Electrical Modelling of Large-area Organic Light-emitting Devices

Evelyne Knapp and Beat Ruhstaller

Institute of Computational Physics, Zurich University of Applied Sciences, Wildbachstr. 21, 8401 Winterthur, Switzerland
evelyne.knapp@zhaw.ch, beat.ruhstaller@zhaw.ch

Summary. Systematic improvement of the performance and lifetime of organic light-emitting devices (OLEDs) are facilitated by electrical characterization through experiments and simulations. We model charge transport in organic disordered materials with the aid of a numerical 1D model for different experimental setups such as current-voltage curves, current transients and electrical impedance spectroscopy. For large-area OLEDs we couple the anode and cathode with the 1D model leading to an efficient 1+2D approach.

1 Introduction

Although the commercial success of organic light-emitting devices (OLEDs) in displays and lighting proceeds rapidly, further research is necessary to improve the efficiency and lifetime. Numerical simulations help to reduce the number of prototype iterations. Electrical characterization of devices and materials is crucial as it sheds light on the physical models of charge carrier transport in disordered, organic semiconductors. Charge transport and recombination models have been introduced several years ago for organic LEDs [1–5]. However, organic semiconductors differ considerably from their inorganic counterparts, not only by low carrier mobilities and long recombination times but also by the disorder. Taking the disordered nature of organic materials into account leads to a description in terms of a Gaussian density of states (DOS) which affects the mobility of charge carriers and the diffusion coefficient. The Gaussian DOS enhances the nonlinearities and the coupling between the equations. These circumstances prevent the use of classical drift-diffusion solvers. With the aid of a one-dimensional numerical OLED model we are able to simulate different operating conditions such as current-voltage curves [6], dark-injection measurements and impedance spectroscopy. We conduct steady-state, transient and small-signal analysis for the 1D OLED model and compare them with experiments. For lighting applications OLED panels are used that need to be as homogeneous as possible. To take this requirement into account we couple the 1D model to two 2D domains.

2 Physical Model

The drift-diffusion model (1) and (2) with the organic model ingredients (such as a Gaussian density of states and the use of the Fermi-Dirac statistics) are discretized with the finite volume method, the current expression (3) with the Scharfetter-Gummel discretization [7]. The resulting system of discretized equations is then solved in a coupled manner with Newton's algorithm for the transient as well as the steady-state case [8].

$$\nabla \cdot (\varepsilon \nabla \psi) = q(n_f + n_t - p_f - p_t), \tag{1}$$

$$\begin{aligned} \nabla \cdot J_n - q(\tfrac{\partial n}{\partial t}) &= \quad qR(n_f, p_f), \\ \nabla \cdot J_p + q(\tfrac{\partial p}{\partial t}) &= -qR(n_f, p_f), \end{aligned} \tag{2}$$

$$\begin{aligned} J_n &= \ -qn_f \mu_n \nabla \psi + qD_n \nabla n_f, \\ J_p &= -qp_f \mu_p \nabla \psi - qD_p \nabla p_f. \end{aligned} \tag{3}$$

For the small-signal analysis, the steady-state voltage V_0 is modulated with a sinusoidal voltage with the amplitude V^{ac} and with the angular frequency ω: $V = V_0 + V^{ac} e^{i\omega t}$. The potential ψ and the charge densities p and n can be expanded into a steady-state and harmonic term, e.g. $\psi(x,t) = \psi_0(x) + \psi^{ac}(x)\mathrm{e}^{\mathrm{i}\omega t}$ where the ac components are complex-valued. To solve the small-signal equations, the solution of the dc problem for $V = V_0$ is required. After inserting the expansions into the linearized drift-diffusion model we obtain a linear system of equations for the unkown ac components and thus for the ac current J^{ac}. From the complex admittance $Y = J^{ac}/V^{ac}$, the small-signal capacitance C and conductance G can be obtained. Charge traps originate in impurities or material degradation and affect the transport. In Fig. 1 we show the effect of different charge trap types on the normalized capacitance at different frequencies. Fast traps are in quasi-equilibrium with free carriers, the transit time is longer than the trapping time whereas for slow traps the transit time is shorter than the trapping time. Slow traps enhance the capacitance at low frequencies while fast traps follow the dynamics of the trap-free case [9]. Similarly, charge traps affect current transients and current-voltage curves.

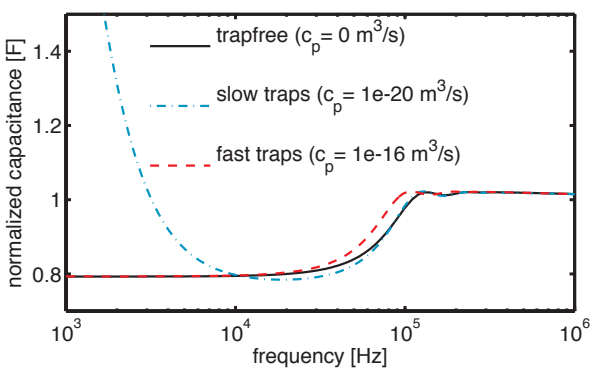

Fig. 1. Normalized capacitance of different trap types at various frequencies.

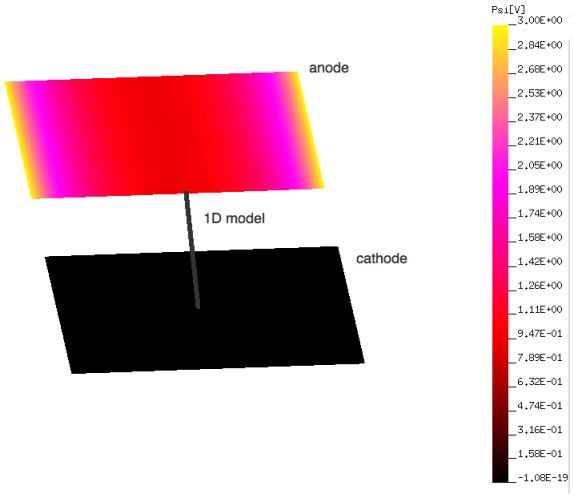

Fig. 2. Coupling of the 1D and 2D domains in an organic LED model. We display the potential drop before a metal grid structure is added.

3 2+1D Approach for Large-area OLEDs

Aiming for a fast PC model for large-area OLEDs we have to take into account that realistic OLED structures consist of transparent anodes with a relatively low electrical conductivity. This affects the homogeneity of the OLED. Metal grid structures are applied to large-area OLEDs to improve the situation. To quantify the potential and temperature drop in large-area OLEDs we extend the 1D modelling of the organic material to higher dimensions. The 2+1D approach captures the important features of the transport process, and accounts for the high aspect ratio between the in-plane and the through-plane dimensions of OLEDs. In comparison to full 3D models, the 2+1D approach requires a reduced number of degrees of freedom, but still provides the lateral potential and temperature distribution. We make use of our in-house FEM tool (SESES) that allows the nonlinear coupling of 2D domains with the aid of the 1D model as shown in Fig. 2. The connection between the anode and cathode can either be:

- a parameterized experimental curve
- an analytical formula
- or a numerical model.

In Fig. 2 we show an OLED panel before optimizing the metal grid layout. No metal structure is present to improve the homogeneity of the OLED.

4 Conclusions

In this paper, we present a 1D model for organic LEDs that is applied to different operating conditions such as steady-state, transient and ac response. We investigate different charge trap types and their influence on the frequency-dependent capacitance. Further, we propose a 2+1D modeling approach for large-area OLEDs.

Acknowledgement. We acknowledge financial support from the European Communitys Seventh Framework program under grant agreement no. 213708 (AEVIOM.eu) and NMP4-SL-2011-295368 (im3oled.eu).

References

1. J.C. Scott and G.G. Malliaras. Charge injection and recombination at the metalorganic interface. *Chem. Phys. Lett.*, 299:115, 1999.
2. B.K. Crone, P.S. Davids, I.H Campbell, D.L. Smith. Device model investigation of bilayer organic light emitting diodes. *J. Appl. Phys.*, 87(4):1974, 2000.
3. P.W.M. Blom, M.J.M. de Jong, J.J.M. Vleggaar. Electron and hole transport in poly(p-phenylene vinylene) devices. *Appl. Phys. Lett.*,68(23):3308, 1996.
4. B. Ruhstaller, S.A. Carter, S. Barth, H. Riel, W. Riess, J.C. Scott. Transient and steady-state behavior of space charges in multilayer organic light-emitting diodes. *J. Appl. Phys.*,89(8):4575, 2001.
5. B. Ruhstaller, T. Beierlein, H. Riel, S. Karg, J.C. Scott, W. Riess. Simulating electronic and optical processes inmultilayer organic light-emitting devices. *IEEE J. Sel. Top. Quantum Electron.*,9(3):723, 2003.
6. S.L.M. van Mensfoort, S.I.E. Vulto, R.A.J. Janssen, R. Coehoorn. Hole transport in polyfluorenebased sandwich-type devices: quantitative analysis of the role of energetic disorder. *Phys. Rev. B*,78(8):085208, 2008
7. D.L. Scharfetter and H.K. Gummel. Large-signal analysis of a silicon read diode oscillator. *IEEE Trans. Electr. Dev.*,16(28):64, 1969.
8. E. Knapp, R. Häusermann, H. Schwarzenbach, B. Ruhstaller. Numerical simulation of charge transport in disordered organic semiconductor devices. *J. Appl. Phys.*,99(9):093304, 2011.
9. E. Knapp and B. Ruhstaller. Numerical impedance analysis for organic semiconductors with exponential density of localized states. *Appl. Phys. Lett.*,108(5):054504, 2010.