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# Studies on correlation of surface and electrical properties in pentacene and thienoacene-based organic thin film transistors

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**Abstract**

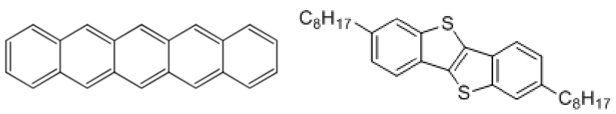
**We fabricated pentacene and thienoacene-based organic thin film transistors (OTFTs) with various types of interfacial layers between $SiO_2$ and organic semiconductor. Surface properties of contact angle and electrical properties of OTFTs include charge carrier mobility, threshold voltage, and on/off ratio were measured to compare and analyze the relationship between them. Based on present studies, some of device properties show a strong correlation, especially the relationship between contact angle and threshold voltage (pentacene-based OTFTs) shows the strong correlation coefficient r of 0.83 compare with others relationship.**

## 1. Introduction

Organic semiconductors have been widely studied for large-area applications, such as, flexible displays, paper-based organic electronics and radio frequency identification (RFID) tags [1]. There are still many challenges and problems need to be solved to improve performance of OTFTs, particularly to achieve high carrier mobility, high on/off current ratio and zero threshold voltage. It has been reported that by controlling dielectric interfaces using surface treatments can increase the OTFTs performance [2][3]. In this study, we used CT4112 (Kyocera Chemical), polymethyl-methacrylate (PMMA), Cytop (Asahi Glass), octadecyltrichlorosilane (OTS), hexamethyldisilazane (HMDS), $Ta_2O_5$, $HfO_2$, and $Si_3N_4$ as an interfacial layer. Each of interfacial layer was fabricated between dielectric layer and organic semiconductor. And, we studied the correlation surface and electrical properties with incorporating the interfacial layer in OTFTs [4].

## 2. Experimental methods

Organic TFT devices using pentacene or 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothiophene (C8-BTBT) as a semiconductor were fabricated with top contact structure, as shown in Fig.2. Heavily doped n-type silicon substrate with 100 nm $SiO_2$ layer was used as a substrate. First, the substrates were cleaned in ultrasonic bath with acetone, isopropanol and deionized (DI) water for each 5 min. Then, the substrates were dried by air gun. Then, an insulating interfacial layer (IIL) was coated on this substrate.



Pentacene C8-BTBT

Fig. 1 Molecular structures under study.

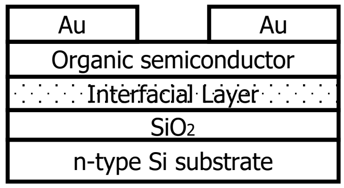



Fig. 2 Structure of top-contact organic TFT.

All the coating layer was prepared on the dielectric layer. Dielectric surface layer was coated with various types of interfacial layer: PMMA, CT4112, CYTOP, OTS and HMDS. High-k materials of $Ta_2O_5$, $HfO_2$, and $Si_3N_4$ were also used as interfacial layers [5]. These high-k materials were deposited using sputtering on $SiO_2$/Si substrate through a shadow mask to a thickness 50 nm. After the formation of IIL, the contact angle was measured in order to analyze the surface state changes. After that, 50 nm pentacene (Sigma-Aldrich, 98% purity) or C8-BTBT [6] as an organic semiconductor was thermally evaporated through a metal mask. The substrate temperatures during evaporation were 60°C for pentacene and 80°C for C8-BTBT. Then, 50 nm gold contact was thermally evaporated on top of device at room temperature. The channel length and width was 500 µm and 1.5 mm, respectively. By using out-of-plane X-ray diffraction (XRD, Bruker AXS) patterns of 50 nm organic materials with different interfacial layer was evaluated.

## 3. Results and discussions

Summary of contact angle, electrical properties and structural properties of pentacene and C8-BTBT OTFTs with nine different interfacial layers are shown in Tables 1 and 2. From the summarized data, we investigated the correlation of device properties and other properties of OTFTs to compare and analyze the relationship between pentacene and C8-BTBT.

Figure 2 shows the correlation of the carrier mobility vs contact angle for (a) pentacene and (b) C8-BTBT TFTs.

Table 1 Device properties of pentacene-based TFT prepared with different interfacial layers.

| Interfacial layers | Contact angle (deg) | Pentacene | | | |
|---|---|---|---|---|---|
| | | μ ($cm^2$/Vs) | $V_{th}$ (V) | $I_{on}/I_{off}$ | Intensity |
| (a) Without | 52 | 0.12 | 2.0 | $10^6$ | 4,789 |
| (b) CT4112 | 82 | 0.012 | -0.4 | $10^5$ | 5,640 |
| (c) PMMA | 75 | 0.004 | -1.0 | $10^5$ | 1,664 |
| (d) Cytop | 113 | $8.5\times10^{-4}$ | -8.6 | $10^3$ | 1,361 |
| (e) OTS | 82 | 0.035 | -0.4 | $10^5$ | 6,007 |
| (f) HMDS | 77 | 0.025 | -1.5 | $10^5$ | 5,766 |
| (g) $Ta_2O_5$ | 64 | 0.068 | 9.4 | $10^5$ | 7,591 |
| (h) $Si_3N_4$ | 37 | 0.005 | 6.4 | $10^4$ | 1,993 |
| (i) $HfO_2$ | 60 | $1.2\times10^{-4}$ | 2.3 | $10^4$ | 1,300 |

Table 2　Device properties of C8-BTBT-based TFT with different interfacial layers.

| Interfacial layers | Contact angle (deg) | C8-BTBT | | | |
|---|---|---|---|---|---|
| | | μ ($cm^2$/Vs) | Vth (V) | $I_{on}/I_{off}$ | Intensity |
| (a) Without | 52 | 1.85 | -5.0 | $10^8$ | 20,859 |
| (b) CT4112 | 82 | 0.26 | -9.4 | $10^7$ | 790 |
| (c) PMMA | 75 | 0.4 | -8.9 | $10^7$ | 1,498 |
| (d) Cytop | 113 | 0.35 | -8.3 | $10^8$ | 2,758 |
| (e) OTS | 82 | 0.11 | -5.0 | $10^7$ | 2,736 |
| (f) HMDS | 77 | 1.7 | -8.0 | $10^8$ | 1,025 |
| (g) $Ta_2O_5$ | 64 | 0.05 | -6.9 | $10^5$ | 24,888 |
| (h) $Si_3N_4$ | 37 | 0.3 | -3.5 | $10^6$ | 13,495 |
| (i) $HfO_2$ | 60 | $3.0\times10^{-4}$ | -0.8 | $10^5$ | 14,944 |

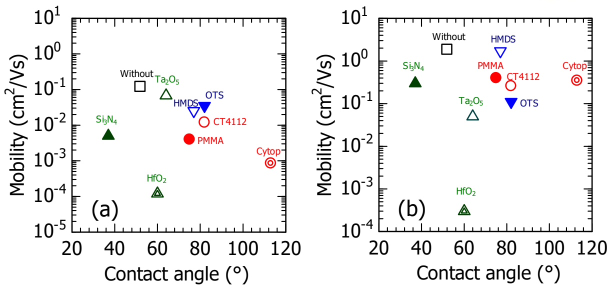



Fig. 2　Relation of the carrier mobility and contact angle for (a) pentacene and (b) C8-BTBT TFTs.

In Pentacene TFT, if we neglect the case of $Si_3N_4$ and $HfO_2$, larger correlation factor between mobility and contact angle of 0.79 is obtained. In C8-BTBT TFT, tendency of field effect mobility was seems to be small when contact angle increase. There only required less energy during vacuum evaporation of organic molecules to assemble and well-ordered thin film [7][8]. In our study, there is small obvious correlation between mobility and contact angle with C8-BTBT TFTs. Possible reason might be due to C8-BTBT molecule has alkyl chain and it affect the crystal growth of organic semiconductor. On the other hands, in Pentacene TFT, the mobility is thought to be maximum at certain value of dielectric constant of insulator. This is future subject for our investigation.

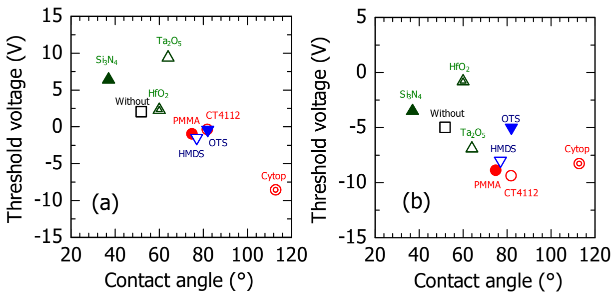



Fig. 3　Relation of the threshold voltage and contact angle for (a) pentacene and (b) C8-BTBT TFTs.

A strong correlation of threshold voltage and contact angle can be observed in Figs. 3 (a) and 3(b). This relationship may be explained the formation of interfacial layer between organic semiconductor and dielectric layer. In addition, the threshold voltage could be shifting become negative or positive depends on the types of interfacial layer and preparation of the surfaces before deposited organic semiconductor. For example, Klauk *et al.* [9] reported that positive threshold voltage obtained using sputtered material. From other researchers also reported that chemical modification using SAM or second polymer materials on $SiO_2$/Si interfaces also can affected low threshold voltage [10].

Interestingly, our results show using sputtering materials $Ta_2O_5$, $HfO_2$, and $Si_3N_4$ on $SiO_2$/Si interfaces for pentacene-based OTFTs, threshold voltage were shifted to positive voltage while using other interfacial layers were shifted to negative voltage. However, as can be seen from these results the relationship pentacene and C8-BTBT TFTs shows same tendency with strong correlation coefficient (r) with 0.83 and 0.61, respectively. This suggests that the shift of threshold voltage is related to density of trapped charge densities between organic semiconductor and dielectric interfaces.

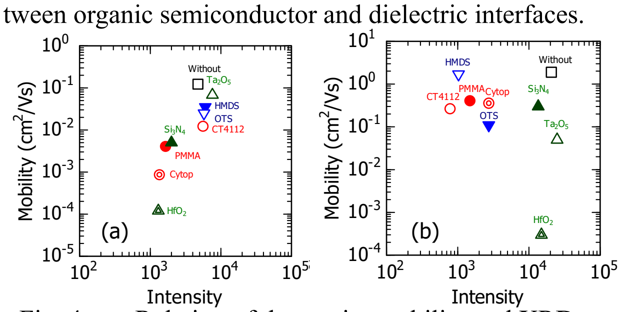



Fig. 4　Relation of the carrier mobility and XRD intensity for (a) pentacene and (b) C8-BTBT TFTs.

Pentacene-based TFTs show obvious correlation of carrier mobility and intensity compare to C8-BTBT TFTs, as shown in Figs. 4 (a) and 4(b). Here, Figure 4 (a) shows that the carrier mobility was significantly increased when the intensity of XRD peak increase. The experimental data for pentacene-based TFT suggest that the quality of crystallization organic thin film deposited on $SiO_2$/Si with and without interfacial layer could changes the carrier mobility. However, the structural properties of C8-BTBT TFT was not clear to show the relationship between mobility carriers of the device. Additional AFM observation will be necessary to clarify the detail of surface morphology to explain the relationship these experimental results.

## 4. Conclusions

We have found the relationship between the surface and electrical properties of pentacene and C8-BTBT OTFTs with different interfacial layers. The relationship between contact angle and threshold voltage in pentacene-based OTFTs shows the strong correlation coefficient of 0.83 compare with others relationship.

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