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Simulations of *C-V* and *C-f* curves for organic MIS capacitor: effects of accumulation layer width and front edge of depletion layer

F. P. Sabino, José A. Giacometti, E. Mantovani and N. Alves*

Faculdade de Ciências e Tecnologia, DFQB – UNESP, Presidente Prudente - São Paulo - Brasil.

e-mail: neri@fct.unesp.br

* Corresponding Author

Abstract: Usually an ideal MIS capacitor is described using two approximations: first, the charge density fall down abruptly to zero in the front of the depletion border and second, the width of accumulation layer is negligible. Using equivalent circuits approach the accumulation layer thickness and the depletion layer with a front edge width not negligible was considered. Simulations results give a more realistic description of capacitance and loss curves usually obtained from an organic MIS capacitor.

Organic field effect transistors (OFETs) and metal-insulator-semiconductor (MIS) capacitors are very attractive for low frequency applications and their performance has improved significantly over the past few years. One can employ a MIS capacitor as a powerful tool to characterize the insulator, the semiconductor and the insulator-semiconductor interface properties [1,2]. For example, semiconductor doping density, electric conductivity, mobility, and interface states density can be extracted from dependences of capacitance and dielectric loss on frequency and voltage [3,4]. In this work capacitance and dielectric loss curves for an organic MIS capacitor are computed through equivalent circuits. It was considered as reference the MIS capacitor made from poly(3-hexylthiophene) (P3HT) 70 nm thick as the semiconductor layer and polysilsesquioxane 100 nm thick as insulator layer.

The charge density profile in the semiconductor is described by the Poisson's equation which gives to the front edge of the depletion region a width of the order of λ_D (Debye length) and the width of the accumulation layer. In silicon devices the depletion approximation is usually employed (referred as ideal MIS capacitor), i.e., the charge distribution at the front edge of depletion region drops abruptly to zero [5] since λ_D << semiconductor thickness. However, for our P3HT MIS capacitors $\lambda_D \sim 6$ nm which is ~10% of the thickness of the organic semiconductor layer. Also, the accumulation layer thickness varies in the range from 0 to $\sqrt{2} \pi \lambda_D/2$ accordingly to the applied voltage (band bending). However, for P3HT $\sqrt{2} \pi \lambda_D/2 \approx 13$ nm, which is also not negligible compared to the semiconductor thickness of our MIS capacitor. Therefore, from the considerations depicted above the model for an ideal MIS capacitor should be improved accounting the front edge of the depletion layer and the accumulation layer thickness.

For the accumulation regime we used the circuit shown in Fig. 1 were the capacitor C_{AC} as added to consider the effect of the accumulation layer which width depends on the applied voltage. For the depletion regime we used the circuit shown in Fig. 2. We added another *RC* parallel circuit whose capacitance and resistance represent the front edge of the depletion layer. Values of R_{FE} and C_{FE} are constant until the front edge reaches the back electrode, thereafter their values are assumed to vary exponentially with the applied voltage and finally they achieve constant values.

Figure 1: Equivalent circuit in accumulation. C_{ins} : insulator capacitance, C_B and R_B : capacitor and resistor of semiconductor bulk.



Figure 2: Equivalent circuit in depletion. C_{FE} and R_{FE} : capacitor and resistor of depletion layer front edge.



Our simulation results showed that the *C-V* curves presented a shape that resembles experimental curves, that is, capacitance variation on the voltage diminishes gradually on frequency without abrupt changes found employing the equivalent circuit for an ideal MIS capacitor. Also, loss versus voltage curves display a peak in the flat-band voltage in agreement with experimental results found in P3HT MIS capacitor. Moreover, the variation of doping density (at constant mobility) also gives a very good picture of experimental results when the MIS capacitor was exposed to air (oxygen produces the increase of doping density in P3HT). Concerning the loss versus frequency curves a peak displacement appears in the accumulation regime as the bias voltage is varied, as usually found in experiments. In conclusion our results showed that the accumulation layer width and front edge of depletion layer are relevant to describe experimental results usually found in organic MIS capacitors.

References:

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