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Electro-thermal modeling of organic semiconductors describing negative differential resistance induced by self-heating

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Abstract—We discuss self-heating of organic semiconductor devices based on Arrhenius-like conductivity laws. The selfconsistent calculation of charge and heat transport explains thermal switching, bistability, and hysteresis resulting from Sshaped current-voltage curves with regions of negative differential resistance (NDR). For large area thin film organic devices we study the appearance of a spatially localized NDR region and the spatial evolution of this NDR region in dependence on the total current. We propose that in organic light emitting diodes (OLEDs) these effects are responsible for spatially inhomogeneous current flow and inhomogeneous luminance at high power.

I. INTRODUCTION

For organic semiconductor devices the well known Arrhenius law applies: The electric conductivity increases with rising temperature. Therefore the electrical current increases and the device gets warm, resulting in a feedback loop which continuously heats up the structure. Often experiments of this kind lead to the destruction of the device. Devices strongly sensible to temperature and thus resulting in such feedback effects are called thermistors and can be used in power electronics.

Nowadays, organic semiconductors reach the range of selfheating, too. Investigations and experiments for the organic semiconductor C_{60} are reported in [1]. Organic devices can heat up in an uncontrollable way leading to thermal breakdown [1] or undesirable spatially inhomogeneous current distributions. For higher light intensities, spatial inhomogeneities in the luminance of large area OLEDs can result from selfheating. In lighting panels the area becomes spotty.

II. SELF-HEATING, BISTABILITY AND THERMAL SWITCHING

The charge transport in organic semiconductors occurs by hopping of electrons between discrete energy levels of molecular sites nearby. These energy states are Gaussian distributed with variance σ and centered at an energy E_0 . The dependence of the mobility μ on the temperature T resulting from the disorder σ can be approximated by an Arrhenius law

$$\mu(T) = \mu_0 \exp\left[-\frac{E_{\rm act}}{k_B T}\right] \tag{1}$$

with an activation energy $E_{\rm act}=2C\sigma^2/(k_{\rm B}T_a)~(k_{\rm B}~{\rm Boltz-mann's}$ constant, T_a ambient temperature, $C\approx~0.4,~\mu_0$

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reference mobility); see [2]. The strong increase of the carrier mobility with the temperature leads to self-amplification of the current and to strong self-heating effects at large currents.

For materials with Arrhenius-like conductivity laws, thermal switching phenomena induced by self-heating appear for activation energies $E_{\rm act} > 4k_{\rm B}T_a$, see [3]. Usual values of the disorder parameter σ of 2 to $6k_{\rm B}T_a$ give activation energies large enough for thermal switching.

We study the self-heating for a thermally activated conductivity in a spatially homogenous situation [4] and suppose an isothermal current-voltage relation of the device given by

$$I_{\rm iso}(U,T) = I_{\rm ref} \left(\frac{U}{U_{\rm ref}}\right)^{\alpha} F(T), \quad \alpha > 0, \tag{2}$$

and a conductivity factor F(T) resulting from an Arrhenius law

$$F(T) = \exp\left[-\frac{E_{\text{act}}}{k_{\text{B}}}\left(\frac{1}{T} - \frac{1}{T_{a}}\right)\right].$$
(3)

The quantities $U_{\rm ref}$, $I_{\rm ref}$, and $P_{\rm ref} = U_{\rm ref}I_{\rm ref}$ denote reference values for voltage, current and power, respectively. The homogeneous steady states of the device are equilibria of the global heat balance equation expressing that the dissipated Joule power *IU* equals the heat loss $\frac{1}{\Theta_{\rm th}}(T - T_a)$ to the surroundings described by the thermal resistance $\Theta_{\rm th}$

$$\frac{1}{\Theta_{\rm th}}(T - T_a) = P_{\rm ref} \left(\frac{U}{U_{\rm ref}}\right)^{\alpha+1} F(T).$$
(4)



Fig. 1. Self-consistent current-voltage characteristics for different activation energies (red). For $E_{\rm act} > 4k_{\rm B}T_a$ they show S-shaped NDR (red dashed). Blue: Isothermal current-voltage curve with $\alpha = 1$, compare [4].

From (2) and (4) one obtains the self-consistent IV characteristic (U(T), I(T)) including self-heating parameterized by the temperature $T \geq T_a$, see [4]. The red curves in Fig. 1 show calculated self-consistent IV curves for a linear isothermal IV characteristics ($\alpha = 1$) and different activation energies. For $E_{\rm act} > 4k_{\rm B}T_a$, a region of negative differential resistance (NDR), $\frac{\mathrm{d}U}{\mathrm{d}I} < 0$ appears.

Along the S-shaped IV characteristics, two stable branches exist: an 'ON' state with high conductivity and an 'OFF' state with low conductivity, whereas the intermediate region of NDR is unstable (dashed red lines in Fig. 1). This bistable behavior of the IV characteristic is related to thermal switching at the turning points, involving a hysteresis loop, where the switching between the OFF and the ON branches occurs. The behavior of the analytic electro-thermal model can be approximated by a thermistor circuit.

For real devices, an additional constant series resistance R_L resulting from the contact resistance and the measurement setup has to be added in series to the S-NDR element. In [4] thermal switching and a pronounced hysteresis loop has been experimentally demonstrated for a C_{60} nin device with small active area of about 0.06 mm² containing a 300 nm thick intrinsic C_{60} layer. The experimental results are in very good agreement with theory, see Fig. 2.

III. LARGE AREA THIN-FILM DEVICES

For OLEDs, the optically transparent top contact is realized using indium tin oxide (ITO) which has a considerably high electrical resistance. In particular, for large area devices this results in a voltage drop along current paths through the top contact (ITO), see Fig. 3. For the typical crossbar contact geometry used for OLEDs this voltage drop leads to a spatial variation of the effective applied voltage across the active OLED layer between top contact (ITO) and bottom contact (metal), see Fig. 3.

Therefore, the application of spatially homogeneous models is no longer justified. OLED lighting panels nowadays have a width in the range of 10 to 20 cm and show an inhomogeneous spatial distribution of current and light intensity at high power. For the explanation of these unwanted effects we investigate the influence of the sheet resistance of the contact material for large area thin film devices by



Fig. 2. Measured hysteresis loop during a voltage sweep upwards and downwards for a C_{60} nin device, see [4]. Blue: isothermal current-voltage curve measured by short voltage pulses.



Fig. 3. Schematic diagram of current paths and potential drop along the top contact (ITO) for an OLED with crossbar contacts.

means of a spatially resolved generalization of the homogenous self-heating model [4]. This electro-thermal model contains a contact resistance, an Arrhenius-type current-voltage relation (2) for the active OLED layer, and a local heat balance instead of a global one (4). We present a study on the appearance of spatially local NDR regions and of the propagation of NDR fronts through the OLED device in dependence on the total current by self-consistent electro-thermal simulations. We propose that NDR phenomena in OLEDs can be present already at moderate temperature rises and therefore could be the reason for an accelerated increase in brightness inhomogeneities.

IV. CONCLUSION

In all organic devices with sufficiently large activation energies, self-heating can lead to S-shaped IV characteristics with NDR regions. This behavior was experimentally verified for nin-C₆₀ crossbar structures and OLEDs at IAPP. Moreover, self-heating can promote spatial inhomogeneities. We investigated the appearance and the evolution of spatially local NDR regions in large area thin-film devices by spatially resolved models including the positive feedback between temperature and an Arrhenius law for the conductivity. Our studies can help to elucidate spatial inhomogeneities of current density and luminance in large area lighting panels at high power.

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