}) \cap \Omega^{\text{dev}}} (|\nabla \varphi_n^D|^2 + \chi_{\text{org}})^{\alpha^*} \, dx \right\}, \end{aligned}$$

where $\varphi_{n0} = \varphi_n - \varphi_n^D$, $\varphi_{p0} = \varphi_p - \varphi_n$. This finishes the proof of Theorem 2.1, since by (A1) there exists a finite number L of sets $\Phi_{x^0}^{-1}(C_{1/24})$ which cover Ω^{dev} . \square

A Proof of Lemma 2.1

For fixed T , let $\tilde{V}_T(C)$ denote the unique solution to

$$\mathcal{H}_1(C, \tilde{V}_T(C)) = 0, \text{ where } \mathcal{H}_1(C, v) := N_{n0} \mathcal{G}\left(\frac{v - E_L}{T}; \frac{\sigma_n}{T}\right) - N_{p0} \mathcal{G}\left(\frac{-v + E_H}{T}; \frac{\sigma_p}{T}\right) - C.$$

1. Because of $\frac{\partial \mathcal{H}}{\partial v}(T, v) = \frac{\partial \mathcal{H}_1}{\partial v}(C, v) = \frac{N_{n0}}{T} \frac{\partial \mathcal{G}}{\partial \eta}\left(\frac{v - E_L}{T}; \frac{\sigma_n}{T}\right) + \frac{N_{p0}}{T} \frac{\partial \mathcal{G}}{\partial \eta}\left(\frac{-v + E_H}{T}; \frac{\sigma_p}{T}\right) > 0$ for all $v \in \mathbb{R}$, $T > 0$, $C \in (-N_{p0}, N_{n0})$, the implicit function theorem can be used to obtain the relations

$$\begin{aligned} V'(T) &= - \left[\frac{\partial \mathcal{H}}{\partial v}(T, V(T)) \right]^{-1} \frac{\partial \mathcal{H}}{\partial T}(T, V(T)), \\ \tilde{V}'_T(C) &= - \left[\frac{\partial \mathcal{H}_1}{\partial v}(C, \tilde{V}_T(C)) \right]^{-1} \frac{\partial \mathcal{H}_1}{\partial C}(C, \tilde{V}_T(C)) = \left[\frac{\partial \mathcal{H}_1}{\partial v}(C, \tilde{V}_T(C)) \right]^{-1} > 0. \end{aligned} \quad (\text{A.1})$$

In other words, in (1.6) for all fixed temperatures, the quantity ψ_0 increases with increasing doping density C . For all $T \geq T_a$ we evaluate and estimate for the values $v = E_L$ and $v = E_H$ the expressions $n - p$ and obtain for $v = E_L$

$$N_{n0}\mathcal{G}\left(0; \frac{\sigma_n}{T}\right) - N_{p0}\mathcal{G}\left(\frac{-E_G}{T}; \frac{\sigma_p}{T}\right) \geq \frac{N_{n0}}{2} - N_{p0}\mathcal{G}\left(\frac{-E_G}{T}; \frac{\sigma_p}{T_a}\right) \geq \frac{N_{n0}}{2} - N_{p0}\mathcal{G}\left(\frac{-E_G}{T_a}; \frac{\sigma_p}{T_a}\right)$$

and for $v = E_H$ that

$$N_{n0}\mathcal{G}\left(\frac{-E_G}{T}; \frac{\sigma_n}{T}\right) - N_{p0}\mathcal{G}\left(0; \frac{\sigma_p}{T}\right) \leq N_{n0}\mathcal{G}\left(\frac{-E_G}{T}; \frac{\sigma_n}{T_a}\right) - \frac{N_{p0}}{2} \leq N_{n0}\mathcal{G}\left(\frac{-E_G}{T_a}; \frac{\sigma_n}{T_a}\right) - \frac{N_{p0}}{2}.$$

Since for every fixed $T \geq T_a$, the map $C \mapsto \tilde{V}(C)$ is increasing, the last 2 estimates ensure for $C \in \mathfrak{C}_{\text{dop}}$ the estimate $E_H \leq \tilde{V}(C) \leq E_L$, meaning that for all fixed $C \in \mathfrak{C}_{\text{dop}}$ we have

$$E_H \leq V(T) \leq E_L \quad \text{for all } T \geq T_a. \quad (\text{A.2})$$

2. We use the abbreviations $\eta_n(T) = \frac{V(T)-E_L}{T}$, $\eta_p(T) = \frac{-V(T)+E_H}{T}$, $z_j = \frac{\sigma_j}{T}$, $j=n, p$. For T and $V(T)$ from (A.2) we have $|\eta_j| \leq \frac{c}{T_a}$ and estimate

$$\begin{aligned} \frac{\partial \mathcal{G}}{\partial \eta}(\eta_j; z_j) &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \exp\left(\frac{-\xi^2}{2}\right) \frac{\exp(z_j \xi - \eta_j)}{(\exp(z_j \xi - \eta_j) + 1)^2} d\xi \\ &> \frac{1}{\sqrt{2\pi}} \int_0^1 \exp\left(\frac{-\xi^2}{2}\right) \frac{\exp(z_j \xi - \eta_j)}{(\exp(z_j \xi - \eta_j) + 1)^2} d\xi \\ &> \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-1}{2}\right) \frac{\exp(-\eta_j)}{(\exp(\frac{\sigma_j}{T_a} - \eta_j) + 1)^2} \geq c > 0. \end{aligned}$$

This ensures $\frac{\partial \mathcal{H}}{\partial v}(T, V(T))T \geq c$ and $\frac{\partial \mathcal{H}}{\partial v}(T, V(T))^{-1} \frac{1}{T} \leq c$. Moreover, we find

$$\frac{\partial \mathcal{H}}{\partial T}(T, V(T)) = \frac{N_{p0}}{T} \left[\frac{\partial \mathcal{G}}{\partial \eta}(\eta_p; z_p) \eta_p + \frac{\partial \mathcal{G}}{\partial z}(\eta_p; z_p) z_p \right] - \frac{N_{n0}}{T} \left[\frac{\partial \mathcal{G}}{\partial \eta}(\eta_n; z_n) \eta_n + \frac{\partial \mathcal{G}}{\partial z}(\eta_n; z_n) z_n \right].$$

Note that

$$\frac{\partial \mathcal{G}}{\partial \eta}(\eta; z) \eta + \frac{\partial \mathcal{G}}{\partial z}(\eta; z) z = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{\xi^2}{2}\right) \frac{\exp(z\xi - \eta)(\eta - z\xi)}{[\exp(z\xi - \eta) + 1]^2} d\xi. \quad (\text{A.3})$$

Using the fact that $|\frac{w e^w}{(e^w + 1)^2}| < 1$ for all $w \in \mathbb{R}$, we obtain from (A.3) that the absolute value of $T \frac{\partial \mathcal{H}}{\partial T}(T, V(T))$ is uniformly bounded. From (A.1) it results the boundedness of the absolute value of

$$V'(T) = - \left[\frac{\partial \mathcal{H}}{\partial v}(T, V(T)) \right]^{-1} \frac{1}{T} T \frac{\partial \mathcal{H}}{\partial T}(T, V(T)).$$

3. Moreover, implicit differentiation gives (here we leave out the arguments)

$$\frac{\partial^2 \mathcal{H}}{\partial T^2} + 2 \frac{\partial^2 \mathcal{H}}{\partial v \partial T} V'(T) + \frac{\partial^2 \mathcal{H}}{\partial v^2} (V'(T))^2 + \frac{\partial \mathcal{H}}{\partial v} V''(T) = 0$$

and results in

$$V''(T) = - \left(\frac{\partial \mathcal{H}}{\partial v} \right)^{-1} \left[\frac{\partial^2 \mathcal{H}}{\partial T^2} + 2 \frac{\partial^2 \mathcal{H}}{\partial v \partial T} V'(T) + \frac{\partial^2 \mathcal{H}}{\partial v^2} (V'(T))^2 \right], \quad (\text{A.4})$$

where it remains to show that T times the term in the brackets stays bounded for $T \geq T_a$ to establish the boundedness of $V''(T)$. We calculate the second derivatives of \mathcal{H} as

$$\begin{aligned}\frac{\partial^2 \mathcal{H}}{\partial v^2} &= \sum_{j=n,p} e_j \frac{N_{j0}}{T^2} \frac{\partial^2 \mathcal{G}}{\partial \eta^2}(\eta_j; z_j), \quad \text{where } e_n := 1, \quad e_p := -1, \\ \frac{\partial^2 \mathcal{H}}{\partial v \partial T} &= - \sum_{j=n,p} \frac{N_{j0}}{T^2} \left[\frac{\partial \mathcal{G}}{\partial \eta}(\eta_j; z_j) + \frac{\partial^2 \mathcal{G}}{\partial \eta^2}(\eta_j; z_j) \eta_j + \frac{\partial^2 \mathcal{G}}{\partial \eta \partial z}(\eta_j; z_j) z_j \right], \\ \frac{\partial^2 \mathcal{H}}{\partial T^2} &= \sum_{j=n,p} e_j \frac{N_{j0}}{T^2} \left[2 \frac{\partial \mathcal{G}}{\partial \eta}(\eta_j; z_j) \eta_j + 2 \frac{\partial \mathcal{G}}{\partial z}(\eta_j; z_j) z_j \right. \\ &\quad \left. + 2 \frac{\partial^2 \mathcal{G}}{\partial \eta \partial z}(\eta_j; z_j) \eta_j z_j + \frac{\partial^2 \mathcal{G}}{\partial \eta^2}(\eta_j; z_j) \eta_j^2 + \frac{\partial^2 \mathcal{G}}{\partial z^2}(\eta_j; z_j) z_j^2 \right].\end{aligned}$$

Note that according to [10, Subsec. 2.1], $\left| \frac{\partial \mathcal{G}}{\partial \eta}(\eta_j; z_j) \right| \leq 1$, $\left| \frac{\partial \mathcal{G}}{\partial z}(\eta_j; z_j) \right| \leq \frac{1}{z_j} (1 + \exp |\eta_j|)$. Moreover, in Step 2 of the proof of [11, Lemma A.2] it was verified that

$$\left| \frac{\partial^2 \mathcal{G}}{\partial \eta^2}(\eta_j; z_j) \right| \leq 1, \quad \left| \frac{\partial^2 \mathcal{G}}{\partial z \partial \eta}(\eta_j; z_j) \right| \leq \frac{1}{z_j} \exp |\eta_j|, \quad \frac{\partial^2 \mathcal{G}}{\partial z^2}(\eta_j; z_j) \leq \frac{1}{z_j^2} \exp |\eta_j|$$

for $j = n, p$, $0 < T_a < T$, and $|v| \leq c$. This together with the boundedness of $V'(T)$ in the relevant arguments gives the boundedness of the term in the bracket in (A.4). Finally, we obtain the desired boundedness of $V''(T)$ for $0 < T_a < T$.

B Some useful tools and inequalities

Lemma B.1 *Let $\Omega_1, \Omega_2 \neq \emptyset$ be open, bounded, disjoint subsets of $\Omega \subset \mathbb{R}^d$ with piecewise smooth boundary, and $\bar{\Omega} = \bar{\Omega}_1 \cup \bar{\Omega}_2$. Moreover, we assume $\varphi|_{\Omega_1} \in H^1(\Omega_1)$, $\varphi|_{\Omega_2} \in H^1(\Omega_2)$ and $\text{Tr}_1 \varphi|_{\partial \Omega_1 \cap \partial \Omega_2} = \text{Tr}_2 \varphi|_{\partial \Omega_1 \cap \partial \Omega_2}$ a.e. on $\partial \Omega_1 \cap \partial \Omega_2$, where $\text{Tr}_i : H^1(\Omega_i) \rightarrow L^2(\partial \Omega_i)$ denotes the trace operator with respect to Ω_i , $i = 1, 2$. Then $\varphi \in H^1(\Omega)$.*

Proof. Let ν denote the outer unit normal with respect to Ω_1 , $\Sigma := \partial \Omega_1 \cap \partial \Omega_2$, and let $\rho \in C_0^\infty(\Omega)$ arbitrarily be given. Then, for all $i \in \{1, \dots, d\}$, Gauss theorem yields

$$\begin{aligned}- \int_{\Omega} \varphi \frac{\partial \rho}{\partial x_i} dx &= - \int_{\Omega_1} \varphi \frac{\partial \rho}{\partial x_i} dx - \int_{\Omega_2} \rho \frac{\partial \varphi}{\partial x_i} dx \\ &= \int_{\Omega_1} \frac{\partial \varphi}{\partial x_i} \rho dx - \int_{\partial \Omega_1} \text{Tr}_1 \varphi \rho \nu_i d\Gamma + \int_{\Omega_2} \frac{\partial \varphi}{\partial x_i} \rho dx + \int_{\partial \Omega_2} \text{Tr}_2 \varphi \rho \nu_i d\Gamma \\ &= \int_{\Omega} \frac{\partial \varphi}{\partial x_i} \rho dx - \int_{\Sigma} (\text{Tr}_1 \varphi - \text{Tr}_2 \varphi) \rho \nu_i d\Gamma = \int_{\Omega} \frac{\partial \varphi}{\partial x_i} \rho dx.\end{aligned}$$

This means $\varphi \in H^1(\Omega)$. \square

The following two lemmas result from Lemma A.3 and Lemma A.4 in [9] for $p = 2$.

Lemma B.2 (Uniform Poincaré-Friedrichs type inequality) *Let $y^0 \in C^+_{\frac{1}{4}}(0)$, $\rho \in (0, \frac{1}{4}]$. Let $G \subset (y^0 + [-3\rho, 3\rho]^2) \cap [-1, 1] \times [0, 1]$ be an axis parallel rectangle with length $(a_0 + a_1)\rho$ and height $a_2\rho$, where $a_0\rho = \text{mes}(\bar{G} \cap \{y \in \mathbb{R}^2 : y_1 \geq 0, y_2 = 0\})$ is the length of the Dirichlet boundary*

and $a_1\rho = \text{mes}(\overline{G} \cap \{y \in \mathbb{R}^2 : y_1 < 0, y_2 = 0\})$. Additionally we assume that $a_0, a_2 \in [1, 6]$ and $a_1 \in [0, 6]$. Then there is a constant $C_{\text{PF}} > 0$ such that

$$\|w\|_{L^2(G)}^2 \leq C_{\text{PF}} \|\nabla w\|_{L^1(G)^2}^2 \quad \forall w \in W_{\Gamma_N}^{1,1}(G)$$

for all G with admissible y^0, ρ, a_0, a_1, a_2 .

Lemma B.3 (Uniform Poincaré-Sobolev type inequality) Let $y^0 \in C_{1/4}(0)$ and $\rho \in (0, \frac{1}{4}]$. Let $G \subset y^0 + [-3\rho, 3\rho]^2 \subset [-1, 1]^2$ be an axis parallel rectangle with side lengths $a_1\rho$ and $a_2\rho$, $a_1, a_2 \in [1, 6]$. Then there is a constant $C_{\text{PS}} > 1$ such that

$$\|w - m_G(w)\|_{L^2(G)}^p \leq C_{\text{PS}} \|\nabla w\|_{L^1(G)^2}^2 \quad \forall w \in W^{1,1}(G), \quad m_G(w) = \frac{1}{|G|} \int_G w(y) \, dy$$

for all G with admissible y^0, ρ, a_1, a_2 .

Lemma B.4 Let $Z(t)$ be a bounded nonnegative function on the interval $[\rho, R]$. Let for all $\rho \leq t < s \leq R$ the inequality

$$Z(t) \leq \left[W(s-t)^{-\mu} + Y \right] + \iota Z(s)$$

with $W, Y \geq 0$ and $\mu > 0$ and $0 < \iota < 1$ be satisfied. Then

$$Z(\rho) \leq c(\mu, \iota) \left[W^{-\mu} + Y \right].$$

This lemma is a special case of [7, Lemma 6.1]. A form of generalized Gehring lemma is

Theorem B.1 (Giaquinta and Modica, Theorem 6.6 and Corollary 6.1 in [7])

Let be $g, h \in L^1(Q_R)$ with $g, h \geq 0$ a.e. and assume that for every pair of concentric cubes $Q \subset \tilde{Q} \subset \subset Q_R$ where \tilde{Q} has six times the diameter of Q , we have for some constant $\omega > 0$

$$\int_Q g \, dx \leq \omega \left\{ \left(\int_{\tilde{Q}} g^a \, dx \right)^{\frac{1}{a}} + \int_{\tilde{Q}} h \, dx \right\},$$

with $0 < a < 1$. Let the function $h \in L^b(Q_R)$ for some $b > 1$. Then there exist constants $c > 0$ and $\alpha^* > 1$ such that g belongs to $L^{\alpha^*}(Q_{R/6})$ and

$$\int_{Q_{R/6}} g^{\alpha^*} \, dx \leq c \left\{ \left(\int_{Q_R} g \, dx \right)^{\alpha^*} + \int_{Q_R} h^{\alpha^*} \, dx \right\}.$$

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