Numerical Analysis of Steady-State and Transient Charge Transport in Organic Semiconductor Devices

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***Abstract*—A one-dimensional numerical model for the simulation of organic light-emitting devices (OLEDs) is presented. The model accounts for the disordered nature of organic semiconductors by a Gaussian density of states and the use of the Fermi-Dirac statistics. It includes density- and field-dependent mobilities and the generalized Einstein relation. The novel model ingredients perform well in combination with the numerical methods which solve the drift-diffusion problem. The results of three different measurement setups are reproduced by the use of different numerical techniques, i.e. we efficiently simulate current-voltage curves, dark-injection transients and impedance spectroscopy. This is crucial for model validation and parameter extraction. We compare the simulations with analytical solutions and measurements.**

I. INTRODUCTION

To improve the performance and structure of organic light-emitting devices (OLEDs) electrical characterization of devices and materials is essential and helps to illucidate the underlying, physical models of charge carrier transport in disordered, organic semiconductors. Besides the commonly used current-voltage curves [1], dark-injection measurements and impedance spectroscopy offer other forms to validate models for organic LEDs and extract model parameters. By means of a one-dimensional numerical OLED model we are able to simulate these different measurement setups. In this paper, we present numerical methods in the physical and numerical framework of reference [2] and solve directly for the steady- and transient state. Further, we conduct a numerical small signal-analysis for OLEDs. The underlying model solves the drift-diffusion equations in a coupled manner for disordered, organic semiconductor. The disordered nature of organic semiconductors affects the density of state, the mobility model, the Einstein relation as well as charge injection. These novel physical model ingredients are integrated in the numerical solver.

II. TRANSPORT MODEL

For the description of charge transport in OLEDs the general semiconductor drift-diffusion equations for electrons and holes are valid. In Poisson's equation

$$\nabla \cdot (\epsilon \nabla \psi) = q(n-p), \tag{1}$$

the electrical potential ψ is related to the electron and hole densities n and p where q is the elementary charge and ϵ the product of the vacuum permittivity ϵ_0 and the relative permittivity ϵ_r of the organic material.

The current equations for electrons and holes read

$$\begin{aligned} J_n =& \quad -qn\mu_n \nabla\psi + qD_n \nabla n, \\ J_p =& \quad -qp\mu_p \nabla\psi - qD_p \nabla p. \end{aligned} \tag{2}$$

where $\mu_{n,p}$ denotes the mobility and $D_{n,p}$ the diffusion coefficient for electrons and holes. The conservation of charges leads to the continuity equations for electrons and holes

$$\begin{aligned} \nabla \cdot J_n - q(\tfrac{\partial n}{\partial t}) =& \quad qR(n,p), \\ \nabla \cdot J_p + q(\tfrac{\partial p}{\partial t}) =& \quad -qR(n,p), \end{aligned} \tag{3}$$

where R denotes the bimolecular recombination rate given by Langevin [3] and t the time. These equations take charge migration and recombination into account. As opposed to inorganic semiconductors the density of states for organic semiconductors is described by a Gaussian DOS

$$N_{Gauss}(E) = \frac{N_0}{\sqrt{2\pi\sigma^2}} \exp\left[-\left(\frac{E-E_0}{\sqrt{2}\sigma}\right)^2\right] \tag{4}$$

since transport is assumed to occur via a hopping process between uncorrelated sites. Thus, polymers and small molecules have broadened HOMO and LUMO energy levels. The DOS in (4) affects the mobility of charge carriers and the diffusion coefficient. Therefore a generalized Einstein relation must be considered [4] for disordered organic materials.

Further, the mobility model consists of a field-, temperature- and density-dependent part. This model is called Extended Gaussian Disorder Model (EGDM) [5], [6] and can be written as the product with the density-enhancement function $g_1(p,T)$ and the field-enhancement function $g_2(F,T)$: $\mu(p,F,T) = \mu_0(T) \times g_1(p,T) \times g_2(F,T)$ where p denotes the density, F the electric field and T the temperature. The enhancement functions $g_1(p,T)$ and $g_2(F,T)$ are nonlinear and increase more strongly, the bigger the disorder in the organic material is.

III. NUMERICAL METHOD

The drift-diffusion equations with the organic model ingredients are discretized with the finite volume method, (2) with the Scharfetter-Gummel discretization [7]. The resulting system is solved in a coupled manner with the Newton

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algorithm for the transient and steady-state case.

For the small-signal analysis, the steady-state voltage V_0 is modulated with a sinusoidal voltage of amplitude V^{ac} and with angular frequency ω: $V = V_0 + V^{ac}e^{i\omega t}$. The potential ψ, the electron and hole densities n and p can be expanded into a steady-state and harmonic term under the assumption of the small-signal analysis:

$$\psi(x,t) = \psi_0(x) + \psi^{ac}(x)e^{i\omega t} \tag{5}$$

$$n(x,t) = n_0(x) + n^{ac}(x)e^{i\omega t} \tag{6}$$

$$p(x,t) = p_0(x) + p^{ac}(x)e^{i\omega t} \tag{7}$$

The above quantities are inserted into the semiconductor equations. This leads to a linear system of equations for ψ^{ac}, n^{ac} and p^{ac}.

IV. RESULTS

We consider a hole-only device with a well-injecting anode for the simulation of the current-voltage curve, dark-injection transients and impedance spectroscopy. The simulation results are compared with analytical solutions and the therefrom derived mobilities for charge carriers. We show and discuss the influence of the EGDM and its components on the results. In Fig. (1) a current-voltage curve is shown for a symmetric hole-only device for the EGDM, constant mobility and diffusion and the analytical solution. The same models are considered for the transients in Fig. (2) and for the impedance spectroscopy in Fig. (3). Moreover, we check the model consistency for the different setups by comparing the simulation results with measurements.

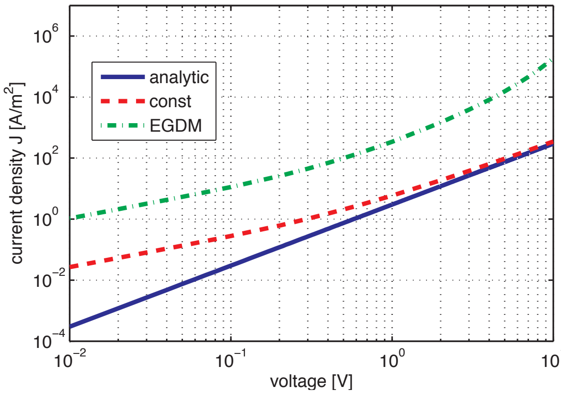

Fig. 1. Current-voltage curve for a hole-only device for a constant mobility and diffusion coefficient, the EGDM and the analytic solution (Mott-Gurney).

V. CONCLUSION

We have shown that our solver is able to simulate different measurement setups for OLEDs. We investigate the influence of the EGDM, its components and the Gaussian density of states on the current-voltage curves, the dark-injection transients and the frequency response for a polymer device. All three characterization curves change significantly, if the disorder model ingredients are taken into account. The simulation results are also compared with analytical solutions.

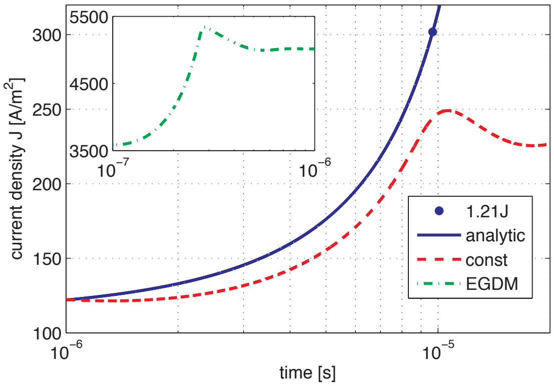

Fig. 2. Dark-injection transients for a hole-only device for a constant mobility and diffusion coefficient and the analytic solution. Inset: transient for the EGDM.

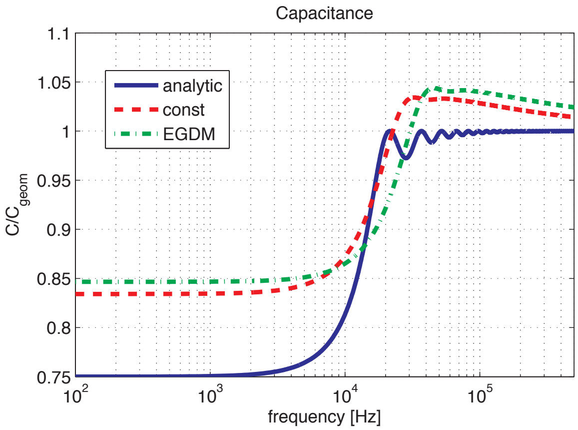

Fig. 3. Frequency dependence of the normalized capacitance in a hole-only device for a constant mobility and diffusion coefficient, the EGDM and the analytic solution.

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