Organic Thin-Film Transistor Compact Model with Accurate Charge Carrier Mobility

T. K. Maiti[1*], T. Hayashi[2], L. Chen[1], M. Miura-Mattausch[1, 2], and H. J. Mattausch[1,2]
[1]HiSIM Research Center, Hiroshima University, 1-3-1 Kagamiyama, Higashi-Hiroshima city, P.C. 7398530, Japan
[2]Graduate School of Advanced Sciences of Matter, Hiroshima University, Higashi-Hiroshima city, P.C. 7398530, Japan
*E-mail: tkm@hiroshima-u.ac.jp

***Abstract*— A physical compact charge carrier mobility model for undoped-body organic thin-film transistors (OTFTs) based on an analysis of the bias-dependent Fermi-energy movement in the band gap is reported. Mobility in localized- and extended-energy states predicts the current transport in week- and strong-inversion regimes, respectively. A hopping mobility model as a function of surface potential is developed to describe the carrier transport through localized trap states located in the band gap. The Poole-Frenkel field effect mechanism is considered to interpret the band-like carrier transport mechanism in extended energy states. Modeled results are compared with the measured DNTT-based high-performance OTFTs data to verify the model.**

Keywords—Hopping Mobility; Poole-Frenkel Effect; Band Gap; Localized Energy States; Extended Energy States ;Trap

I. Introduction

OTFTs have recently shown higher mobility and better performances [1]. Charge carrier mobility in OTFTs differs significantly from MOSFETs due to the energetic and spatial disorder of organic materials. Some organic materials exhibits hopping transport, some exhibits band-like transport, and some shows both in an OTFT [1]. Previously reported mobility models are not capable to reproduce the transport effects seen in OTFTs caused by localized states located in the band gap of organic semiconductor [2].

In this paper, we report a new compact mobility model to describe an OTFT operation in week- and strong- inversion regimes. In week-inversion regime, the Fermi level (E_F) is located at the localized state energy inside the band gap (E_g) of thin-film organic semiconductors. With increase of gate voltage (V_{gs}), E_F moves towards the band edge and the carriers located in the localized states are able to jump which results in hopping mobility. Miller-Abrahams jump-rate equation and Einstein diffusion relation are used to develop a hopping mobility model as a function of surface potential. In strong-inversion regime, high V_{gs} pushes E_F to extended energy states and causes field-effect mobility. With increase of V_{gs}, field-effect mobility approaches the band mobility and is considered *via* the Poole-Frenkel mobility model. We have used both hopping mobility and Poole-Frenkel formalism to predict the OTFT operation. The proposed model accurately describes the currents in week- and strong-inversion regimes in an OTFT. Modeled results are compared with the measured DNTT-based high-performance p-channel OTFTs data [3].

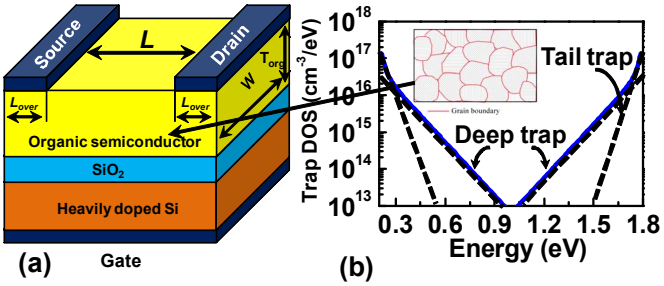
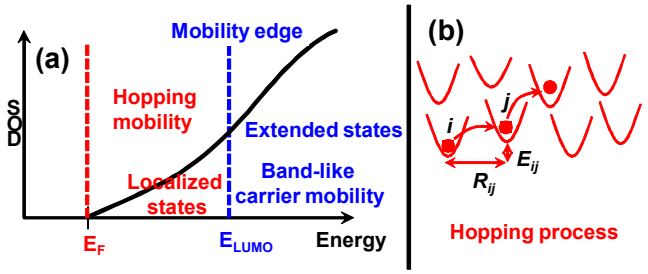


Fig. 1. (a) Schematic diagram of an organic thin-film transistor (OTFT). (b) Density of grain boundary trap states located in the band gap of the organic semiconductor thin-film layer.



***E_{ij}*: Energy difference between two sites *i* and *j*.**
***R_{ij}*: Special distance between two sites *i* and *j*.**

Fig. 2. (a) Sketch shows the density of localized states distribution in the upper half of the energy band gap in organic semiconductors. The hopping mobility and the band-like mobility are dominating for the localized states and the extended states, respectively. (b) Hopping takes place between two closely neighbouring localized states.

II. Model Description

A schematic diagram of an OTFT is shown in Fig.1 (a). Grain boundary trap states are present in the band gap of organic thin-film semiconductor and are approximated in the developed model by the sum of the localized deep and tail trap states (Fig.1 (b)). Charge carrier mobility in organic semiconductors is manly characterized by the localized trap states. The charge carriers are localized due to (a) energetic (E_{ij}) and (b) spatial (R_{ij}) disorder present in the bulk. Variation of localized states with respect to energy is shown schematically in Fig.2 (a). The localized energy states and the extended energy states are separated by the mobility edge at energy E_{LUMO} (Lowest Unoccupied Molecular Orbital energy). Carriers located above the mobility edge can easily conduct. But, the conduction below the mobility edge is complicated

and takes place by carrier hopping between two neighboring localized states as shown schematically in Fig. 2(b). In 1956, R. A. Marcus proposed a theory known as "Marcus theory" to describe the rate of the carrier transfer process between two neighboring sites which is usually used in multi-scale simulation [4]. Miller and Abrahams also proposed a carrier transition model which is used for generic simulation without considering the molecules and is given by [4].

$$\nu_{ij}\left(\varepsilon_i,\varepsilon_j,R_{ij}\right)=\nu_{ij0}\exp\left(-\frac{\varepsilon_j-\varepsilon_i}{k_BT}\right) \quad for\ \varepsilon_j>\varepsilon_i \tag{1}$$

$$\nu_{ij}\left(\varepsilon_i,\varepsilon_j,R_{ij}\right)=\nu_{ij0} \quad for\ \varepsilon_j<\varepsilon_i$$

Here, $\nu_{ij0} = \nu_0 \exp(-2\gamma R_{ij})$, $\exp(-2\gamma R_{ij})$ describes the tunneling contribution, R_{ij} is the average jumping distance between two sites i and j, ε_i and ε_j are the corresponding energies, γ is the inverse of localization radius, ν_0 is the hopping frequency, k_B is the Boltzmann constant and T is absolute temperature. We used Miller-Abrahams rate equation as an appropriate model for compact modeling to derive the hopping mobility model.

A. Hopping Mobility Model

In organic semiconductors the conduction process occurs *via* hopping of charge carriers between the localized energy states in the band gap. If $g(\varepsilon)$ describes the density of localized states and $f(\varepsilon)$ describes the Fermi function with the Fermi level (E_F) in thermal equilibrium, then the total concentration of carriers (n) can be described as,

$$n=\int_{-\infty}^{\infty} g(\varepsilon)f(\varepsilon)d\varepsilon=\int_{-\infty}^{\infty}\frac{g(\varepsilon)d\varepsilon}{1+\exp\left[(\varepsilon-E_F)/k_BT\right]} \tag{2}$$

To consider the energy disorder effect in carrier conduction we assumed that the charge carriers which are located in occupied energy states or starting energy states (E_i) are jumping to unoccupied states or target states. We therefore use the following expression to calculate the occupied carrier concentration (N_T) within the E_i as,

$$N_T=\int_{E_i}^{\infty} g(\varepsilon)f(\varepsilon)d\varepsilon \tag{3}$$

We applied the concept of threshold radius (R) from the percolation theory to consider the spatial effect on hopping conduction. R is the distance between two close neighbour sites where a carrier can jump from one site to the other [4], [5] and follows the expression:

$$\frac{4\pi}{3}R^3N=B \tag{4}$$

with percolation threshold $B \approx 2.7 \pm 0.1$ restricting the hopping distance [4]. Here, N is the concentration of unoccupied localized energy states and can be expressed as,

$$N=\int_{E_i}^{\infty} g(\varepsilon)\left[1-f(\varepsilon)\right]d\varepsilon \tag{5}$$

where $[1-f(\varepsilon)]$ is the probability of a site to be unoccupied. By combining equation (4) and (5) we end up with the following expression for the typical jumping distance (R),

$$R=\left[\frac{4\mu}{3B}\int_{E_i}^{\infty} g(\varepsilon)\left[1-f(\varepsilon)\right]d\varepsilon\right]^{-1/3} \tag{6}$$

We derive an average hopping transition rate $<\tau>$ inside the band gap by using Miller-Abrahams transition rate equation (1) over the distribution of unoccupied (target) localized states and by using the relation $[1-f(\varepsilon)]=\exp((\varepsilon-E_F)/k_BT)f(\varepsilon)$,

$$\left\langle\tau\right\rangle=\frac{\nu_{ij0}^{-1}\exp\left(\frac{E_{LUMO}-E_F}{k_BT}\right)\int_{E_i}^{\infty} g(\varepsilon)f(\varepsilon)d\varepsilon}{\int_{E_i}^{\infty} g(\varepsilon)\left[1-f(\varepsilon)\right]d\varepsilon} \tag{7}$$

Here, we assumed that $\varepsilon_j = E_{LUMO}$, since we are interested in the carrier transport between localized states within the band gap. For low field, the mobility (μ) can be calculated from the Einstein relation $\mu=qD/k_BT$. Here, q is the elementary charge and D is the diffusion coefficient. The diffusion coefficient for organic semiconductors can be estimated as $D=<\tau>^{-1} R^2$ [4]. Therefore, μ can be expressed as,

$$\mu=\frac{qD}{k_BT}=\frac{q}{k_BT}R^2\left\langle\tau\right\rangle^{-1} \tag{8}$$

From (3), (5) and (6) and by inserting the hopping transition equation (Eq. (7)) into (8), we obtained the hopping mobility equation as,

$$\mu=\nu_{ij0}\frac{q}{k_BT}\frac{3B}{4\pi RN_T}\exp\left(\frac{E_F-E_{LUMO}}{k_BT}\right) \tag{9}$$

Here, the energy difference ($E_F - E_{LUMO}$) is calculated as a function of surface potential (ϕ_s) in eV to transform into gate voltage (V_{gs}) as [6],

$$E_F-E_{LUMO}=\phi_s-E_g+k_BT\ln\left(\frac{N_L}{n_i}\right) \tag{10}$$

where, E_g is the band gap of the organic semiconductor. N_L and n_i are effective density of states and intrinsic carrier concentration, respectively. In case of OTFT, at a low V_{gs}, if the Fermi level (E_F) falls below the mobility edge with characteristic energy (k_BT2) of the exponential variation of the tail states, then k_BT2 is not equal to the k_BT at room temperature. So, k_BT in (9) should be replaced by k_BT2 and we consider it as a model parameter *TFTE2*. We also considered $\nu_{ij0}(q/k_BT)(3B/4\pi RN_T) = MUB$ as a model parameter. Therefore, the hopping mobility (μ_{HOP}) equation becomes:

$$\mu_{HOP}=MUB.\exp\left(\frac{E_F-E_{LUMO}}{TFTE2}\right) \tag{11}$$

If $E_F < E_{LUMO}$, we expect that the mobility will be dominated by the charge carriers jumping from E_F to the localized states just below the mobility edge. If the E_F is above the E_{LUMO}, we expect that the carrier transport in is limited by the carrier scattering with molecular vibrations, leading to field dependent band-like charge carrier mobility and followed by field and temperature dependent Poole-Frenkel (*PF*) mobility which is discussed below.

B. Poole-Frenkel Mechanism

The Poole-Frenkel mobility describes several experimental results of OTFTs [7]-[9]. For accurate prediction of the electrical behavior of an OTFT, we used following Pool-Frenkel mobility expression [7],

$$\mu_{PF} = PFMU0.\exp\left(-\frac{PFDELTA}{k_B T}\right) .\exp\left[\left(\frac{PFBETA}{k_B T} - PFGAMMA\right)\sqrt{E_{\|}}\right] \quad (12)$$

Here, $E_{\|} = (\phi_{sL} - \phi_{s0})/(L_{eff} - \Delta L)$ is the parallel electric field in the direction of current flow. ϕ_{s0} and ϕ_{sL} are the source- and drain-side surface potential, respectively. L_{eff} and ΔL are the effective channel length and the length of the pinch-off region under the saturation condition. *PFMU0* is the constant low field mobility; *PFBETA* and *PFGAMMA* are the Poole-Frenkel fitting parameters. *PFDELTA* is the activation energy at zero electric field for charge carriers. We treated *PFMU0*, *PFDELTA*, *PFBETA*, and *PFGAMMA* as model parameters. Fig.3 shows the schematic view of hopping conduction,

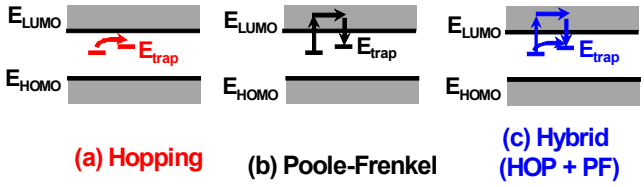


Fig. 3. (a) Hopping conduction is carrier jumping between localized states. (b) Poole-Frenkel mechanism is free carrier movement through delocalized states. (c) Hybrid means both hopping (HOP) + Poole-Frenkel (PF).

Poole–Frenkel (*PF*) conduction, and the combination of both hopping and PF conduction, called hybrid-conduction model. We consider the hybrid model which describes the carrier hopping through localized trap states and field-assisted carrier transport from trap states to conductive band *via* the *PF* mechanism [9]. Both models are combined using Matthiessen's rule with the following expression,

$$\frac{1}{\mu} = \frac{1}{\mu_{HOP}} + \frac{1}{\mu_{PF}} \quad (13)$$

Equation (13) is used to predict the mobility from low V_{gs} (low field) to high V_{gs} (high field) regimes of operation, (i.e. in week- and strong- inversion regimes).

III. Results and Discussion

Mobility as a function of carrier energy ($E_F - E_{LUMO}$) is shown in Fig.4 (a). We also plotted ($E_F - E_{LUMO}$) as a function of V_{gs} (seen in Fig.4 (b)) to interpret the relation between ($E_F - E_{LUMO}$) and V_{gs}. At low V_{gs}, E_F located in the band gap and charges carriers are hopping from occupied localized states to unoccupied localized states which establishes hopping mobility in OTFTs. With increasing V_{gs}, E_F moves exponentially closer to E_{LUMO} (i.e. closer to the band edge) causing larger mobility. Exponential variation of ($E_F - E_{LUMO}$) with respect to V_{gs} occurs due to exponential distribution of

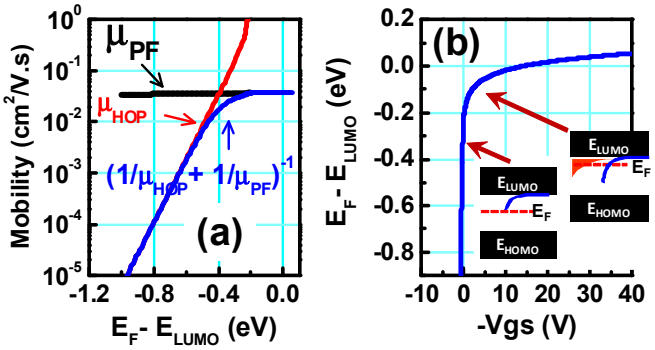


Fig. 4. (a) Modeled carrier mobility as a function of energy ($E_F - E_{LUMO}$). (b) ($E_F - E_{LUMO}$) as a function of gate voltage (V_{gs}).

localized trap states as shown in Fig.4 (b). At high V_{gs}, trap states located in the band gap are filled and more mobile charge can be accessed in the extended energy states which results in higher field effect mobility which is closer to the band-like mobility for some organic semiconductors [1]. In this regime, Poole-Frenkel mobility model is considered to describe the carrier transport. Combination of both hopping and *PF* mobility *vs*. V_{gs} is shown in Fig.5 (a) and measured mobility is seen in Fig.5 (b). Modeled mobility results show similar behaviour as measurements at high V_{gs} and deviated at low V_{gs} due to two-dimensional (2D) effects, observed from 2D device simulation [10] as shown in Figs.6 (a) and (b). The 2D effect on the electric-field ($E_{\|}$) distribution for different organic semiconductor layer thickness (T_{org}) throughout the device is shown in Fig.6 (b) from which we concluded that $E_{\|}$ decreases with increased T_{org}. Fig.6 (a) shows exponential

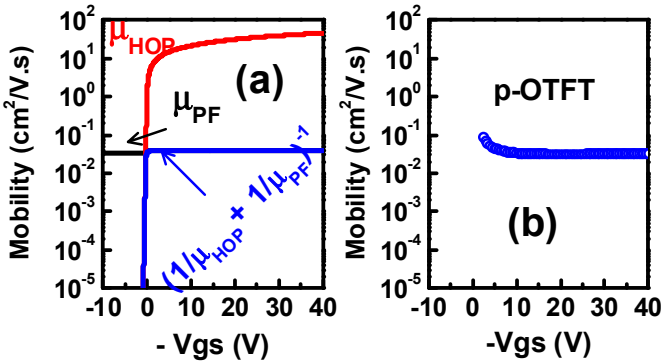


Fig. 5. (a) Mobility (μ) *vs*. Gate voltage (V_{gs}) together with hopping and *PF* model (b) Measured mobility at V_{ds} = -0.1V as a function of gate voltage (V_{gs}).

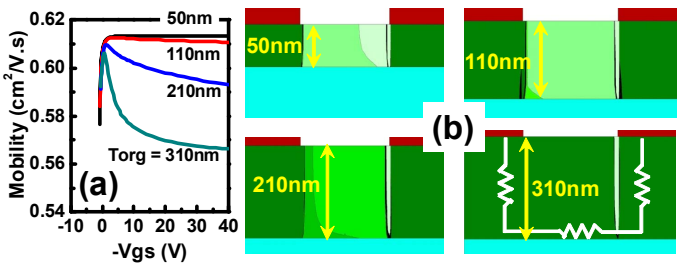


Fig. 6. (a) 2D-device simulated result shows the effect of organic semiconductor layer thickness (T_{org}) on mobility (μ). (b) 2D-device simulated parallel electric-field ($E_{\|}$) distribution throughout the device for different T_{org} at V_{gs} = - 40V and V_{ds} = - 0.1V shows two-dimensional effect. $E_{\|}$ decreases with increase of T_{org} causing exponential decrease of μ with V_{gs}.

decrease of mobility as a function of V_{gs} with increased T_{org} caused by a decreased parallel electric field ($E_{||}$) due to traps and resistances effects. Fig.7 (a) shows the effect of traps on mobility behaviour. OTFTs without traps exhibits greater mobility than OTFTs with traps due to the trap effects on the electric field. Modeled μ *vs.* V_{gs} for low- and high-trap density is shown in Fig.7 (b) which exhibits a mobility decrease with high trap density. It is also possible to predict an exponential decrease of μ by adjusted trap and γ (*PFGAMMA*) (see. Eq. (12)) model parameters as observed in Fig.7 (b). We developed a surface potential model equation with the inclusion of trap charge densities [11], drain current (I_{ds}) equation as the function of surface potential and backside potential [12-15], and the resistance model [12]-[13]. We verified the effect of mobility on I_{ds} as shown in Fig.8 (a). It is confirmed that subthreshold current is controlled by the hopping mobility and above-threshold current is controlled by the band-like carrier mobility. Modeled I_{ds} is verified against measurements as seen in Fig.8 (b) and is able to predict I_{ds} in week- and strong-inversion regimes of a p-channel OTFT with channel length (L_g) 190µm and width (W) 1500µm .

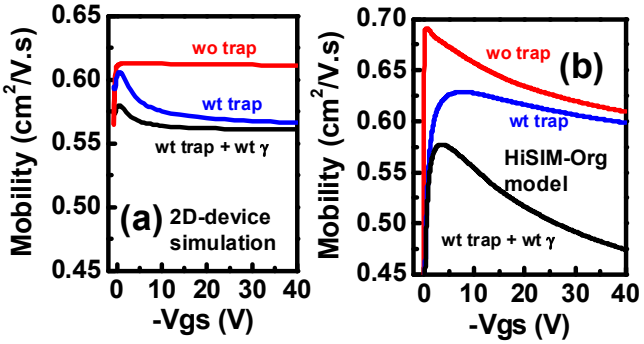


Fig. 7. (a) OTFTs without traps show greater mobility (μ) than OTFTs with traps (2D-device simulation). μ degradation caused by decrease of $E_{||}$ due to presence of traps. (b) Modeled μ *vs.* V_{gs} for different trap density and γ.

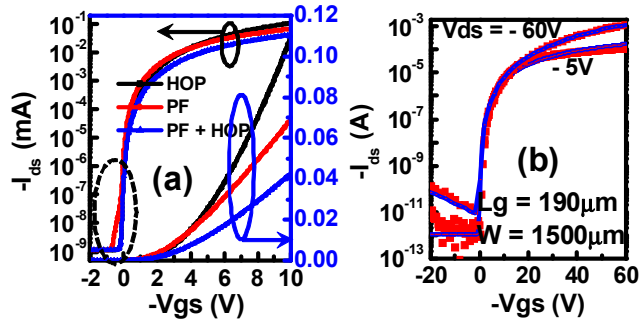


Fig. 8. (a) Mobility effect on drain current (I_{ds}) of a p-channel OTFT. Hopping mobility affects I_{ds} in subthreshold regime whereas Poole-Frenkel mobility affects I_{ds} in above-threshold regime. (b) Model verification against measurements of a p-channel OTFT for channel length (L_g) 190µm and width (W) 1500µm for I_{ds} is shown. (Symbols: Measurements, Lines: HiSIM-Org model).

IV. Conclusion

We have presented a surface potential based compact model for undoped-body OTFTs with a new charge carrier compact mobility model including both hopping and the band-like charge carrier mobility effects. Increase of gate voltage (V_{gs}), pushes the Fermi level from localized trap-energy levels to above band edge (i.e. extended energy levels) which results in mobility transition from hopping to band-like. The verification of model results with measured data demonstrates the predictivity of the model. We implemented the developed model using Verilog-A code to give easy access to this compact model by the OTFT community for circuit design.

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