Electro-thermal Drift-diffusion simulations for organic light-emitting diodes

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Abstract— **A coupled electrothermal model is presented for 1D non-isothermal drift-diffusion simulations to analyze self-heating in organic light-emitting diodes. Governing equations, boundary conditions, discretization scheme and structure preserving properties are discussed. The simulation of simple organic device structures shows that the model can reproduce non-linear electrothermal effects. Thermal parameter variation yields results that are in line with experimentally observed trends. Simulations are shown to reproduce properties of the solution that are predicted from analytic theory. The model achieves successful integration of thermal effects into a full opto-electronic device simulation tool.**

Keywords—Electro-thermal, Drift-diffusion, OLED, Self-heating

I. INTRODUCTION

Continuing adoption of organic light emitting diodes (OLED) in display and lighting application raises the requirements for brightness [1] (>1000 cd/m^2) and presents the issue of self-heating known from traditional electronics applications where high-power throughput is required. The issue is further accentuated by the fact that organic materials exhibit a temperature-activated conductivity (TAC) [2] creating a setup whereby a strong, two-way coupling is observed between electronic and thermal properties of the device. This coupling leads to highly non-linear phenomena such as S-shaped current-voltage curves and negative differential resistance (NDR) or even sudden burn-in phenomena [3]. To understand such phenomena several approaches have been suggested including, fully analytical models based on the power balance equation [4], p-Laplace thermistor models[5] or numerical drift diffusion (DD) models [6] [7]. The later approach allows us to understand how charge injection, transport and recombination affect self-heating phenomena and vice versa. Modern OLED devices are comprised of complex multi-layer structures. Integrating thermal models with industrial-strength tools like SETFOS is necessary in order to model realistic device setups and assess the impact of thermal effects on device efficiency.

II. MODEL DESCRIPTION

A. Governing equations

The starting point for our analysis is the 1D non-isothermal drift-diffusion system comprising of the current continuity equations and the Poisson equation. The self-heating behavior of OLED originates from microscopic processes like Joule heating and non-radiative recombination. Generation and transport of heat is described by the diffusion equation and its source terms H_J, H_R:

$$-\nabla(\kappa\nabla T) = H_J + H_R \qquad (1)$$
$$H_J = -j_n(\nabla\varphi_n + P_n\nabla T) - j_p(\nabla\varphi_p + P_p\nabla T) \qquad (2)$$
$$H_R = qR(\varphi_p - \varphi_n) \qquad (3)$$

The thermal conductivity κ is a material property, T stands for the variable temperature, $j_{n(p)}$ is the electron (hole) current density, φ_n is the quasi-Fermi potential (QFP), P_n is the thermopower coefficient according to the Kelvin formula [8] and R is the recombination rate. Since organic materials do not exhibit strong thermoelectric effects, we neglect Peltier-Thomson heating-cooling. This formulation of H_J avoids averaging exponentially varying densities while ensuring the non-negativity of the source terms in the presence of thermal gradients.

B. Boundary Conditions

For the electrical boundary conditions (BC) we use Dirichlet (BC) for the potential and ohmic BC for the injected charge species, $n_b = N\exp\left(-\frac{W_n - E_{LUMO}}{k_B T}\right)$, where N is the effective density of states w_n is the metal work function, k_B is Boltzmann's constant and T is the temperature of the device at the boundary. The reciprocal densities are calculated so that the intrinsic Equation, $n_b \cdot p_b = N^2$, is satisfied. The contact density for the BC is re-computed every time the temperature changes so that charge equilibrium is ensured at elevated temperatures. This way the electrochemical potential remains pinned at the applied voltage throughout the simulation. In the domain outside the electrical stack there are no heat sources, thus the incoming thermal current density, $j_{th} = -k\nabla T$, is conserved. Considering an effective thermal resistance R_{th}, describing the OLED package, and an ambient temperature T_a the boundary temperature T_b is given by:

$$T_b = T_a + R_{th} \cdot P_{th} \qquad (4)$$

where P_{th} is the power resulting from integrating j_{th} over the contact area A.

C. Finite difference discretization scheme

The semiconductor equations follow the generalized Scharfetter-Gummel discretization scheme. The discrete Joule heating term $H_{n,i+1/2}$, adapted from [8] is well defined at half integer nodes $i\pm1/2$ in between vertices:

$$H_{n,i+1/2} = -j_{n,i+1/2}\left(\frac{\varphi_{i+1}-\varphi_i}{h_{i+1/2}} + P_{n,i+1/2}\frac{T_{i+1}-T_i}{h_{i+1/2}}\right) \quad (5)$$

$$P_{n,i+1/2} = \frac{k_B}{q} \cdot \frac{(T_{i+1}-T_{i+1/2})w_{i+1}-(T_i-T_{i+1/2})w_i}{T_{i+1}-T_i} \quad (6)$$

$$n_i = N\,e^{w_i} \quad (7)$$

where n is the charge density, h is the grid spacing, and w denotes a generalized Fermi energy.

III. Results

Steady state (SS) simulations performed using H_J and H_R as sources satisfy energy conservation, meaning injected electrical power per unit area P_{el} equals the sum of thermal power P_{th} exiting at the contacts. To showcase electrothermal effects we chose a simple setup consisting of a unipolar, p-type, single layer 100 nm thick doped (10^{19} cm^{-3}) organic semiconductor device employing a temperature dependent mobility law [4] modeled according to an Arrhenius equation:

$$\mu = \mu_0 \exp\left(\frac{-E_a}{k_B T}\right) \quad (8)$$

We chose a typical value for the activation energy of $E_a =$ 0.5 eV, and a mobility perfector $\mu_0 = 5\times 10^{-6}$ cm^2/Vs. Figure 1a shows current-voltage (J-V) curves for different values of the R_{th}. For non-zero R_{th} values the curve exhibits the S-shaped J-V characteristic of the positive electrothermal feedback. Due to the nonlinear power temperature relation $P_{th}(T)$ Eq. (4) features two solution branches for a given voltage. The top solution branch has NDR corresponding to the higher temperature state as seen in figure 1b. The model correctly reproduces the physical trends observed in experiments [5] and simulation [7]. The temperature for the first turn-over point, where the differential resistance becomes 0, can be calculated as a function of activation energy according to the analytic formula [4]:

$$T_0 = \frac{E_\alpha}{2k_B}\left(1 - \sqrt{1-\frac{4k_B T_a}{E_a}}\right) \quad (9)$$

From figure 1a-b we can see that the turnover point stays constant with respect to different R_{th}. For an effective activation energy of ~ 0.5 eV and ambient temperature of 296 K we expect $T_0 \sim 312.87$ K for all R_{th}, matching well with our results.

IV. Conclusions

We have shown the numerical implementation of a non-isothermal drift-diffusion scheme capable of simulating self-heating phenomena in organic semiconductor devices. Charge equilibrium density boundary conditions were modified to account for the temperature dependent state. Thermal boundary conditions were implemented based on the thermal resistance of the OLED package. A self-consistent discretization scheme was adapted from literature that satisfies energy conservation and energy balance. Electrothermal simulations confirmed negative differential resistance regions and positive feedback effects for organic devices with temperature-activated conductivity. The model paves the way for full electro-thermal-optical OLED device simulation.
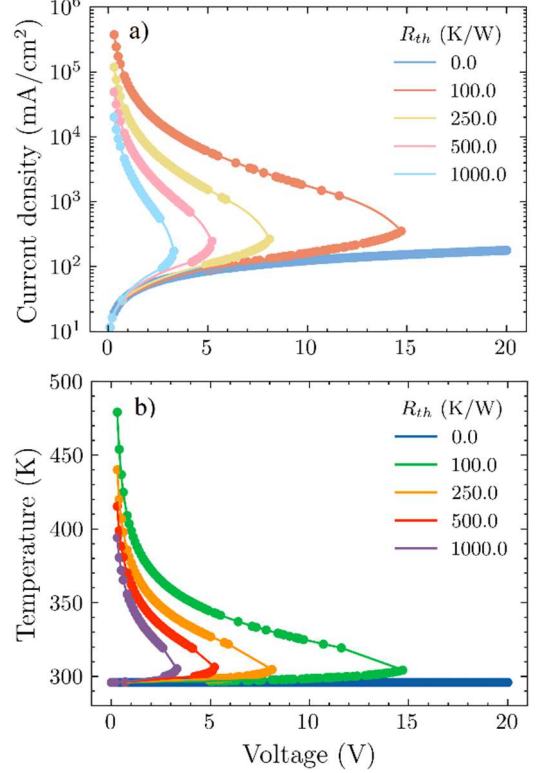

Fig. 1. (a) J-V of organic device with TAC for different values of the thermal resistance R_{th} (b) Corresponding average electrical stack temperature. Data points mark simulations results while lines represent a linear interpolation to guide the eye.

VI. References

[1]   A. Fischer *et al.*, "Full Electrothermal OLED Model Including Nonlinear Self-heating Effects," *Phys Rev Appl*, vol. 10, no. 1, Jul. 2018.

[2]   H. B. Anna Köhler, *Electronic Processes in Organic Semiconductors: An Introduction*.

[3]   A. Kirch, A. Fischer, M. Liero, J. Fuhrmann, A. Glitzky, and S. Reineke, "Electrothermal Tristability Causes Sudden Burn-In Phenomena in Organic LEDs," *Adv Funct Mater*, vol. 31, no. 47, Nov. 2021.

[4]   A. Fischer *et al.*, "Self-heating, bistability, and thermal switching in organic semiconductors," *Phys Rev Lett*, vol. 110, no. 12, Mar. 2013.

[5]   A. Kirch, A. Fischer, M. Liero, J. Fuhrmann, A. Glitzky, and S. Reineke, "Experimental proof of Joule heating-induced switched-back regions in OLEDs," *Light Sci Appl*, vol. 9, no. 1, Dec. 2020.

[6]   E. Knapp and B. Ruhstaller, "Analysis of negative capacitance and self-heating in organic semiconductor devices," *J Appl Phys*, vol. 117, no. 13, p. 135501, Apr. 2015.

[7]   D. H. Doan, A. Fischer, J. Fuhrmann, A. Glitzky, and M. Liero, "Drift–diffusion simulation of S-shaped current–voltage relations for organic semiconductor devices," *J Comput Electron*, vol. 19, no. 3, pp. 1164–1174, Sep. 2020.

[8]   M. Kantner, "Generalized Scharfetter–Gummel schemes for electro-thermal transport in degenerate semiconductors using the Kelvin formula for the Seebeck coefficient," *J Comput Phys*, vol. 402, Feb.