Heat and carrier flow in organic semiconductor devices – Modeling, analysis, and simulation

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The temperature activated hopping transport of charge carriers in organic semiconductors results in a strong interplay between electric current and heat flow. It gives rise to interesting phenomena like S-shaped current-voltage relations with regions of Negative Differential Resistance or leads to inhomogeneous luminance in large-area Organic Light Emitting Diodes (OLEDs) (see Figure 1 and [1]). Moreover, electrothermal effects influence the performance of transistors [2].

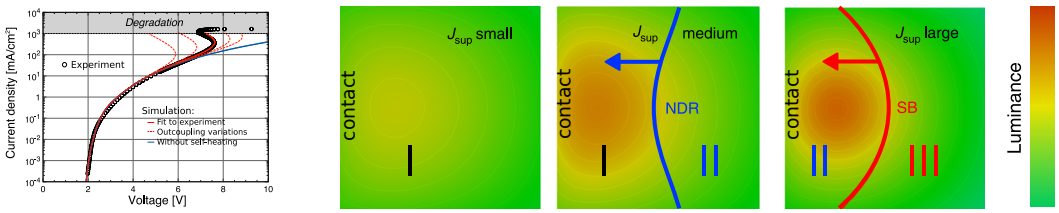

FIGURE 1. Left: Measured and simulated S-shaped current-voltage relations (up to thermal degradation) for OLED device, Right: Simulated luminance in OLED cross-section for increasing supplied current, I, II, III refer to different operation modes that propagate through the device: normal, local NDR, and switched-back. In the latter mode, the local currents, and hence also the luminance, decreases.

As demonstrated in [1], p-Laplace thermistor models that describe the total current and heat flow in a device, are able to capture the positive temperature feedback in OLEDs. Especially, they can reproduce experimentally observed S-shaped CV-relations and inhomogeneous current density and temperature distributions in large-area OLEDs. But, details such as separate electron and hole current flow, generation-recombination and related heat productions, as well as energy barriers at material interfaces cannot be included. Thus a description of the electrothermal behavior of organic semiconductor devices via more detailed drift-diffusion models is required. In these models the specialities of organic semiconductors have to be taken into account: On the one hand the statistical relation between chemical potentials and charge carrier densities is given by Gauss–Fermi integrals leading to bounded charge carrier densities. On the other hand the mobility functions μ_n, μ_p depend on temperature, density, and electrical field strength. The mobility laws are fitted from a numerical solution of the master equation for the hopping transport in a disordered energy landscape with a Gaussian density of states [3, 4].

In this talk, we give an overview over modeling the electrothermal behavior of organic devices with thermistor- and drift-diffusion-type models as well as hybrid concepts, summarizing [6, 5, 7, 8]. We discuss the mathematical analysis of the underlying equations, the numerical approximation via finite-volume methods based on modified Scharfetter–Gummel schemes, and present simulation results using path-following techniques for recovering the S-shaped current-voltage relations.

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