SPICE Optimization of Organic FET Models Using Charge Transport Elements

Vaibhav Vaidya, Jungbae Kim, Joshua N. Haddock, Bernard Kippelen, and Denise Wilson

***Abstract*—We report on a modeling technique that uses charge transport equations to calculate channel current in organic field effect transistors (OFETs) by numerical solution in the SPICE simulation program. SPICE is also used to optimize the model and achieve a fit to measured characteristics within 5% error. The overall modeling technique is a bridge between physical models of charge transport and a SPICE model useful in circuit simulation without requiring a closed-form drain-current equation. The automatic optimization of the simulation to measured curves will also allow, in the future, the empirical weighing of various charge transport effects in search of physical device operation, given sufficient empirical data. This modeling technique was applied to the measured characteristics of an OFET using pentacene in which the mobility was dependent on the voltage in the channel. The accuracy of the fit was better than 5% for 40 V $> V_{\rm DS} >$ 7 V and better than 20% for $V_{\rm DS} <$ 7 V. Simulation was completed within 3 min for this optimization on a modern personal computer.**

***Index Terms*—Charge transport, organic electronics, organic field effect transistor (OFET), OTFT, SPICE, SPICE optimization.**

I. Introduction

ORGANIC FIELD effect transistor (OFET) technology is at a stage where useful commercial electronic circuits are possible for applications such as active matrix displays [1], [2] and flexible systems [3], and future applications such as printable RFID tags are under active development [4]. As circuit applications of OFETs are researched, a pressing need for accurate models of the OFETs for use in electronic circuit simulators is evident. Along with the development of the fabrication processes for OFETs, various such physical and empirical models have been developed to explain OFET behavior [5]–[12]. Since OFET physics is still an actively researched topic, these models are mathematically devised for single device calculations and present a significant difficulty for adapting to circuit simulators such as SPICE. Furthermore, since the actual physical mechanisms underlying OFET operation have not yet achieved consensus, present literature shows a large variation in the type and scope of OFET models. Given the increasing advancement of organic devices in commercial markets, the need for useful circuit models is obvious. Inherent differences between the OFET and the silicon-based MOSFET, however, pose some challenges to developing effective models for widespread use in the circuit community. In this paper, we propose a basic model that enables flexibility and accuracy in matching physical equations to measured OFET characteristics; this approach is important in developing practical models for a wide variety of OFETs for use in SPICE-based simulation. The model is based on utilizing the ability of SPICE to numerically calculate node voltages to evaluate boundary conditions in a finite-element approach to modeling the OFET channel. Details of the model and performance for pentacene OFETs are presented herein.

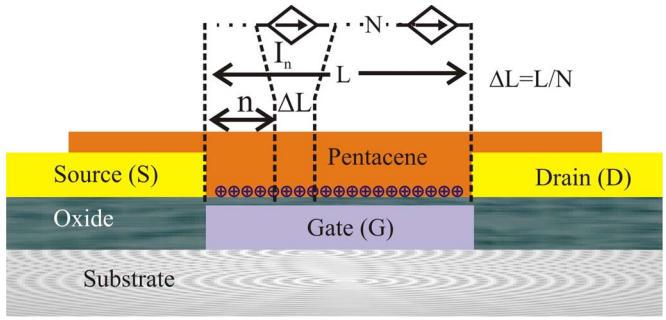

Fig. 1. Multielement channel model of OFET charge transport.

II. Model Description

The model for charge conduction used in this paper divides the OFET channel into a finite series of elements, each of length $\Delta L = L/N$ (Fig. 1). An assumption that the electric field and material properties such as mobility are constant across the length of each element is then made. With this assumption, charge transport in each element can now be described as a function of basic physical parameters such as mobility and switch-on voltage for the FET, and circuit parameters such as gate and terminal voltage. This approach is similar to the analytical derivation of the gradual channel approximation model for FETs. However, whereas the analytical method seeks a closed-form solution for the current in the channel, the element-based SPICE model arrives at this solution numerically as a by-product of simulation. Essentially, SPICE calculates the boundary conditions for the elements such that the current through them is the same and that this same current is also

Manuscript received June 10, 2008; revised October 10, 2008. Current version published December 19, 2008. This work was supported in part by the National Science Foundation under Agreement DMR 0120967 through the STC program and in part by the Office of Naval Research. The review of this paper was arranged by Editor J. Kanicki.

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Digital Object Identifier 10.1109/TED.2008.2008164

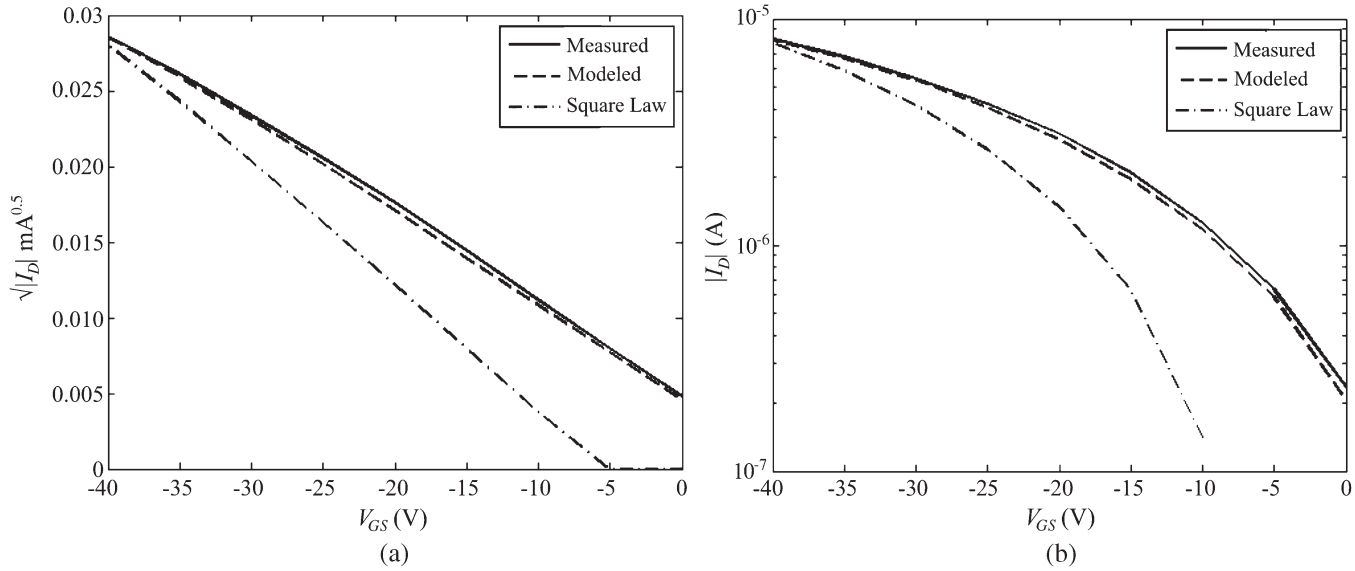

Fig. 2. (a) Plot of $\sqrt{|I_D|}$ versus $V_{\rm GS}$, with models optimized for $V_{\rm GS} = -40$ V. (b) Plot of $\log(|I_D|)$ versus $V_{\rm GS}$, with models optimized for $V_{\rm GS} = -40$ V.

a function of both the gate and drain voltages. One of the concerns of using a finite number of elements is that such a model begins to lose accuracy when high fields are concentrated in a very small region of the channel (near the drain), which occurs frequently at high drain-source voltages. In order to alleviate this concern, we conducted tests changing the number of elements through an order of magnitude and comparing the accuracy and simulation time. For the model used in this work, the error between measured and modeled characteristics with 20 elements was of similar magnitude as that with 200 elements, although the simulation time in the latter case was significantly higher. The error was also found to change more with the model used for charge transport, as described in Section IV. This charge transport element approach can be very useful in cases where an analytical derivation of channel current is prohibitively complex or requires special numerical techniques [8]. As long as the basic charge transport equations can be evaluated with convergence in SPICE, the OFET can be modeled without requiring a closed-form equation for current.

A schematic of the element-based SPICE model used in this paper is shown in Fig. 1. For our simulations, HSPICE from Synopsys was used. Each element is represented in HSPICE as a dependent current source ("G element"). The equation for the current in this element is the mathematical representation of the physical model selected to define charge transport in the OFET. A downside of this approach is that only mathematical functions available in SPICE can be used to describe charge transport, which can be limiting in some cases [8]. However, the available math primitives were more than sufficient to describe a simple square-law MOS-like model and also other more complex models such as the Poole–Frenkel model for field-dependent mobility [6], which we use as a part of the charge transport equation used in our OFET models.

III. Optimization Procedure

OFETs modeled in this work were fabricated [11] on heavily n-doped silicon substrates (resistivity of 0.005 $\Omega \cdot$ cm), which acted as the gate electrode with 200 nm of thermally grown oxide (SiOx, $\varepsilon_r = 3.9$) as the gate dielectric. Bottom contact source and drain electrodes (e-beam evaporated Ti/Au, 10/100 nm) with a channel width of 500 μm and channel length of 50 μm were fabricated on the oxide surface using lift-off photolithography. An external common gate contact of e-beam evaporated Ti/Au (10/100 nm) was deposited on the backside of the substrate. Commercially available pentacene was first purified using zone gradient sublimation and then thermally evaporated onto the source/drain contacts at a rate of $0.2/$s and at a pressure below 10^{-7} torr. The fitting procedure was automated in HSPICE. An initial estimate and probable ranges for each of the equation parameters were provided to HSPICE based on hand calculations on measured data, and then, dc optimization was performed to achieve the best fit to measured characteristics. Although optimization can iterate up to 100 cycles (limited to 100 by the simulation file) of the entire characteristics, a 50-element model took only 125 s (for 45 optimization cycles) to simulate on an Intel Core 2 Duo 2.3-GHz computer with 2-GB RAM. Thus, for small and medium transistor counts, which are common in OFET circuits, this model yields sufficient computational speed in simulation.

The generation of the multielement channel netlist was automated with a MATLAB script, yielding easy control over the number of elements tested. Changing the number of elements over an order of magnitude (10–200) did not demonstrate a significant change in the accuracy of the model, implying that the finite-length-element simplification was reasonable for the models we considered in this paper.

The model was optimized to both a single output curve (only one value for $V_{\rm GS}$) and the full measured output characteristics. Optimizing to a single curve yielded a model that has minimal error in the region of $V_{\rm GS}$ closest to the optimized curve and progressively increasing error toward the extremes of $V_{\rm GS}$. Fig. 2 shows a square-law model to the OFET model described herein, both optimized to a single output characteristic at $V_{\rm GS} = -V_{\rm DD}$.

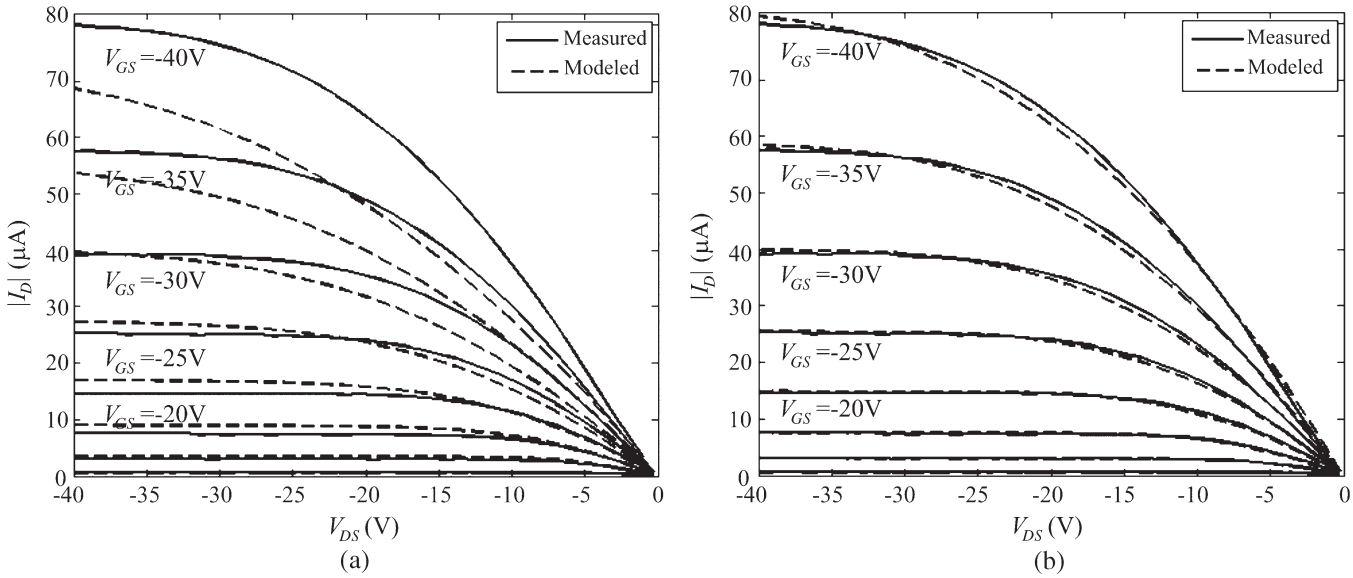

Fig. 3. (a) Optimized simple square-law-like model. (b) Optimized OFET model.

A concern with optimizing using HSPICE is ensuring convergence. Certain conditions on simulation can cause convergence to fail, such as choosing initial estimates for parameters that are outside reasonable range and many orders of magnitude change in measured characteristics.

IV. Results and Discussion

The optimization was first tested with a simple model with a linear region channel current equation

$$I_D = \mu C_{\rm OX} \frac{W}{\Delta L} (V_{\text{G-CH}} - V_{\rm SO}) \cdot V_{\Delta \rm CH} \tag{1}$$

where I_D is the current through the channel, μ is the charge mobility, $C_{\rm OX}$ is the unit area capacitance of the gate insulator, W and ΔL are the width and length of the element being considered, $V_{\text{G-CH}}$ refers to the gate voltage with respect to the channel voltage at the element being considered, $V_{\rm SO}$ is the "switch on" or "threshold" voltage, and $V_{\Delta \rm CH}$ refers to the voltage across the channel element. It should be noted here that the saturation region was modeled as a constant impedance once the onset of saturation was detected for every channel element (i.e., saturation mode when $V_{\text{G-CH}} \sim 0$ for an element). With a gradual channel approximation, this equation yields the standard MOS square-law model. The results of the optimization are shown in Fig. 3(a), which illustrates some of the inconsistencies that would arise from simulating OFET circuits with a simple LEVEL 3 or 15 SPICE model. The behavior of current with change in $V_{\rm GS}$ is not explained well over the entire current characteristics, nor is the low $V_{\rm DS}$ nonlinear behavior represented well. These artifacts can be due to field-dependent contact resistance or channel mobility, and a judgment on the same can only be arrived at after extensive study. To the end of evaluating our modeling framework, however, we added a linear gate dependence to the mobility to explain the super-square-law gate dependence of drain current

$$\mu_g = \mu_0 \left(1 + \delta \cdot (V_{\text{G-CH}} - V_{\rm SO})\right) \tag{2}$$

where μ_0 is the zero field mobility and δ is the proportionality parameter to be optimized, and a Poole–Frenkel-type [6] longitudinal field dependence approximated to the first order to model the low-field nonlinearity

$$\mu = \mu_g \left(1 + \beta \frac{\sqrt{V_{\Delta \rm CH}}}{kT}\right) \tag{3}$$

where k is the Boltzmann constant, T is the absolute temperature, and β is the fitting parameter to be optimized.

These effects were added directly to each charge transport element, without the need to arrive at a closed-form solution for the entire channel. The result of these additions is shown in Fig. 3(b). The parameters of μ_0, δ, and β were automatically optimized by HSPICE using dc simulation with Levenberg–Marquardt least squares optimization to $\mu_0 = 4 \times 10^{-1}$ cm^2/Vs, $\delta = 37 \times 10^{-3}$ V^{-1}, and $\beta = 5.2 \times 10^{-6}$ eV/V$^{0.5}$, and $V_{\rm SO} = 0.16$ V, with $W = 200\,\mu$, $L = 20\,\mu$, and $N = 100$.

Although automatic optimization provides one set of parameters that seem to give minimal error in measured characteristics, conclusions about the actual physical values of the parameters should not be drawn without more extensive tests. For example, in the context of this paper, the parameters of unit oxide capacitance ($C_{\rm OX}$) and base mobility (μ_0) have the same weight in the final equation. Even though the product $\mu_0 \cdot C_{\rm OX}$ might be properly optimized by HSPICE, their individual values might not be true to the underlying physics. Optimization to multiple data sets such as transient data, time-of-flight measurements, and similar data will likely yield a model that is both more accurate and true to the underlying FET operation. However, for the purposes of dc circuit simulations, considered herein, the present optimization procedure is sufficient. We

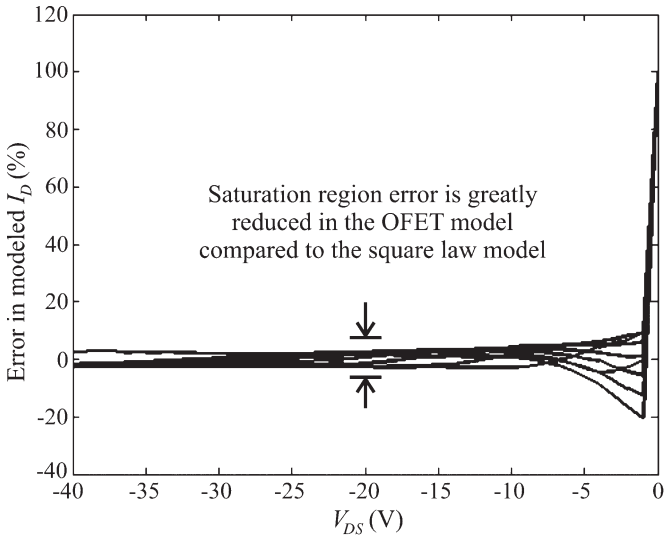

Fig. 4. Error performance of optimized OFET model.

have used the model optimized in such a way to simulate simple OFET circuits such as active matrix OLED drivers and oscillators. For low transistor count circuits where up to ten devices are used, we have used the presented model with up to 100 elements with resulting simulation times of less than 1 min. Simulation time increases with model-equation complexity.

The accuracy of the predicted current values optimized to our model as shown in Fig. 3(b) is shown in Fig. 4. As can be seen, the error in higher field regions is lower than 5%, whereas in lower field regions where $V_{\rm DS}$ is low, the error climbs to 20%. The latter results imply either that HSPICE has reached the limit of overall error tolerances without the need to reduce this error by adjusting β further or that the Poole–Frenkel model for the linear field dependence of mobility does not completely explain the behavior of these OFETs. This effect (in the underlying physics of the OFET) is the subject of continued study.

V. Conclusion

In conclusion, this work demonstrated a technique to form a bridge between physics-based charge transport models and practical device simulation in SPICE. To facilitate simulation without the need for a closed-form solution of channel current, a finite-element model was used for channel conduction. A model accuracy of 95% was achieved for $V_{\rm DS} > 7$ V, demonstrating the effectiveness of exploring the parameter space using SPICE for a given physical model of OFET charge transport. The direct optimization of the model in SPICE means that further circuit simulation does not require any additional effort before using the optimized form of the model. Our future work will include extending this approach to OFETs made with different geometries and materials. Finally, the set of models yielded from optimization will be used to design and simulate practical OFET circuits.

Acknowledgment

The authors would like to thank Prof. D. Yoder from the Georgia Institute of Technology for the insightful discussions on modeling in SPICE and device physics. This work was performed in part at the Microelectronics Research Center, Georgia Institute of Technology, a member of the National Nanotechnology Infrastructure Network, which is supported by the NSF under Grant ECS- 03-35765.

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