1. Introduction

Organic field-effect transistors (OFET), which were first demonstrated by Tsumura et al in 1986 [1], utilize organic semiconductors in place of conventional inorganic semiconductors. The device performance of OFETs has significantly improved by virtue of a better understanding of materials and fabrication processes [2]. Thanks to the improved device performance, system-level applications based on OFETs are currently sought for RF-ID tags [3–5], display backplanes [6, 7], and sensors [8].

In the early stage, physical modelling of organic semiconductors used in OFETs at a material level were of primary interest. It allowed a profound understanding of the electronic structure and the related charge carrier transport and injection processes in organic semiconductors [9, 10]. However, at a device level, it is pointed out that considerable work remains to be done to model the device physics of OFETs because the classical models, which fit well into conventional silicon based metal-oxide-semiconductor filed-effect transistors (MOSFETs), often fail to describe the behaviour of OFETs [11].

The primary benefit of physical modelling of OFETs is to improve the device performance further. In addition, results of physical modelling can be used to improve the accuracy of compact models, which consist of simple mathematical descriptions of device behaviour needed for the simulation of integrated OFET circuits [12, 13]. The rigorousness of compact modelling strongly relies on the input parameters such as the charge carrier mobility $\mu$, contact resistance $R_c$, and threshold voltage $V_T$, which have usually been considered as constant fitting parameters [12–15]. Among them, $V_T$ is particularly important for OFETs because of the following reasons.

Firstly, there is a lack of analytical model for $V_T$ in OFETs. Because OFETs operate in the accumulation regime, they cannot borrow the definition of $V_T$ from conventional MOSFETs, which operates in inversion regime as the voltage needed to create minority charge carriers to an amount equal to that of the majority carrier [11]. This accounts for the lack of an automatic extraction functionality for $V_T$ of OFETs in most device simulators [16]. Secondly, $V_T$ must be controllable to realize circuit-level applications. In circuit-level applications,
it is possible to compensate spatial deviations of $V_T$ with the knowledge of $V_T$. In addition, this allows us to achieve a low voltage operation. Thirdly, $V_T$ is highly correlated to other key parameters. For example, $V_T$ is used to describe channel resistance $R_{ch} = 1/|\mu C_s (V_G - V_T)|$ in the extraction of contact resistance $R_s$ by transmission-line method. In addition, other parameters are often expressed as a function of $V_G - V_T$.

In OFETs, $V_T$ is defined as the voltage at which accumulation of charge starts [11]. For device evaluation and characterization, $V_T$ is estimated by parameter extraction methods from simulated or experimentally obtained transfer characteristics $I_D(V_G)$. One of the authors applied a second derivative method to OFETs for a reliable extraction of $V_T$, which can exclude the effect of drain voltage $V_D$ on $V_T$ [17]. However, the correlation between the extracted value of $V_T$ with the definition of $V_T$ has not yet been clearly demonstrated.

In this paper, a systematic study on physical modelling of organic field-effect transistors (OFETs) is performed based on a two-dimensional (2D) finite-element method (FEM). Through the systematic numerical simulation based on FEM, we try to clarify the contributions of device parameters on $V_T$, which is necessary to formulate a more rigorous analytical model.

### 2. Simulation methods

A numerical modelling is conducted by using ATLAS simulator (SILVACO) which self-consistently resolves the drift-diffusion current equation and the Poisson’s equation. With FEM-based ATLAS simulator, not only the transfer characteristics $I_D(V_G)$ of OFETs but also physical parameters, such as electric potential and electron and hole concentration, can be calculated at each mesh, which are small domains constructing the device. Figure 1 shows the simulated p-type OFET structure with a bottom-gate/top-contact (BG/TC) configuration. The physical dimensions of the device and the point of origin on a 2D plane are not changed throughout the simulation.

The physical and electrical properties of the materials used in the simulation are summarized in table 1. The electronic structure of the simulated p-type OFET is determined by the work functions $W$ of the metal electrodes, and the highest-occupied molecular orbital (HOMO) level and band gap $E_g$ of the organic semiconductor. It is particularly important to note that we assume a zero-doped and defect-free organic semiconductor. Organic semiconductors are usually used without intentional doping for OFETs; we showed that the unintentional dopants incorporated with a moderate concentration (roughly up to $10^{14}$ cm$^{-3}$) do not significantly affect the device characteristics as has been shown for organic diodes [18], organic metal-semiconductor field-effect transistors (OMESFETs) [19] and OFETs (see the supporting material). Moreover, the defect-free case is assumed in order to study $V_T$ in relation to the electronic structure of the OFET, excluding any role of defects which have been reported to have a significant effect on $V_T$ [17, 20–23]. The defect (or trap) states created in the forbidden gap accommodate and immobilize charge carriers, which modify the electronic structure and the charge carrier concentration in OFETs. Because the defect-free case is hard to achieve experimentally, it is a distinctive merit of simulation to be able to neglect the effect of traps.

Threshold in OFETs occurs at a low voltage. In addition, it has been reported that the injection property at the metal-organic semiconductor junction is one of the most significant aspects that governs the device operation at low voltages [18]. In this context, we varied the injection barrier height $E_b$ at source (and drain) by varying the ionization energy (IE) of the organic semiconductor while keeping $E_g$ constant to study the effect of charge carrier injection on $V_T$. Because we did not directly change the Fermi level of the source and drain electrodes, the flat-band potential $V_{FB}$, which is defined as...
the Fermi level difference between gate and source (or drain) electrodes, was unaffected by the modification of \( E_0 \).

### 3. Results and discussion

#### 3.1. Threshold voltage extraction and the ‘structure-unique’ threshold voltage

A rigorous analytical model for \( V_T \) of OFETs is still lacking. Therefore, \( V_T \) was extracted from simulated transfer characteristics \( I_D(V_G) \) in order to be used for device analysis. The linear-regime drain current \( I_D(V_G) \) of a p-type OFET is expressed as,

\[
I_D(V_G) = - \frac{W}{L} \mu C_i \left\{ V_G - \left( V_T + \frac{V_D}{2} \right) \right\} V_D,
\]

where \( W \) and \( L \) are the channel width and length respectively, \( \mu \) is the field-effect mobility, \( C_i \) the capacitance of the insulator, and \( V_D \) the drain voltage. Extraction methods used for conventional MOSFETs such as the constant current method [24], linear extraction method (LEM) [24, 25], and second derivative method (SDM) [26] are also applicable to OFETs. However, it has been often overlooked that \( V_T \) should be a structure-unique value. By the term ‘structure-unique’, we emphasize the dependence of \( V_T \) only on the electronic structure of the device without the dependence on the bias condition and the extraction method.

A reliable extraction method should be able to determine \( V_T \) as a single constant. In LEM, \( V_T \) is estimated at the intercept of the voltage axis with the \( I_D(V_G) \) line. The approximation is made at the voltage point corresponding to the maximum slope of \( I_D(V_G) \) curve [27]. However, the maximum slope point is uncertain when the \( I_D(V_G) \) curve deviates from an ideal straight line. For example, if the \( I_D(V_G) \) curve is bended downward over \( V_T \) (concave down with positive slope) due to mobility degradation and/or the existence of a source and drain contact resistance \( R_C \), the point of maximum slope becomes dependent on the mobility degradation and \( R_C \). Similarly, if the \( I_D(V_G) \) curve is bended upward (concave up with positive slope), the point of the maximum slope does not even exist. Although a range of \( V_G \) that allows the best possible linear fit, can be arbitrarily chosen [28], the extracted value of \( V_T \) becomes dependent on the choice of bias range. On the other hand, in SDM, \( V_T \) is defined as the \( V_G \) at which the second-order derivative of \( I_D(V_G) \) curve is maximum. It corresponds to \( V_G \) where the change of conductivity is the fastest, which is not affected by \( R_C \). In most cases, it is possible to specify \( V_T \) from the distinctive peak of the second-derivative \( \partial^2 I_D(V_G)/\partial V_G^2 \).

Secondly, a reliable extraction method should exclude the dependency of \( V_T \) on \( V_D \). Instead of impetuously neglecting the second-order term \( V_D^2/2 \) in equation (1) for linear regime approximation, it is more desirable to collect the common \( V_D \) factor,

\[
I_D(V_G) = - \frac{W}{L} \mu C_i \left\{ V_G - \left( V_T + \frac{V_D}{2} \right) \right\} \frac{V_D}{2}, \tag{2}
\]

where \( V_T + V_D/2 \) is defined as the effective threshold voltage \( V_T^{eff} \). Then, \( V_D \) independent \( V_T \) can be determined as the y-intercept of an extrapolation line of \( V_T^{eff} \) with respect to \( V_D \), which can be obtained from different \( I_D(V_G) \) curves at different \( V_D \).

In figure 2, numerically simulated linear-regime \( I_D(V_G) \) and \( \partial^2 I_D(V_G)/\partial V_G^2 \) are shown for a BG/TC OFET biased at \( V_D = -0.1, 0.3, -0.5, -0.7 \), and \(-1.0 \) V. While the injection barrier height \( E_0 \) is kept unchanged at 0.3 eV. It is observed that a slight upward-bending and a leftward-shift of the simulated \( I_D(V_G) \) occur as the drain voltage increases (figure 2(a)). This reflects the dependence of \( V_T^{eff} \) on \( V_D \) which is demonstrated by the leftward-shifted peak of \( \partial^2 I_D(V_G)/\partial V_G^2 \) as shown in figure 2(b). In addition, the voltages can be specified without any ambiguity by referring to the peaks of \( \partial^2 I_D(V_G)/\partial V_G^2 \). The \( V_T^{eff} \) extracted from figure 2(b) is plotted as a function of \( V_D \) (see figure 4). At the y-intercept of the extrapolated linear line for \( V_T^{eff} \), the structure-unique \( V_T \) is determined as 0.5 V for the case of \( E_0 = 0.3 \) eV.

In many reports, \( V_T \) is regarded as equivalent to the flat-band voltage \( V_{FB} \) when no dipole moment and trapped charges exist at gate/insulator and insulator/organic semiconductor interfaces [28, 29]. In the meantime, \( V_{FB} \) has been determined without clear remarks on the free carrier concentration in organic semiconductor layer at equilibrium. For OFETs
using intentional doping to achieve high carrier concentration, the conventional definition for \( V_{FB} \) of the MOS structure in MOSFETs, defined from the Fermi level difference of the gate electrode and the organic semiconductor, is equally valid for OFETs. On the other hand, when organic semiconductors are not doped as in the case of this study, \( V_{FB} \) is defined in a different manner. It was well demonstrated that, for non-doped organic diodes, the depletion region extends up to the organic semiconductor/metal interface due to (i) much smaller thickness of organic layer (around 100 nm) compared to silicon wafer (around 0.7 mm) and (ii) extremely low carrier concentration (typically 10^{14} \text{ cm}^{-3}) \[18, 30\]. This makes possible an analogy of the organic layer with an insulator in the metal-insulator-metal (MIM) model. Similarly, the electronic structure of OFETs is often seen as the metal-insulator-insulator-metal (MIIM) structure comprising the source electrode \[31\]. Accordingly, \( V_{FB} \) is defined from the Fermi level difference of the gate and source electrode, which will be used as the definition for \( V_{FB} \) herein.

Based on the MIIM model, the energy diagram of an OFET at \( V_{FB} = V_{FB} \) can be schematically drawn, as in figure 3. If we assume that the MIIM model is applicable at all \( E_b \), \( V_T \) should be equal to \( V_{FB} \) and should be invariant with respect to \( E_b \) because \( E_b \) is varied while keeping the Fermi levels of gate and source constant. However, as shown in figure 4, a direct impact of \( E_b \) on the structure-unique \( V_T \) is indeed observed. Figure 4(b) shows that \( V_T \) is equal to \( V_{FB} \), and thus the MIIM model is strictly valid only for an electronic structure, \( E_b = 0.4 \text{ eV} \). However, the MIIM model cannot be adopted to estimate \( V_T \) when \( E_b < 0.4 \text{ eV} \) even if no interface charges and defects are considered. This demonstrates the importance of injection properties at organic semiconductor/source interface in defining the threshold behaviour in OFETs. When \( E_b \) gets higher than 0.4 eV, the drain current is strongly reduced and the transfer curve deviates from a straight line, thus hindering any reliable estimation of the threshold voltage. We also note that such a high barrier height is not realistic for any practical application of the transistor \[32\].

### 3.2. Physical meaning of the threshold voltage

In the previous section, we demonstrated that the structure-unique threshold voltage \( V_T \) is not equal to the flat-band voltage \( V_{FB} \) determined from the MIIM model when the hole injection barrier height \( E_b \) is smaller than 0.4 eV. This result accounts not only for the modified injection properties, but also for the fact that the OFET is a two-dimensional (2D) device as opposed to the one-dimensional (1D) organic diodes. In this respect, the threshold behaviour needs to be understood not only across the channel, which corresponds to the MIIM structure, but also along the channel.

Figure 5 shows the numerically simulated hole concentration \( p_{xy} \) in the organic layer of an OFET with a hole injection barrier height of 0.3 eV at different gate bias: (a) for \( V_G = 0 \text{ V} \), (b) for \( V_G = V_{FB} = -0.6 \text{ V} \), and (c) for \( V_G = -5 \text{ V} \). At equilibrium, \( V_G = 0 \text{ V} \) (see figure 5(a)), \( p_{xy} \) greatly varies inside the organic layer. Near the center of the channel \( x = 15 \mu \text{m} \), \( p_{xy} \) shows an extremely low value (around \( 10^5 \text{ cm}^{-3} \)).
In contrast, $p_{xy}$ along $x = -5$ and $x = 35 \mu m$, which corresponds to the MIIM structure, takes 7–10 order of magnitude larger value because of the effect of source and drain electrode. At $V_G = V_{FB} = -0.6$ V, injected holes are filling the center of the channel, and the spatial distribution of $p_{xy}$ is nearly, but not perfectly, uniform in the organic layer. At $V_G = -5$ V, $p_{xy}$ is several orders of magnitude higher at the insulator/organic semiconductor interface than in the bulk, due to accumulation by a large negative bias applied at gate electrode, thus reaching to the creation of the conducting channel. The spatial distribution of $p_{xy}$ greatly changes along the $x$-axis, especially for an OFET in sub-threshold regime, so that a systematic analysis is desirable to compare the spatial distribution of $p_{xy}$ at two characteristic lines along $y$-axis, that is the center of channel ($x = 15 \mu m$) and at the center of source electrode ($x = -5 \mu m$).

Figure 5. Simulated hole concentration in the OFET at different bias conditions: (a) $V_G = 0$ V, (b) $V_G = V_{FB} = -0.6$ V and (c) $V_G = -5$ V. For each condition, $V_D = 0$ V and $E_b = 0.3$ eV. The $y$-coordinate represents the distance from insulator/organic semiconductor interface, while the $x$-axis is parallel to the interface. The center of channel and the center of source electrode corresponds to $x = 15$ and $x = -5 \mu m$.

Figure 6. Simulated hole concentration across the channel (along y-axis) sectioned (a) at the center of channel ($x = 15 \mu m$) and (b) at the center of source electrode ($x = -5 \mu m$) for two bias conditions: $V_G = V_{FB} = -0.6$ V and $V_G = V_T$. The hole injection barrier height $E_b$ is varied from 0.0 to 0.4 eV. Accordingly, the value of threshold voltage $V_T$ varies following the electronic structure of each OFET (figure 4(b)).

In contrast, $p_{xy}$ along $x = -5$ and $x = 35 \mu m$, which corresponds to the MIIM structure, takes 7–10 order of magnitude larger value because of the effect of source and drain electrode. At $V_G = V_{FB} = -0.6$ V, injected holes are filling the center of the channel, and the spatial distribution of $p_{xy}$ is nearly, but not perfectly, uniform in the organic layer. At $V_G = -5$ V, $p_{xy}$ is several orders of magnitude higher at the insulator/organic semiconductor interface than in the bulk, due to accumulation by a large negative bias applied at gate electrode, thus reaching to the creation of the conducting channel. The spatial distribution of $p_{xy}$ greatly changes along the $x$-axis, especially for an OFET in sub-threshold regime, so that a systematic analysis is desirable to compare the spatial distribution of $p_{xy}$ at two characteristic lines along $y$-axis, that is the center of channel ($x = 15 \mu m$) and at the center of source electrode ($x = -5 \mu m$).

Figure 6(a) shows the spatial distribution of $p_{xy}$ at the center of the channel ($x = 15 \mu m$) across the channel (along y-axis) of OFETs with various electronic structures for two gate bias conditions: $V_G = V_{FB} = -0.6$ V (squares in navy), and $V_G = V_T$ (circles in orange). The hole injection barrier height $E_b$ is varied as 0.0, 0.1, 0.2, 0.3, and 0.4 eV, where the
structure-unique threshold voltage $V_T$ changes correspondingly as shown in figure 4(b). When the flat-band voltage $V_{FB}$ based on the MIIM model $-0.6$ V is applied, the spatial distribution of $p_N$ across the channel is flat only for the case of $E_b = 0.4$ eV, where $V_{FB}$ happens to be equal to $V_T$. For other barrier heights, $E_b = 0.0, 0.1, 0.2,$ and $0.3$ eV, the OFETs are already turned on when $V_{FB}$ is applied because $V_{FB}$ is bigger than $V_T$. On the other hand, when $V_G = V_T$, the spatial distribution of $p_N$ across the channel is constant for every electronic structure, and hence the potential. This demonstrates that the threshold voltage can be defined as the voltage at which charge starts to accumulate at the insulator/organic semiconductor interface at the center of the channel. In addition, this physical meaning of threshold voltage is a universal description which is valid for every electronic structure, and well represented by the structure-unique $V_T$ other than $V_{FB}$.

Figure 6(b) shows the spatial distribution of $p_N$ at the center of source electrode ($x = -5 \mu m$) across the channel (along y-axis), which corresponds to MIIM structure, of OFETs having various electronic structures for two gate bias conditions: for $V_G = V_{FB} = -0.6$ V (squares in navy), and $V_G = V_T$ (circles in orange). The hole concentration at the organic semiconductor/source interface is determined by

$$p_n = N_v \exp \left(-\frac{E_b}{kT}\right),$$

where $N_v$ denotes the HOMO effective density-of-states (DOS), $E_b$ hole injection barrier height, $k$ Boltzmann constant, and $T$ temperature (300 K). As the injection of holes becomes more favoured thanks to lowered $E_b$, the concentration of holes injected from the organic semiconductor/source interface increases. As a consequence, potential in organic layer deviates from a perfectly linear line and shows significant bending near organic semiconductor/source interface when $E_b < 0.4$ eV. For this reason, it is hard to define either $V_{FB}$ or $V_T$ at the center of source or drain electrode.

3.3. Sub-threshold current

A reliable extraction method of $V_T$ based on the SDM demonstrates to compute a structure-unique $V_T$ which excludes the effect of drain voltage $V_D$ and inherent ambiguity from some extraction methods, and which is coherent to the physical meaning of threshold voltage. In this section, sub-threshold characteristics are studied in reference to structure-unique $V_T$.

Figure 7(a) shows the simulated transfer characteristics $I_D(V_G)$ of OFETs in semi-log plot. The drain voltage $V_D$ is varied as $-0.1, -0.3, -0.5, -0.7$ and $-1.0$ V, and hole injection barrier height $E_b$ is set to $0.3$ eV, where the structure-unique $V_T$ is $-0.5$ V and effective-threshold voltage $V_{TEF}$ is $-1.2$ V for $V = -1.0$ V (see figure 4). With the help of two guide lines for $V_T$ and $V_{TEF}$ in figure 7, it is shown that the current at gate voltage $V_G$ larger than $V_T = -0.5$ V shows $V_D$ dependence, which demonstrates that the current is realized by both diffusion and drift of charge carriers. On the other hand, for $V_G$ smaller than $V_T = -0.5$ V, it is shown that the current does not depend on $V_D$. Figure 7(b) shows $I_D(V_G)$ read at $V_D = -0.25$ V as an example. The variation of $V_D$ does not affect $I_D(V_G)$, which is a characteristic of conduction solely mediated by diffusion of carriers. This proves that the sub-threshold region of OFETs can be successfully defined by the structure-unique $V_T$ obtained from aforementioned method.

4. Conclusion

We have investigated the threshold behaviour of OFETs. The proposed extraction method for threshold voltage $V_T$ based on second-derivative method (SDM) enabled determination of a structure-unique $V_T$ excluding the effects of drain voltage $V_D$. By the structure-unique $V_T$, we defined the threshold voltage as the voltage where accumulation starts at the center of channel, which is shown to be universally valid for all electronic structures. At the same time, the flat-band voltage $V_{FB}$ adopted form the metal-insulator-insulator-metal model was shown to have limited applicability for OFETs with hole injection barrier height ($E_b = 0.4$) in the definition of $V_T$. In the gate voltage range smaller than the structure-unique $V_T$,
the sub-threshold region of OFETs could be successfully determined, where only the diffusion of carriers contributes to drain current.

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