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Analysis of Pentacene Based Organic Thin Film Transistors through Two Dimensional Finite Element Dependent Numerical Device Simulation

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ABSTRACT

Pentacene based Organic Thin Film Transistors (OTFTs) analysis are performed for bottom and top contact structures using Silvaco ATLAS two dimensional finite element dependent numerical device simulations. Various OTFT structures are simulated using organic TFT display module. The transistor sizes for all the proposed structures are kept same, for valid comparison among them. The characteristic parameters of organic transistors are evaluated from output and transfer characteristics of different structures. Characteristics parameters have been evaluated in terms of mobility, on/off current ratio, threshold voltage, Sub-threshold slope, transconductance and drain current. OTFTs are considered as promising devices for future development of low-cost and large-area electronics applications such as flexible displays and sensors. Further this paper thoroughly discusses the overall performance and applications of OTFTs in various fields.

General Terms

Channel Length,Performance Parameters, Top and Bottom Contact.

Keywords

DNA Sensor, Organic Light Emitting Diode, Organic Thin Film Transistor, Pentacene

1. INTRODUCTION

The interest for Organic Thin Film Transistors (OTFTs) has been significantly increased over the last few years, and they have extensively studied for many applications such as low cost flexible displays [1], organic memories, key components for radio frequency identification tags (RFIDs), low end electronics, polymer integrated circuits, and sensors [2, 3]. Flexible electronics is a new technology for building electronic circuits by depositing electronic devices on flexible substrates such as plastic, paper, or even cloth. Compared with inorganic electronics, organic electronics or flexible electronics has following advantages. First of all, it can be fabricated at low temperature and at considerably low cost. Secondly it is thin, light weight, foldable, bendable, strong optical absorption, unbreakable, mechanical flexibility, consumes much less energy and efficient emission. Thirdly it has low cost due to cheaper material and lower cost deposition process techniques. Finally it can be used for large area applications. The most widely studied organic semiconductor material used for OTFT is pentacene [3]. OTFT based on Pentacene material have a typical field effect mobility of around 1 cm2/V.sec [4]. This is of comparable value to amorphous hydrogenated silicon (a-Si: H). OTFTs provide two important advantages over TFTs based inorganic semiconductors which can be defined in terms of fabrication at lower temperature and at considerably lower cost. OTFTs fabricated with light weight flexible substrates are expected to replace hydrogenated amorphous TFT applications on glass substrate. Researchers have already replaced the semiconductor layer by an organic material such as Pentacene, Poly (3-octylthiophene) P3OT, Pentacene, poly (3-hexylthiophene) P3HT and Poly (3-alkylthiophene) P3AT [1] and are currently targeting to replace the dielectric layer by suitable organic insulating materials for the development of completely flexible displays. The importance of two dimensional device simulations is growing for familiarization with basic device operation and optimization of novel device structures.

In order to enhance the device speed, considerable research effort has been devoted for increasing the mobility of organic materials by improving deposition conditions. As a result of this effort, mobility for OTFT exceeding 1 cm2 /V.sec for Pentacene and 0.1 cm2 /V.sec for poly(3-hexylthyophine) P3HT [5]. In addition of mobility, other ways of improving performance of OTFTs are scaling of channel length and with variation in active layer thickness. OTFTs are commonly fabricated as an inverted structure with gate at the bottom and source and drain at top [6]. Although the merits and demerits of these devices in terms of processing, mobility and contact resistance [2] are well recognized, the implications of structural differences for circuit performance have not been elucidated so far. This paper describes the impact of structural differences on performance of OTFT devices. All structures shows in Fig. 1 to Fig. 4 are realized using two dimensional ATLAS TCAD numerical device simulators. Various important device parameters are also being summarized here. Top and bottom contact, indicating the location of the source and drain electrodes with regard to the organic semiconducting layer, are the most widely used. Top contacts OTFTs typically have the highest performance. This is most probably because of reduced contact resistance at the source and drain electrodes. This paper contains seven sections. The present section 1 introduces the contents of the paper. Structures and working principle is described in section 2. Results and discussion are explained in section 3 thereafter in section 4; OTFTs characteristics parameters have been described. Finally various applications, conclusion and references are drawn in section 5, 6 and 7 respectively.

2. OTFTs STRUCTURES AND WORKING PRINCIPLE

An organic thin film transistor is a transistor made up of active thin film current carrying organic semiconductor, a dielectric layer and three contact electrodes. Two of the electrodes, source and drain are in direct contact with organic semiconductor and the third, gate (G) electrode is isolated from organic semiconductor thin film layer by suitable dielectric layer. Firstly, the main difference between the geometry of conventional Transistor and Organic thin film transistors (OTFTs) is that latter does not have a fourth terminal that is bulk, thus making these transistors free of body effect. Secondly, in conventional transistors the conducting channel is formed by an inversion layer while in OTFTs, it is because of accumulation. Researchers have recently proposed various structures which are discussed in following subsection along with their working principle.

2.1 OTFTs Structures

Today, MOSFETs dominate current technology; there are millions of them in the processors used in personal computers, cellular phones and many other microelectronic devices. Though these give direct access to charge carrier mobility, besides their numerous technological applications. OTFTs have been gaining attention over past few years. It shows that these transistors are out breaking their performance and becoming very attractive for range of applications in large area electronics. OTFTs adopt the architecture of Thin Film Transistor (TFT), which has proven it's adaptability with low conductivity materials. It contains three electrodes source, drain and gate, a dielectric layer and active organic semiconducting (OSC) layer. The main structural difference between the geometry of conventional MOSFETs and OTFTs is that the latter does not have a fourth terminal that is body, thus making these transistors free of the body effect. Secondly, in the former the conducting channel is formed by an inversion layer while in OTFTs, it is because of accumulation layer. Majority of OTFTs that have been studied are p-type devices, however, recently n-types have also been examined. Pentacene acts as a p-type semiconductor where majority carriers are holes. Based upon the relative position of the source/drain and gate contacts with respect to OSC layer different structures can be made for OTFTs.

The structure can be top gate or bottom gate and further both structures can be divided into top contact and bottom contact alternatives as shown in Fig.1 to Fig.4. The deposition of organic semiconductor layer on the insulator is much easier than the reverse due to fragile nature of organic semiconductor materials; hence bottom gate structure is built in majority for current OTFTs. In top contact structure contacts are deposited through shadow mask where as in bottom contact microlithography technique is used [2].

Well known structure for standard silicon MOSFETs is top-gate-top-contact (TGTC), however for simulation of OTFT bottom-gate-top-contact (BGTC) and bottom-gate-bottom-contact (BGBC) structure has been modeled mostly. Certain advantages and disadvantages are associated with each of four TFT structures. For example it is expected to obstruct the exchange of charge carriers between contacts and semiconductor, due to presence of an energy barrier at the interface between source and drain contacts and organic semiconductor. In case of BGBC; gate dielectric layer and source/drain contacts are prepared before organic semiconductor is deposited. It is very advantageous because methods involving solvents and/or thermal treatments can be safely employed to prepare the gate dielectric and contacts without harming the semiconductor layer.

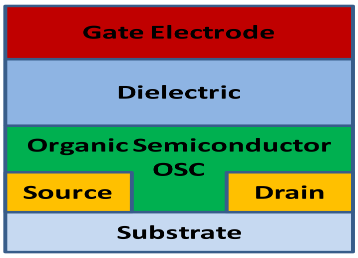

Fig 1: Top Gate Bottom Contact (TGBC) OTFT structure.

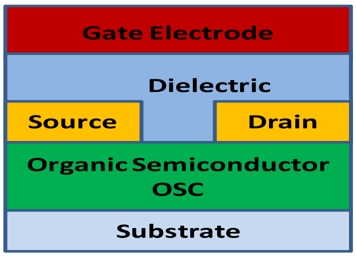

Fig 2: Top Gate Top Contact (TGTC) OTFT structure.

In terms of mobility among both the structures, BGTC structure shows better performance in comparison with BGBC structure. The better mobility for top contact OTFT is due to less contact resistance than that of a bottom contact one [5]. The performance of OTFTs in a BGBC bottom contact device structure is generally observed to be lower as compared to top contact device configuration [9, 13]. The reason for this performance difference is often explained by the large metal-semiconductor contact resistance due to interface contact barrier and irregular deposition or poor morphology of the semiconductor film around the already patterned source and drain contacts. The contact resistance is lower in TGBC structure due to large injection area which enables higher currents for the same applied voltages in comparison to BGBC structure. In TGBC structure source/drain contacts are patterned on a substrate rather than on a dielectric or OSC layer, so it is easier to fabricate the structure. On the other hand BGBC structure has been more often used to make high resolution display.

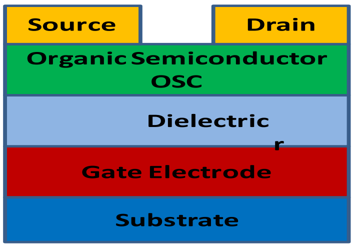

Fig 3: Bottom Gate Top Contact (BGTC) OTFT structure.

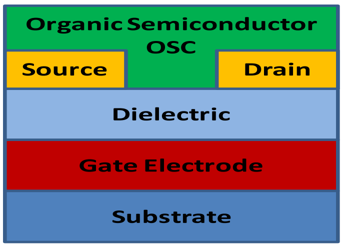

Fig 4: Bottom Gate Bottom Contact (BGBC) OTFT structure.

2.2 Working Principle

The operating principle of OTFT in this paper is explained using the schematic diagram of BGTC structure, as shown in Fig. 5. The device consists of pentacene organic semiconductor material with source/drain and gate electrodes made of Au and Al, respectively. The Fermi level of gold and the HOMO: LUMO (Highest Occupied Molecular Orbital: Lowest Unoccupied Molecular Orbital) levels of pentacene are shown in Fig. 6. Fundamentally, an OTFT operates like a capacitor. At zero gate voltage an intrinsically undoped organic semiconductor is devoid of charge carriers. Charge carriers are induced into the organic material by injection from the source and drain electrode is drawn in the vicinity of the dielectric. When a negative/positive gate voltage is applied, positive/ negative charges are induced in the semiconductor and a p-type / n-type conducting channel is formed [5]. If the work function of the source/.drain metal is close to the HOM-LUMO level of the OSC, then positive/ negative charges can be extracted by the electrodes by applying a voltage, VD between drain and source.

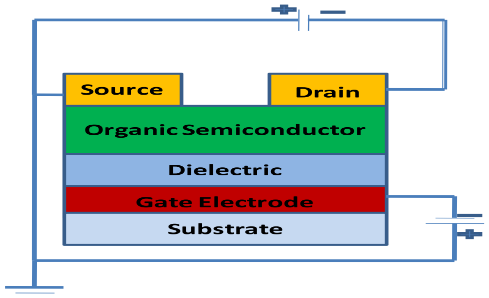

Fig 5: Schematic of BGTC OTFT operation, pentacene as active semiconductor layer, with Al2O3 as dielectric, S/D of gold and Al as gate contact electrodes.

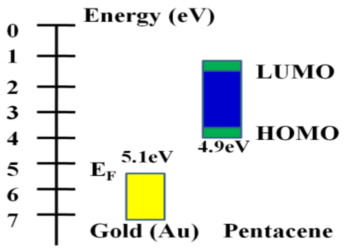

Fig 6: Energy band of the gold and pentacene interface

Pentacene acts as a *p*-type semiconductor where majority carriers are holes. When a negative gate voltage is applied, an electric field is formed across the dielectric, causing an accumulation region of holes at the dielectric-semiconductor boundary. Applying a voltage to the source-drain terminals allows a current to flow across this accumulation layer between the contacts [13]. All the way through discussion the source serves as the reference (grounded) electrode. Fig. 1 to Fig. 4 are illustrate widely used various OTFTs structures. There are several alternative ways of arranging the structure of device. Operating principle and current- voltage characteristics of OTFT are shown in Fig. 7 through 14. These characteristics are measured on a device made of pentacene as the semiconductor layer and gold are used as source and drain electrodes, aluminum as gate electrode respectively.

In the linear region, $V_D << V_G - V_T$ the channel is continuous and I_D is given by

$$I_{D,lin} = \frac{W\mu C_i}{L}\left[(V_G - V_T)V_D - \frac{V_D^2}{2}\right]$$

(1)

Where C_i is the capacitance per unit area of gate dielectric material, *L* and *W* are channel length and channel width of OTFT, respectively. Further increasing $V_D > V_G - V_T$ causes electric field to become zero at the drain contact. Due to this, a depletion area is created around the drain contact which is called pinch off. Beyond this pinch off point, the saturation regime begins and the drain current is now independent of drain voltage which is being controlled by gate voltage alone. In this region, the drain current varies quadratically with the field:

$$I_{D,lin} = \frac{W\mu C_i}{2L}(V_G - V_T)^2$$

(2)

Equation 1-2 represents the expression used to calculate mobility in OTFTs. The mobility can be estimated for various structures from their transfer characteristics. Mobility in the linear region is given by transconductance, which is defined by

$$g_m = \frac{\partial I_{D,lin}}{\partial V_G} \tag{3}$$

For small and constant V_D, mobility in the linear region is calculated from the relationship

$$\mu_{lin} = \frac{L g_m}{W C_i V_D} \tag{4}$$

In the saturation region mobility is calculated using

$$\mu_{sat} = \frac{2L}{W C_i}\left(\frac{\partial\sqrt{I_{Dsat}}}{\partial V_G}\right)^2 \tag{5}$$

3. RESULTS AND DISCUSSION

This section analyzes the functioning of various OTFT structures. The major parameters used in this simulation for channel length (L), Channel width (W), Al2O3 insulator thickness (tox), source and drain length (tS, tD), and Pentacene active layer thickness (tP) are of 20 µm, 100µm, 5.7 nm, 20 nm and 30 nm respectively. The properties of pentacene organic semiconductor material used in simulation include energy gap of 2.2 eV, electron affinity of 2.8 eV, electron density of state of 2.0 x 1021 per cm3 in valance band, 1.7 x 1021 per cm3 in conduction band and permittivity is 4 [5, 14]. All the structures are simulated in the above organic module known as ATLAS environment. The proposed structure of OTFT in bottom gate-top contact is showing superior characteristics [14] in terms of drain current and mobility as compared to bottom gate bottom contact structure.

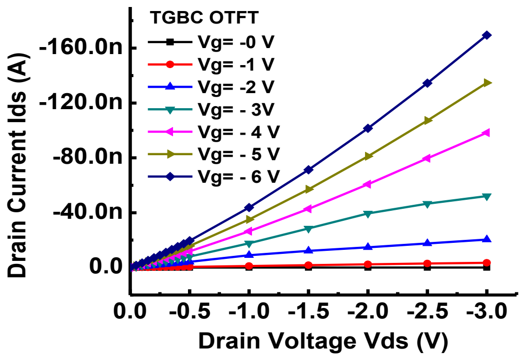

Fig 7: Top Gate Bottom Contact (TGBC) OTFT output characteristics.

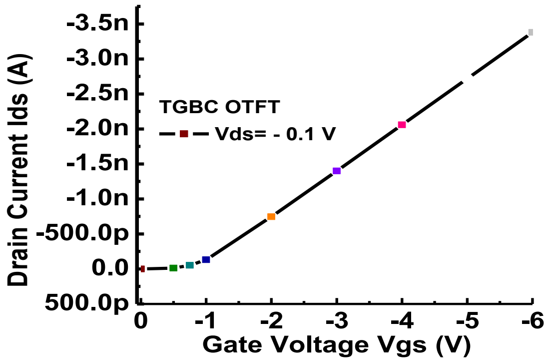

Fig 8: Top Gate Bottom Contact (TGBC) OTFT transfer characteristics.

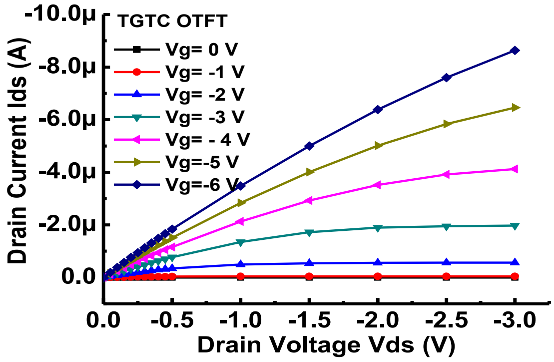

Fig 9: Top Gate Top Contact (TGTC) OTFT Output characteristics.

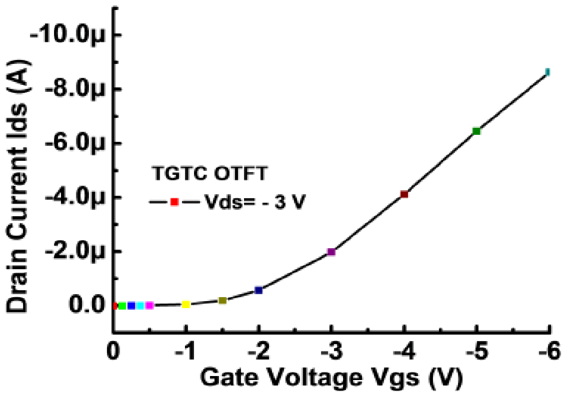

Fig 10: Top Gate Top Contact (TGTC) OTFT transfer characteristics.

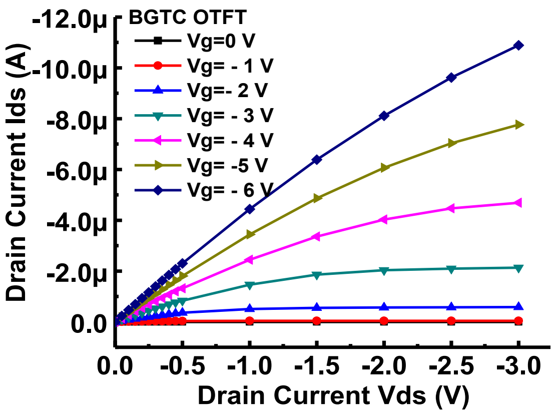

Fig 11: Bottom Gate Top Contact (BGTC) OTFT Output characteristics.

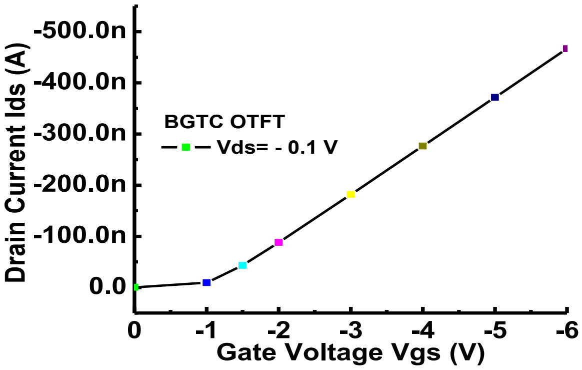

Fig 12: Bottom Gate Top Contact (BGTC) OTFT transfer characteristics.

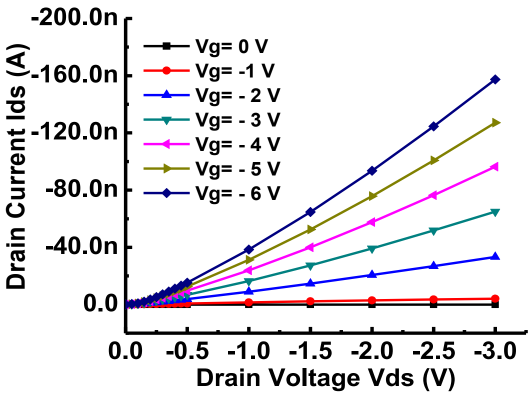

Fig 13: Bottom Gate Bottom Contact (BGBC) OTFT Output characteristics

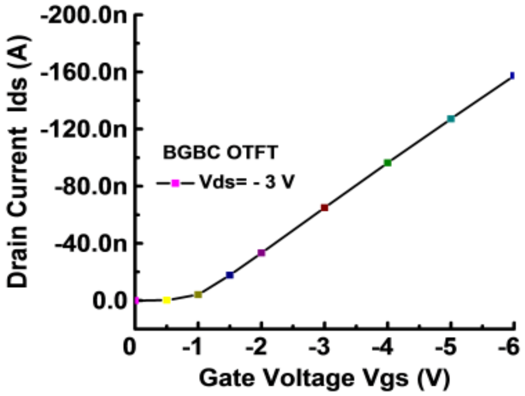

Fig 14: Bottom Gate Top Contact (BGTC) OTFT transfer characteristics.

OTFT at given source-drain bias voltage VSD, drain-source current ID is the function of conductivity of organic semiconductor thin film. This conductivity has to be controlled by source-gate bias voltage VSG. Since gate insulator prevents currents flow from gate, one has to deduce a charge enhancement for the polymer due to gate electric field in order to obtain ID-VSG dependence curve. The output and transfer characteristics of OTFTs have been analyzed by use of proper boundary condition and physics of OTFTs. The output and transfer characteristics are examined for TGBC, TGTC, BGTC and BGBC OTFTs, and the simulated results are shown in Fig. 7 to Fig. 14 respectively. As indicated in Fig. 7 through Fig. 14 drain current (Idmax) of TGBC, TGTC, BGTC and BGBC are of -0.169 µA, -8.63 µA, -10.9 µA, and -0.157 µA, respectively, at specified gate voltage and drain voltage of -6.0 V and -3 V respectively. Thus maximum drain current (Idmax) of bottom gate top contact device is higher than that of other structures of OTFT for same structural parameters. It implies that more current flows in bottom gate top contact devices as compared to any other structure without pretentious any structural or electrical behavior differences of the organic semiconductor-metal contact barrier. Consequently, the difference of bottom contact and top contact device characteristics are due to device structures.

4. CHARACTERISTIC PARAMETERS

The performance parameters such as mobility, threshold voltage, Sub-threshold slope, transconductance, on/off current ratio and drive current are extracted from characteristic plots of various OTFT structures. The resulting characteristics parameter values are presented in Table 1.

Table 1. Extracted parameters for various organic thin film transistors structures

Parameters	TGBC	TGTC	BGTC	BGBC
Mobility (μ) cm^2/V.s	0.0019	0.245	0.0278	0.0111
Threshold Voltage (V_T) V	- 0.89	- 2.24	- 1.10	- 0.95
On/Off Current Ratio (I_{ON}/ I_{OFF})	10^6	10^5	10^6	10^7
Sub-threshold Slope (*SS*) V/decade	0.195	0.113	0.198	0.148
Transconductance (g_m) μ S	0.031	2.33	0.095	0.032
Maximum Drive Current (µA) at V_{GS} = - 6 V, and V_{DS} = - 3 V	-0.169	-8.63	-10.88	-0.175

It is observed that OTFT structures with top contact demonstrate superior performance as compared to those with bottom contact. Higher injection area and reduced drain and source contact resistances are main reasons for better behavior of top contact based OTFT architectures. Among all OTFT structures, BGTC structure.

The analysis in section 3 shows that a larger mobility is obtained for top contact rather than the bottom one. The results, tabulated in Table 1, indicate that TGBC and TGTC have much lower mobility than BGBC and BGTC structures, respectively. Moreover, simulation results indicate that device structure by itself is not the only factor that affects mobility devices. Other factors, which may be responsible for their performance, depend on the device fabrication process and electrical, mechanical optical and chemical properties of materials.

5. APPLICATIONS

Organic thin film transistors find wide applications in OLEDs, RFID tags and DNA sensors

5.1 Organic Light Emitting Diodes (OLEDS)

OTFTs can be utilized to make displays on glass, or plastic Liquid crystal display can be fabricated with organic thin film transistors and Active Matrix Organic Light Emitting Diode (AMOLED) with dot patterns. But the AMOLED shows significant non-uniformity in the brightness. On the other hand, OTFTs can be used to make superior displays of E-paper or LCD because it requires only high on/off current ratio.

An organic light emitting diode (OLED) is a thin film device whose emissive layers are made of organic compound [10, 13] and does not require any back light function. New emissive technology called organic/polymer light emitting diode (OLEDs/PLEDs) displays has been developed. Many OLEDs together on a screen make up a picture. OLEDs require no backlighting, so they have high luminous efficiencies. They are used in mobile phones, televisions and display systems.

5.2 Radio Frequency Identification (RFID) Tags

Development of RFID tags for item-level tracking of individual goods of consumer. Such tags are expected to dramatically improve inventory control, automation, and purchasing/checkout operations [7, 13]. Several approaches have been developed to realize item-level RFIDs [8]. In most conventional approach, low-cost silicon RFID tags were developed. But there usages are restricted in water- and metal-contaminated environments.

Moreover, silicon based RFIDs are not bendable which limits their applicability in general flexible items. In contrast, organic electronic devices find wide applications in alternative flexible RFIDs. To realize low cost individual RFID tags, efforts have been made for development of item level RFID tags by use of OTFTs and printed electronics technologies.

6. DNA SENSORS

Presently used fluorescent scanning and imaging techniques for the analysis of DNA microarrays are not portable and has a limited spatial resolution and sensitivity. Moreover, these techniques require labeling of targets, which is time-consuming, more complex and expensive. DNA sensors have been developed based on various types of FETs, including single crystal silicon FETs, polycrystalline or amorphous silicon thin-film transistors (TFT), silicon nanowire transistors, carbon nanotube transistors, graphene transistors and organic TFTs (OTFT). OTFT fabricated on an insulating substrate is low-cost and flexible. OTFTs show great advantages over devices based on silicon wafers especially in disposable applications. Being mature technologies they can be directly transferred to sensing applications, including high-density DNA sensors [11].

Zhang et al. [11] reported an OTFT-based single-stranded DNA (ssDNA) and double stranded DNA (dsDNA) sensor. Fig. 15 shows ssDNA molecules immobilized on the surface of semiconductor layer (Pentacene). The immobilized DNA molecules dope the organic semiconductor, causing a threshold voltage shift. Zhang et al. observed substantial difference in the resultant threshold voltage shift due to different net doping and immobilization efficiencies of ssDNA and dsDNA molecules [11, 12].

This enables the direct electrical detection of hybridization through the measurement of TFT saturation current. However, the DNA molecules that need to be immobilized on the surface of pentacene may decrease the stability and repeatability of the device since pentacene film is sensitive to moisture and some ions. Furthermore, it is not convenient to firmly bind biomolecules to the surface of pentacene.

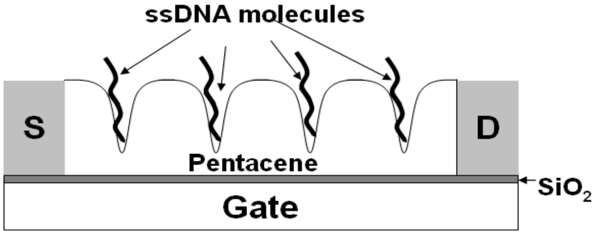

Fig 15: OTFT with a bottom gate. DNA molecules naturally immobilize itself in grain boundaries and other troughs on the semiconductor surface due to hydrophobic interactions [11].

Yan et al. [12] demonstrated an improved OTFT based DNA sensor where DNA molecules were immobilized on gold source and drain electrodes. Both ssDNA and dsDNA molecules are differentiated successfully due to dramatic change in the performance of the devices, which is attributed to the increase in contact resistances at the source/drain electrodes. OTFTs successfully find wide applications in DNA sensors. An overall analysis time of less than 40 minutes is required with OTFT based DNA sensor as compared to around 24 hours of testing time using conventional techniques [11]. Thus OTFTs are capable of deploying fast and ultra-low-cost DNA detection.

7. CONCLUSION

OTFTs have been going through a perpetual and reliable enhancement since last five years. Simulation results analyze for the performance of devices designed by using bottom and top gate organic thin film transistors. It is observed that OTFT structures with top contact demonstrate superior performance as compared to those with bottom contact. These improvements in performance are achieved in terms of mobility, Transconductance and maximum drain current. Higher injection area and reduced drain and source contact resistances are main reasons for better behavior of top contact based OTFT structures. Higher on-off current ratio is achieved for bottom contact devices. Along with all important applications, simple manufacturing process of OTFT with low production cost and non-breakable impacts that can be bended and folded, has been argued to be the most important research area. OTFTs may be demonstrated as novel circuits for future sophisticated engineering applications.

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