Monte Carlo Simulation of the Dynamic Charge Hopping Transport in Organic Thin Film Transistors

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***Abstract*—Technology of thin film transistors based on organic semiconductor (OTFTs) materials had gained great progress in recent years. A technology computer aided design (TCAD) model is needed to further investigate the devices physics and shortcut the fabrication process. In this article, based on hopping transport mechanism, we proposed a physical model for charge transport process in OTFTs. By Monte Carlo simulation we can get a visualized charge transport and carriers' distribution map in OTFTs and finally get its I-V characteristics, indicating that it can serve as the prototype TCAD model for OTFTs, which gives us a way for understanding the physical process in OTFTs and for predicting the performance of OTFTs before device fabrication.**

Keywords*—Organic thin film transistors (OTFTs); Hopping transport; Monte Carlo (MC) simulation; Technology computer aided design (TCAD) model.

I. INTRODUCTION

Organic thin film transistor (OTFT) is the key elemental component for the flexible, low cost and large area electronic device [1-3]. The performance of OTFTs have been greatly developed in recent years, with field effective mobility promoted from 0.01 to 10 cm^2/Vs [4, 5], however still can't meet the mass commercial application needs. Much efforts in the research of OTFTs focus on optimizing organic semiconductor materials with highest mobility [6, 7] and process of organic layer growth [8, 9], choosing of self-assemble molecular (SAM) layers [10, 11], contact electrode and structure with smallest contact resistance [12-14], and best structure for transistor performance [15], and so on. It results in thrive of organic electronic materials and devices [16], however most of the time, we do not have a clearly routine for further development of the performance of OTFTs. Traditionally, in silicon based electron devices, there are technology computer aided design (TCAD) software [17] based on Poisson-Boltzmann law and current continuity equation, which can provide the inner physics and predict the electric performance of devices, and highly lower the redundancy of fabrication. However, due to whole different charge transport mechanism, TCAD model for OTFTs is still scarce. Hopping charge transport mechanism [18-22] is considered as the predominant transport theory for organic semiconductor materials, whereas the research of transport theory is limited in bulk materials, no simulation in device level has been presented. In this work, we proposed a physical TCAD model for charge transport in OTFTs based on hopping theory. By using Monte Carlo (MC) simulation base on the proposed model, the charge transport and carrier distribution map in OTFTs were depicted visually, moreover, the I-V characteristics could also be obtained. This method provides a way to understand the physical process of charge transport in OTFTs and predict the performance of OTFTs.

II. MODEL AND METHOD

Charge transport in OTFTs, unlike in bulk organic semiconductor materials, would be highly affected by the structure and dimension of OTFTs and the voltage bias applied source/drain and gate electrode. As shown in Figure 1a, the carriers would firstly be injected from source electrode to organic semiconductor, then move by hopping transport in organic semiconductor area, finally jump to the drain electrode. The injected carrier in organic semiconductor would be accumulated in organic layer and feed back to the distribution of electronic potential induced by source/drain and gate voltage.

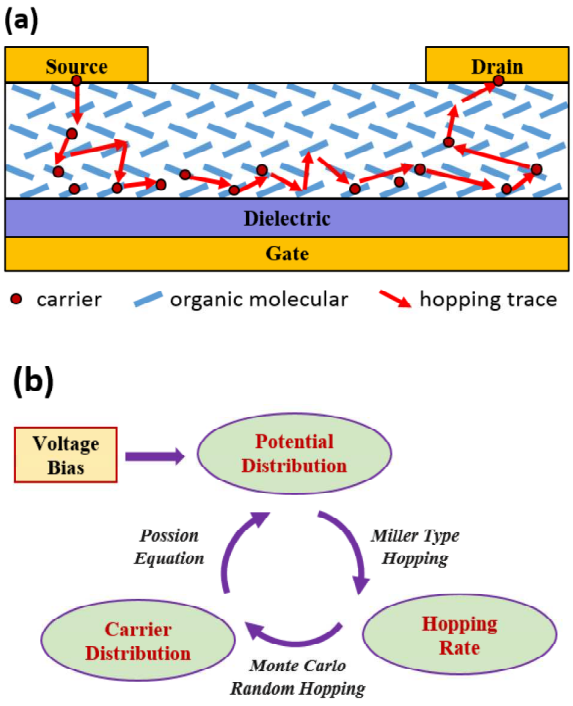

Fig. 1 (a) Schematic diagram of charge hopping and accumulation in OTFTs. (b) Workflow of the MC simulation process.

The hopping rate v_{ij} of the carrier jump from molecular i to j can be represented as Miller-Abrahams type [23-25],

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$$\nu_{ij} = \nu_0 \exp(-\gamma \frac{\Delta R_{ij}}{a}) \exp(-\frac{q(\varphi_j - \varphi_i)}{kT}), \quad (1)$$

where ν_0 is the electronic wave function overlap related prefactor, γ is also the overlap parameter, ΔR_{ij} is the distance of the two molecules, a is the average lattice distance, φ_i and φ_j is the potential in the molecular i and j respectively, q is the element charge, k is Boltzmann constant, T is temperature. Similarly, it is reasonable to assume that the source/drain electrode as an additional point for carrier can jump from and to, respectively. The hopping rate of a carrier jump from source electrode to an adjacent molecular j and a carrier jump from a molecular i around drain electrode to drain can be represented as,

$$\nu_{Sj} = \nu_e \exp(-\gamma \frac{\Delta R_{Sj}}{a}) \exp(-\frac{q(\varphi_j - V_S)}{kT}), \quad (2)$$

and

$$\nu_{iD} = \nu_e \exp(-\gamma \frac{\Delta R_{iD}}{a}) \exp(-\frac{q(V_D - \varphi_i)}{kT}), \quad (3)$$

where ν_e is the prefactor related to electronic wave function overlap between molecular and source/drain electrode, V_S and V_D is the source and drain voltage, respectively. The probability that a carrier jumps from site i to site j within a critical radius is [24, 26]

$$P_{ij} = \nu_{ij} \Big/ \sum_{i \neq j} \nu_{ij} . \quad (4)$$

The waiting time before the jump being executed is

$$t_i = \left(\sum_{j \neq i} \nu_{ij} \right)^{-1} . \quad (5)$$

The carrier with the shortest waiting time have the priority to hopping to its next position. The potential distribution φ with the influence of injected charge carrier distribution can be obtained by solving Poisson equation,

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = -\frac{\rho}{\varepsilon}, \quad (6)$$

where ρ is the charge density represented by each carriers' position, ε is the permittivity of organic semiconductor. After each carrier jumped, the potential distribution should be recalculated by Equation 6.

Based on this model, a two dimensional charge hopping transport process in OTFTs is simulated by using Monte Carlo method. For simplifying the simulation, we assume that the organic molecules are fixed in the grid of organic semiconductor area (which is for the single crystal situation). A top contact OTFT with channel length of 200 nm, organic thickness of 50 nm, dielectric layer of 50 nm, source/drain contact length of 25 nm, and space of the organic molecules of 1 nm, was simulated in this article. At the beginning of the simulation, we assume there is no carrier exist in OTFTs, the potential distribution is all induced by given voltage bias applied to source, drain and gate electrode. After that, carriers begin to be injected from source electrode and transport in organic semiconductor area with the circumstance potential distribution according to the hopping model as presented above. In the meantime, the injected carriers' distribution would feed back to the potential distribution by equation 6. The workflow the simulation process can be seen from Fig. 1b. After a long enough simulation process, the number of carriers jump from source and to drain as function of device operation time would be stable (the source/drain current is stable), where we can end the simulation.

III. Results and Discussion

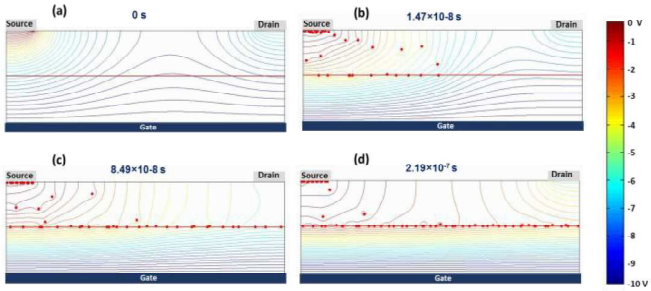

Fig. 2 (a-d) MC simulation of time evolution of the dynamic charge carriers' transport and potential distribution in OTFTs. (Line: contour of potential distribution; Red points: carriers.)

The device operation time dependent potential and carrier distribution of charge hopping transport process in OTFTs is illustrated in Fig. 2, with voltage bias of Vg = -10V, Vs = 0V, Vd = -5V. At the beginning of the simulation, the source, drain and gate voltage induced potential distribution was calculated (Fig. 2a). Then, carriers begin to spread from source electrode, and transport in semiconductor area (Fig.2b). After that, as shown in Fig. 2c, carriers are gradually accumulated in the interface of dielectric and organic semiconductor layers and the transport channel thus forms in this interface. At the end the carriers in the tail of the channel begin to hop to drain electrode (Fig. 2d). The potential distribution is highly affected by the transient distribution of the carriers.

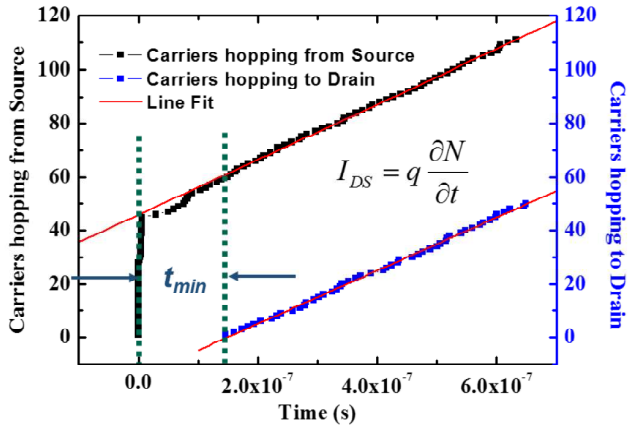

Fig. 3 Total number of carriers hopping from source (black box) and to drain (red box) as the function of device operate time.

During the simulation, the number of carriers jump from source electrode and hopping to drain electrode was counted as the function of device operation time, as shown in Fig.3. In Fig. 3, one can see that after a specific time, the total number of carriers jump from source and to drain would linearly increase with the device operation time, which suggests that the source/drain current of the simulated OTFT is stable. Then the DC source/drain current can be calculated by

$$I_{DS} = q\frac{\partial N}{\partial t}. \quad (7)$$

The specific time t_{min} (in Fig. 3), before both source and drain currents are stable, is the time the OTFT device needed for establishing the inner electronic and current fields after a bias voltage applied to it. It can be seen as the intrinsic frequency characteristic of the OTFTs without considering the parasitic capacitance or resistance.

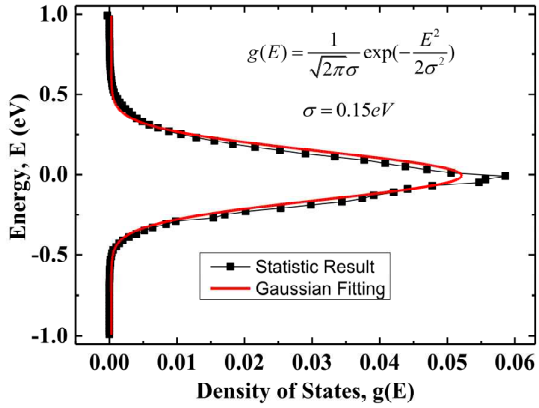

Fig. 4 Statistical result of the Gaussian distribution of the molecular energy.

Statistical result of the transient potential deviation from average potential at each point shows Gaussian distribution [4], as shown in Fig. 4. It shows that the Gaussian density of states (DOS) of the organic molecular can be explained as the result of the Coulomb interaction of the dynamic carriers and bias induced potential distribution.

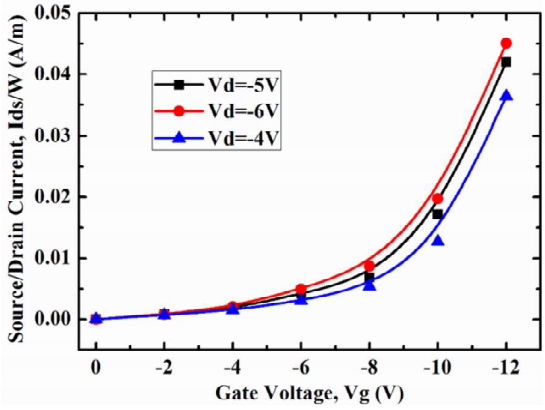

Fig. 5 Transfer characteristics of the OTFTs obtained by varying the gate bias in the simulation.

Changing the gate voltage bias, we can see that the higher gate voltage, the more the carriers would be accumulated in the channel, and the channel become more effective to transport carriers from the area beneath the source electrode and the area beneath the drain electrode. The source/drain current would increase with the increase of gate voltage, which is agreement with the experimental fact. By varying the gate voltage, we can get the transfer characteristics of the OTFTs, as shown in Fig. 5 (Points: MC simulation results; Lines: B-spline fitting lines). Similarly, we can change the source/drain voltage in the simulation. If we change the source/drain voltage bias in the simulation, we would find that the higher source/drain voltage would result in higher gradient of potential distribution between source and drain electrodes in organic semiconductor area, and, as we can expected, higher source/drain current. By varying the source/drain voltage, we can get the output characteristics of the OTFTs, as shown in Fig. 6.

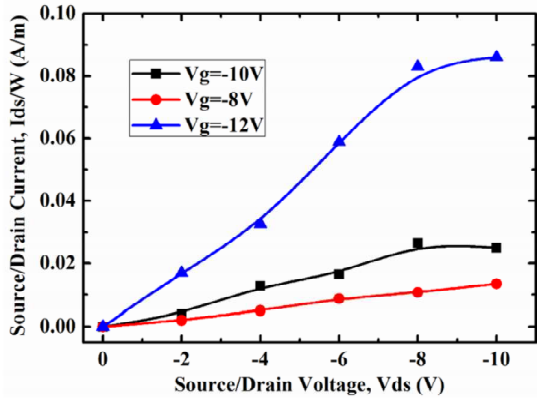

Fig. 6 Output characteristics of the OTFTs obtained by varying the source/drain voltage in the simulation.

IV. Conclusion

In summary, a MC simulation model for OTFTs based on hopping transport mechanism and charge carriers feed back to the potential distribution is proposed. Based on the proposed model, we simulate the dynamic charge transport process in OTFTs, and the visualization map of the charge transport and carriers' distribution process are presented. The results can give an insight view of the device physics in OTFTs, carriers' accumulation to form the channel, channel spread near the source/drain contact, et al. By varying the voltage bias applied to source/drain or gate electrode, the I-V characteristics of the OTFTs can be obtained. As a result, a prototype pure physical TCAD model for OTFTs was developed.

Acknowledgment

This work was supported in part by the Strategic Priority Research Program of the Chinese Academy of Sciences, Grant No. XDB12030400, the National 973 Program under Grant 2011CB808404 and Grant 2013CB933504 and in part by the National Science Foundation of China under Grant 60825403, and Grant 61102025.

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