Numerical Estimation of the Impact of Energetic Disorder on the Low-Frequency CV Characteristics of Organic MOS Structures

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Summary. We propose a numerical model for estimating the low frequency Capacitance-Voltage (CV) characteristics of organic MOS structures and we use it to study the dependence of CV curves on the DOS. Preliminary results seem to suggest that low frequency CV measurements could be a viable means to estimate the DOS width of a material independently of its transport properties.

1 Introduction

Conjugated polymers are attracting increasing interest as viable semiconducting materials for various applications such as Organic Solar Cells (OSCs) [4], Field Effect Transistors (FETs) [7],Organic Light-Emitting Diodes (OLEDs) [5], photodetectors [1]. For this reason, much effort has recently gone in developing numerical tools for the simulation of this new class of devices [3, 8]. In particular regarding charge transport it must be reminded that organic semiconductors are generally amorphous and as such are to be modelled as disordered systems with localized states whose distribution is assumed to be in the simplest case a Gaussian with variance centered at the Lowest Unoccupied Molecular Orbital (LUMO) for electrons and centered at the Highest Occupied Molecular Orbital (HOMO) for holes. Charge carrier mobilities are modeled assuming that transport occurs as a hopping process (a thermally activated tunnelling) between localized sites and the variance of the Density of states appears as a parameter in the models. A method for determining the value of for a given material independently of its transport properties would greatly improve the predictive ability of numerical simulations. In this communication, we propose a numerical model for estimating the low frequency Capacitance-Voltage (CV) characteristics of organic MOS structures and we use it to study the dependence of CV curves on the DOS. In addition to the Gaussian DOS, we explore the effect on CV of more elaborate DOS models, such as two Gaussian distributions or a space-dependent distribution given by a Guassian with an exponential tail close to the insulator interfaces which fades into a Gaussian towards the bulk, simuating the effect of disordered electric dipoles within the insulator. Preliminary results seem to suggest that low frequency CV measurements could be a viable means to estimate the DOS width of a material independently of its transport properties.

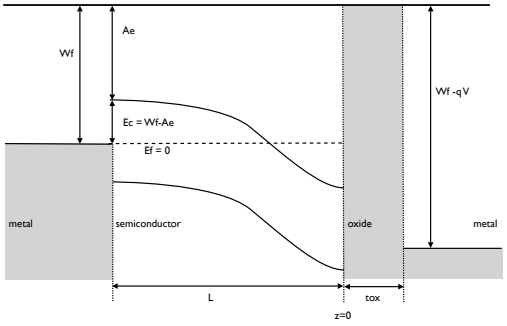

Fig. 1. Device geometry and relevant energetic levels involved with a positive voltage applied at the gate contact. Solid lines in the semiconducotr refer to the LUMO and HOMO levels.

2 Model

A schematic representation of the device we consider is given in Fig. 1 together with the relevant energetic levels involved. It consists of a slab of thickness t_{ox} of insulating material on top of a semiconducting layer of thickness L sandwiched between two metals. If we neglect gate leackage currents, the Fermi energy level E_F is constant throughout the device, so we can set $E_F = 0$ without loss of generality. The electric potential $\varphi := -E_{LUMO}/q$ in the device can be computed by solving the equation

$$\begin{cases} -\mathrm{div}\,(\varepsilon\nabla\varphi) = -q\,n(\varphi) & \text{in } (-L,\,0) \\ -\mathrm{div}\,(\varepsilon\nabla\varphi) = 0 & \text{in } (0,\,t_{ox}) \\ \varphi|_{-L} = \varphi_0; \quad \varphi|_{t_{ox}} = \varphi_{ox} + V \end{cases} \tag{1}$$

where ε denotes the electric permittvity, q the quantum of charge V the externally applied potential and the boundary condition values and are determined from the contact metal work function and the semiconductor material electron affinity as shown in Fig. 1. The accurate modeling of dependence of n on φ, which is crucial for understanding the impact of energetic disorder. If we assume the DOS to be a Gaussian centered at the LUMO, n may be expressed as

$$n = \int_{-\infty}^{\infty} g_\sigma (E - E_{LUMO})\ f(E)\ dE \qquad (2)$$

where

$$g_\sigma (x) = \frac{N_0}{\sigma\sqrt{2\pi}}\ \exp\left\{-\frac{x^2}{2\sigma^2}\right\} \qquad (3)$$

and $F(E)$ is the Fermi distribution function. Although the ansatz (3) is very common, it has been shown in [6] that the energy level distribution may vary greatly near the insulator-semiconductor interface due to non-vanishing dipole density in the gate insulator material rendering (3) quite inaccurate. As the approach given by [6] for the modification of the DOS due to such effect has a very high computational cost, we take an alternative approach in order to account for this effect while retaining an acceptable level of model complexity. We introduce a modified density of state which we assume to take the following form

$$g_{\sigma,\lambda} (x) = g_\sigma (x) + \frac{\lambda N_\lambda}{2}\ \exp\{-\lambda |x|\} \qquad (4)$$

and compute the parameters σ and λ in (4) via an automatic optimization procedure in order to fit the model of [6]. Fig. 2 shows a comparison of the simplified model (4) with that of [6].

3 Numerical algorithms and results

The CV characteristics are obtained from equations (1)-(4) via the numerical method, based on a Newton iteration, described in [2]. Suitable quadrature rules have been devised to compute the integrales appearing in (3) and (4) which need to be evaluated many times at each iteration step. The preliminatry numerical results shown in Fig. 3 show a strong dependence of the CV curves (and of its derivative) on the disorder parameter σ. Ongoing research is directed towards the solution of the inverse problem of determining σ from measured CV characteristics.

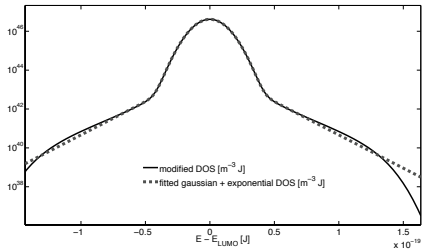

Fig. 2. Comparison of the simplified DOS model (5) with the model of [6]. The comparison is done one nanometer away from the interface.

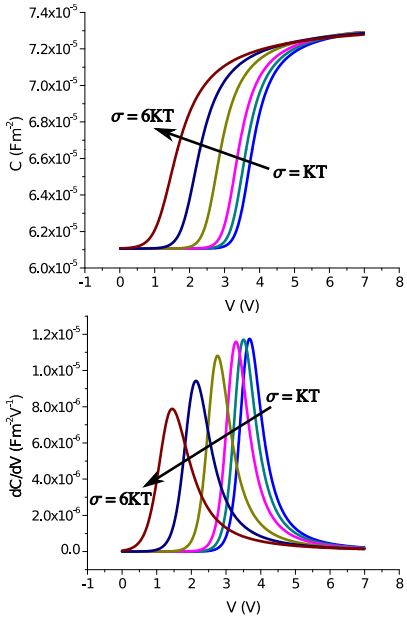

Fig. 3. Dependence of the CV curve (top) and of its derivative (bottom) on the DOS for a device with the following parameters: $T = 300K$, $N_0 = 4e27\ m^{-3}$, $L = 75e\text{-}9\ m$, $t_{ox} = 300e\text{-}9\ m$, $\varepsilon = 3\ \varepsilon_0$ (semiconductor), $\varepsilon = 2.5\ \varepsilon_0$ (insulator).

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