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Matthias Liero      Axel Fischer      Jürgen Fuhrmann  
Thomas Koprucki      Annegret Glitzky

Preprint September 2016

MATHEON preprint  
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# A PDE model for electrothermal feedback in organic semiconductor devices

Matthias Liero, Axel Fischer, Jürgen Fuhrmann, Thomas Koprucki,  
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**Abstract** Large-area organic light-emitting diodes are thin-film multilayer devices that show pronounced self-heating and brightness inhomogeneities at high currents. As these high currents are typical for lighting applications, a deeper understanding of the mechanisms causing these inhomogeneities is necessary. We discuss the modeling of the interplay between current flow, self-heating, and heat transfer in such devices using a system of partial differential equations of thermistor type, that is capable of explaining the development of luminance inhomogeneities. The system is based on the heat equation for the temperature coupled to a  $p(x)$ -Laplace-type equation for the electrostatic potential with mixed boundary conditions. The  $p(x)$ -Laplacian allows to take into account non-Ohmic electrical behavior of the different organic layers. Moreover, we present analytical results on the existence, boundedness, and regularity of solutions to the system. A numerical scheme based on the finite-volume method allows for efficient simulations of device structures.

**Keywords:** Organic semiconductor devices, thermistor model,  $p(x)$ -Laplacian, heat flow, electrothermal feedback, Arrhenius law, finite-volume method

**MSC 2010:** 35J92, 65M08, 35J57, 35Q79, 80M12

## 1 Introduction

Nowadays organic (i.e. carbon-based) semiconductors are extensively used in smartphone displays and increasingly in TV screens. Lighting applications are of great interest due to the fascinating properties of organic light-emitting diodes (OLEDs), e.g. large-area surface emission, semi-transparency, flexibility. However, lighting applications require a much higher brightness than displays and hence higher currents are necessary. These cause substantial Joule self-heating accompanied by unpleasant brightness inhomogeneities of the panels. An appropriate simulation tool

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A. Fischer

Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden 01062 Dresden, GERMANY e-mail: axel.fischer@iapp.de

M. Liero, J. Fuhrmann, Th. Koprucki, A. Glitzky

Weierstrass Institute Berlin, Mohrenstraße 39, 10117 Berlin, GERMANY, e-mail: liero@wias-berlin.de, fuhrmann@wias-berlin.de, koprucki@wias-berlin.de, glitzky@wias-berlin.de

can help to validate cost-efficient device concepts by accounting for nonlinear self-heating effects.

The appearance of the inhomogeneities, which show a saturation of the luminance in the panel center, can neither be explained with high sheet resistances of the optically transparent electrode nor with a degradation of the organic materials due to high temperatures. In [1, 2] it was demonstrated that the complex interplay of temperature activated transport of the charge carriers and heat flow in the device lead to inhomogeneous current distributions resulting in inhomogeneous luminance.

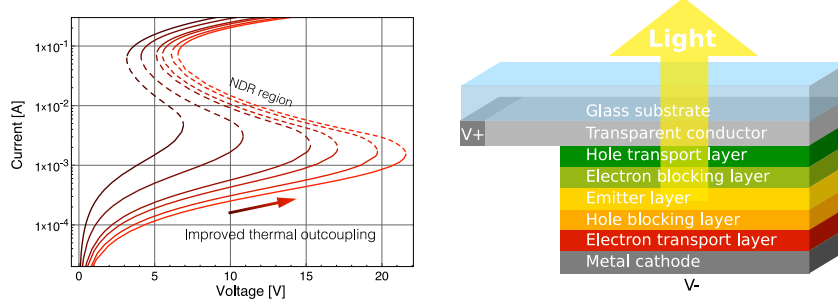
Indeed, applying a voltage to an organic semiconductor device induces a current flow which leads to a power dissipation by Joule heating and hence also a temperature rise. As higher temperatures improve the conductivity in organic materials, higher currents occur. Thus, a positive feedback loop develops that can result in a complete destruction of the device by thermal runaway if the generated heat cannot be dispersed into the environment. The temperature dependence of the conductivity is often [1] modeled by an exponential law of Arrhenius type, which features an activation energy that is linked to the energetic disorder in the organic material.

Devices that show such an electrothermal interplay are called thermistors with negative temperature coefficient. The current-voltage characteristics of such thermistors are S-shaped with regions of negative differential resistance (S-NDR), where currents increase despite of decreasing voltages, see Fig. 1 (left). A thermistor-like behavior of organic semiconductors induced by self-heating has been verified for the organic material  $C_{60}$  in [1] and for organic materials used in OLEDs in [2].

However, due to the huge aspect ratios of OLED panels, such devices cannot be regarded as a single spatially homogeneous thermistor device, but rather as an array of thermistor devices that can exchange heat. In particular, the self-heating, and hence also the local differential resistance, is now a collective property of neighboring thermistors.

In [2] we demonstrated that a new operation mode appears that is not present in the spatially homogeneous case: Eventually, the S-NDR regime has propagated through the whole panel. Now, regions in the panel do not warm up enough to remain in an S-NDR mode so that both, local voltages and currents, decrease although the externally applied voltage is still increasing. This “switched-back” regime is ultimately the reason for the observed saturation of luminance in the panel center, in fact, one even has to expect a decline of luminance as the local currents are decreasing.

In the following we present a mathematical model for the current and heat flow in organic semiconductor devices consisting of a coupled PDE system for the electrostatic potential and the temperature, see Section 2. This PDE modeling approach gives much more flexibility concerning variations in geometry and material composition than for example network models. Moreover, our model contains also a PDE-type description of the active organic zone whereas in other PDE simulation approaches the organic layer is reduced to the information from empirical characteristics. The crucial feature of our PDE model is that the current flow equation is of  $p(x)$ -Laplace type, where the exponent  $p(x)$  takes the non-Ohmic behavior of the organic layers into account. In particular, the exponent is in general discontinuous



**Fig. 1** Left: Simulated current-voltage characteristics for different thermal outcoupling regimes, regions of negative differential resistance are dashed. Right: Schematic picture of OLED stack.

as the different functional layers exhibit different power laws. In Section 3, we summarize the analytical results of [3, 4, 5] and present in Section 4 a numerical scheme that allows us to efficiently simulate the current and heat flow in OLEDs. One of the major challenges is the derivation of a stable scheme for the  $p(x)$ -Laplacian, which we address by using a hybrid finite-volume/finite-element approach.

## 2 Modeling of current and heat flow

A typical OLED device structure is depicted in Fig. 1 (right). To describe the interplay of current and heat flow in organic semiconductor devices the following PDE model was proposed in [6]. It consists of the current flow equation for the electrostatic potential  $\varphi$  and the heat equation for the temperature  $T$

$$\begin{aligned} -\nabla \cdot S(x, T, \nabla \varphi) &= 0, \\ -\nabla \cdot (\lambda(x) \nabla T) &= H(x, T, \nabla \varphi) \quad \text{on } \Omega \subset \mathbb{R}^d. \end{aligned} \quad (1)$$

The system is complemented by Dirichlet and no-flux boundary conditions for the potential  $\varphi$  at the contacts  $\Gamma_D$  and the insulating parts  $\Gamma_N$  of the boundary, respectively, and Newton boundary conditions for the temperature to describe the coupling to the environment

$$\begin{aligned} \varphi &= \varphi^D \text{ on } \Gamma_D, \quad S(x, T, \nabla \varphi) \cdot \nu = 0 \text{ on } \Gamma_N, \\ -\lambda(x) \nabla T \cdot \nu &= \gamma(x)(T - T_a) \text{ on } \Gamma = \partial \Omega, \end{aligned} \quad (2)$$

where  $T_a > 0$  denotes the fixed ambient temperature. The special features of the model are the Arrhenius-like temperature law as well as the non-Ohmic current-voltage relations incorporated by a power law in the current expression  $S$ , namely

$$S(x, T, \nabla \varphi) = \kappa_0(x) F(x, T) |\nabla \varphi|^{p(x)-2} \nabla \varphi, \quad F(x, T) = \exp \left[ -\frac{E_{\text{act}}(x)}{k_B} \left( \frac{1}{T} - \frac{1}{T_a} \right) \right].$$

Here,  $\kappa_0$  and  $E_{\text{act}}$  are material dependent effective conductivity and an activation energy, respectively. The exponent  $p$  of the power law is also material dependent, taking different power laws in the various layers of the device into account. Hence, the first equation in (1) becomes of  $p(x)$ -Laplacian type with discontinuous measurable exponent  $p$ . In particular, we have  $p(x) \equiv 2$  in Ohmic materials such as electrodes and  $p(x) > 2$  (e.g.  $p(x) = 9.7$ , see [2]) in organic layers.

The Joule heat term in the second equation of (1) takes the form

$$H(x, T, \nabla\varphi) = (1 - \eta(x, T, \nabla\varphi)) \kappa_0(x) F(x, T) |\nabla\varphi|^{p(x)},$$

where  $\eta(x, T, \nabla\varphi) \in [0, 1]$  represents the light-outcoupling factor. Note that  $H$  is a priori only an  $L^1$  function which hampers the analytical treatment of the system.

### 3 Analytical results

The first and foremost question is, whether the system in (1), (2) is well-defined, i.e. existence of (weak) solutions. Due to the definition of the flux function  $S$  with spatially dependent exponent  $p$  it is clear, that we cannot work in the classical Lebesgue and Sobolev spaces. Following [7], we introduce for measurable exponents  $p$  with

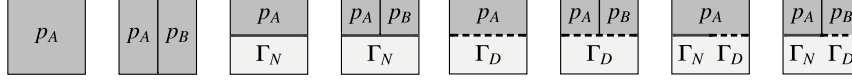
$$1 < p_- := \text{ess inf}_{x \in \Omega} p(x) \leq \text{ess sup}_{x \in \Omega} p(x) =: p_+ < \infty \quad (3)$$

the generalized Lebesgue space  $L^{p(\cdot)}(\Omega)$  as the set of all measurable functions  $f$  with finite modular  $\rho_{p(\cdot)}(f) := \int_{\Omega} |f(x)|^{p(x)} dx < \infty$ , which equipped with the corresponding Luxemburg norm is a reflexive and separable Banach space. Moreover, we define the generalized Sobolev space  $W^{1,p(\cdot)}(\Omega) := \{f \in W^{1,p_-}(\Omega) : \nabla f \in L^{p(\cdot)}(\Omega)^d\}$  being also a separable and reflexive Banach space with the norm  $\|f\|_{W^{1,p(\cdot)}} := \|f\|_{W^{1,p_-}} + \|\nabla f\|_{L^{p(\cdot)}}$ . By  $W_D^{1,p(\cdot)}(\Omega) \subset W^{1,p(\cdot)}(\Omega)$  we denote the subspace of functions with Dirichlet value 0 at  $\Gamma_D$ . The following theorem guarantees the existence of solutions, we refer to [4, 5] for details.

**Theorem 1.** *Besides an  $L^\infty$  setting for the material parameters we suppose (3),  $T_a > 0$ , and  $d \geq 2$ . Then the  $p(x)$ -Laplace thermistor problem (1), (2) has a solution  $(\varphi, T)$  with  $\varphi \in \Phi^D + W_D^{1,p(\cdot)}(\Omega)$  and  $T \in W^{1,q}(\Omega)$  for all  $q \in [1, \frac{d}{d-1})$ . Especially,  $T$  is an entropy solution to the heat equation and  $T \geq T_a$  a.e. in  $\Omega$ .*

There are two strategies to prove the existence result without improved regularity of the Joule heating term  $H$ . In [4] a more constructive way is proposed, where an truncation  $H_\varepsilon$  of the Joule heat term is applied such that it remains bounded. The regularized problems are solved by Galerkin approximation. By verifying a priori estimates not depending on the truncation parameter  $\varepsilon$  and a suitable passage to the limit the existence result for (1), (2) is obtained. The second method is based on Schauder's fixed point theorem on the set  $\mathcal{M} := \{T \in L^1(\Omega) : \|T\|_{W^{1,1}} \leq \tilde{c}, T \geq T_a\}$

and the concept of entropy solutions for the heat equation with Newton boundary conditions, see [5].



**Fig. 2** Model sets with different exponents  $p_A < p_B$  and different types of boundary conditions.

An alternative approach to verify the existence of solutions to (1), (2) is to improve the regularity of the Joule heating term  $H$  such that the concept of weak solutions for the  $p(x)$ -Laplace thermistor problem is applicable. In [3], we proved higher regularity of the gradient of the electrostatic potential in two spatial dimensions and for  $p(x) \geq 2$  piecewise constant, and such that the localized geometric situation is covered by one of the eight cases in Fig. 2. The proof is based on a localization argument, Caccioppoli estimates, and a Gehring-type lemma. With this, we obtain  $\nabla \varphi \in L^{sp(\cdot)}(\Omega)$  and  $H(\cdot, T, \nabla \varphi) \in L^s(\Omega)$  for some  $s > 1$ . Defining a fixed point map for the temperature on the set  $\mathcal{M} = \{T \in W^{1,q}(\Omega) : \|T\|_{W^{1,q}} \leq c_q, T \geq T_a\}$  for some  $q > 2$  Schauder's fixed point theorem leads to the following improved existence result.

**Theorem 2.** *Let additionally  $d = 2$ ,  $\varphi^D \in W^{1,\infty}(\Omega)$  and  $p(x) \geq 2$  be piecewise constant. We assume that the geometric structure can be locally transferred to the situation of one of the eight cases in Fig. 2, where  $p_B > p_A$ . Then the problem (1), (2) has a solution  $(\varphi, T)$  with  $\varphi \in \varphi^D + W_D^{1,sp(\cdot)}(\Omega)$  and  $T \in W^{1,q}(\Omega)$  for some  $s > 1$  and  $q > 2$ . Especially,  $T$  is continuous and fulfils  $T_a \leq T \leq c_T$ .*

Note that Schauder's theorem does not give uniqueness of fixed points and hence of solutions. However, uniqueness of solutions for the  $p(x)$ -Laplace thermistor system (1), (2) cannot be expected due to the hysteretic behavior induced by the positive feedback with respect to temperature described in the introduction. Even in the spatially homogeneous setting of self-heating in organic devices (see [1] and [6, Sect. 2.1]) S-shaped current-voltage characteristics occur. Here, three different currents are possible for the same applied voltage.

## 4 Numerical scheme

As we have to deal with piecewise constant functions  $p(x)$ , we subdivide the computational domain  $\tilde{\Omega} = \bigcup_{r \in \mathcal{Q}} \tilde{\Omega}_r$  into disjoint subdomains coinciding with the regions of continuity of the coefficients. We call the boundary between two neighboring regions *hetero interface*. To solve the PDE system (1), (2) numerically we use a finite-volume method on Voronoi cells as control volumes which are constructed based on a Delaunay grid. The latter is supposed to be boundary conforming with

respect to exterior boundaries and hetero interfaces, see e.g. [8]. We assume that each control volume contains a collocation point  $x_K \in \overline{\Omega}$ .

We apply Gauss's theorem to the integral of the flux divergence to obtain for the current flow equation in (1) the flux balance with further subdivision into contributions from adjacent subdomains:

$$0 = \int_K \nabla \cdot S(x, T, \nabla \varphi) \, dx = \sum_{r \in \mathcal{R}} \sum_{L \sim K} \int_{\partial K \cap \partial L \cap \Omega_r} \kappa_{0,r} F_r(T) |\nabla \varphi|^{p_r-2} \nabla \varphi \cdot \nu_{KL} \, da, \quad (4)$$

where  $L \sim K$  indicates that  $L$  is adjacent to  $K$  and  $\nu_{KL}$  is the unit normal vector pointing from  $K$  into  $L$ .

Note that the normal flux over a surface  $\partial K \cap \partial L \cap \Omega_r$  does not only depend on the normal components of  $\nabla \varphi$  but on the modulus of the full gradient. To take this into account we compute the approximation of  $|\nabla \varphi|^2$  on  $\partial K \cap \partial L \cap \Omega_r$  as the average squared norms of the P1 finite element gradients  $\nabla_\tau \varphi$  over the set  $\mathcal{T}_{K,L,r}$  of all simplices (triangles in 2D) in the underlying Delaunay triangulation adjacent to the edge  $\overline{x_K x_L}$  and belonging to  $\Omega_r$ :

$$|\nabla \varphi|^2|_{\partial K \cap \partial L \cap \Omega_r} \approx G_{K,L,r}^2(\varphi) := \frac{\sum_{\tau \in \mathcal{T}_{K,L,r}} |\tau| |\nabla_\tau \varphi|^2}{\sum_{\tau \in \mathcal{T}_{K,L,r}} |\tau|}.$$

This approach allows us to introduce an approximation of the right-hand side of (4) consisting in replacing the surface integral by a simple quadrature, and the gradient projection by a finite difference expression leading to

$$0 = \sum_{r \in \mathcal{R}} \sum_{L \sim K} \frac{|\partial K \cap \partial L \cap \Omega_r|}{|x_K - x_L|} \kappa_{0,r} F_r(T_{KL}) G_{K,L,r}(\varphi)^{p_r-2} (\varphi_L - \varphi_K).$$

The same approach of calculating the conductivity in the Joule heat term is combined with the approach suggested in [9] which allows us to calculate the Joule heating approximation by edge contributions: Applying Gauss's theorem leads to

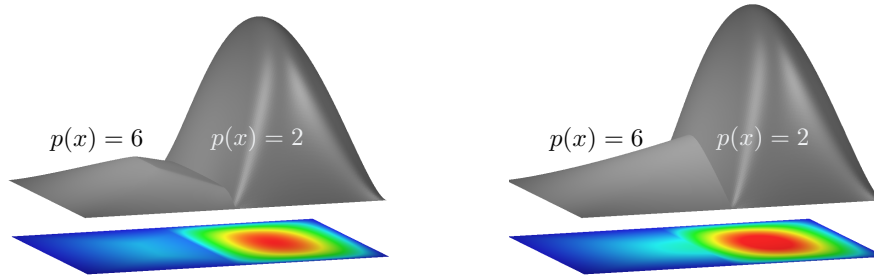
$$\begin{aligned} 0 &= \int_K (\nabla \cdot (\lambda(x) \nabla T) + H(x, T, \nabla \varphi)) \, dx \\ &= \sum_{L \sim K} \int_{\partial K \cap \partial L} \lambda(x) \nabla T \cdot \nu_{KL} \, da + \int_K (1 - \eta(x)) \kappa_0(x) F(x, T) |\nabla \varphi|^{p(x)} \, dx, \end{aligned} \quad (5)$$

and the suggested approach yields the approximation of the heat flow equation on  $K$

$$\begin{aligned} 0 &= \sum_{r \in \mathcal{R}} \sum_{L \sim K} \left( \frac{|\partial K \cap \partial L \cap \Omega_r|}{|x_K - x_L|} \lambda_r (T_L - T_K) \right. \\ &\quad \left. + d \frac{|\partial K \cap \partial L \cap \Omega_r|}{|x_K - x_L|} (1 - \eta_r) \kappa_{0,r} F_r(T_{KL}) G_{K,L,r}(\varphi)^{p_r-2} (\varphi_L - \varphi_K)^2 \right), \end{aligned}$$

where  $T_{KL} = (T_K + T_L)/2$ .

It is important to take care of the hetero interface when calculating the average of the gradient norm. An averaging over all simplices adjacent to a given edge regardless of the hetero region they belong to leads to an artificial diffusion along the hetero interface (see Fig. 3) which does not diminish with grid refinement. The validity of this approach and the way it has been implemented hinges on the fact that all the measures  $|\partial K \cap \partial L \cap \Omega_r|$  can be calculated from contributions from each simplex which at the hetero interfaces have to stay nonnegative. It is guaranteed by the boundary conforming Delaunay property of the underlying triangulation.



**Fig. 3** Discrete solutions of  $p(x)$ -Laplace equation with constant right-hand side, Dirichlet boundary conditions, and piecewise constant  $p(x)$ . Left: Wrong approximation with two local maxima due to gradient averaging ignoring the hetero interface. Right: Correct approximation.

**Acknowledgement.** A.G. and M.L. gratefully acknowledge the funding received via Research Center MATHEON supported by ECMath in project D-SE2.

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