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Keywords: *pentacene; simulation; organic thinfilm transistor; Poole-Frenkel mechanism; threshold voltage; gate-electrode; workfunction.*

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SIMULATIONBASEDCHARACTERIZATIONOFTHETRANSPORTCHANNELPARAMETERSOFPENTACENETHINFILMTRANSISTOREFFECTOFGATEINSULATORTHICKNESSANDGATEELECTRODEWORKFUNCTION

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Simulation based Characterization of the Transport Channel Parameters of Pentacene Thin Film Transistor: Effect of Gate Insulator Thickness and Gate Electrode Work Function

W. Wondmagegn [α] & R. J. Pieper [σ]

Abstract- In this paper we have presented the simulation and analysis of the channel field, potential, mobility, hole concentration, and the threshold voltage of pentacene thin film transistor with gate metal work function and gate insulator thickness. The top contact transistor from pentacene active material, paryelene dielectric and gold source/drain electrodes, has been used for our simulation. The simulations have been performed using Silvaco's Atlas device simulator. The Poole-Frenkel transport model was used in the pentacene active material. The results of the simulation have shown an impact of the gate metal work function on threshold voltage, channel potential, channel charge concentration, channel field, and mobility of the device. When the high work function gate electrode is used, there exists a built in field in the transistor channel. As a result there exists built in channel charge concentration at zero gate voltage and increased channel mobility is observed. As expected, when the gate insulator thickness decreases, the channel charge density increases due to increased vertical field and this increases the drain current. The field effect mobility decreases as the thickness of the dielectric decreases. The threshold voltage changes with gate electrode work function but remains the same when the thickness of the dielectric changes.

Keywords: pentacene; simulation; organic thinfilm transistor; Poole-Frenkel mechanism; threshold voltage; gate-electrode; workfunction.

I. Introduction

Pentacene Field Effect Transistors (FETs) have been attractive for applications in the areas of Flexible display, RFIDs, sensors because its performances are similar to that of amorphous silicon thin film transistors [1-5]. Apart from these comparable electronic characteristics and promising low-cost fabrication, there are still important parameters of the device that needs better understanding and precise control for proper operation of the device. Some of the key issues are environmental stability, leakage current, threshold voltage and mobility [6-12].

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In general organic FETs have higher threshold voltages than normally required for integrated circuit applications. The threshold voltage can depend on different factors such as gate bias stress [13,14], gate dielectric [15], and the thickness of the active layer material [16]. Properties of gate electrode and dielectric are also important parameters that affect the performance of the transistor. The dependence of threshold voltage on gate metal work function has also been reported [17,18]. In this paper we have simulated a top contact transistor and systematically studied the effect of gate work function and gate insulator thickness on channel parameters such as field, potential, charge concentration, threshold voltage, and field effect mobility.

II. Simulation

Bottom contact pentacene Thin Film transistor is simulated and matched with experimental data, previously reported by our group [19-21]. Poole-Frenkel-like electric-field dependence (equation below), which is the inverse variation in activation energy against the square root of electric-field strength [22,23], has been employed for pentacene active channel. Nonlinear transport organic semiconductor materials is intensively explained through Poole-Frenkel (PF) transport mechanism [24-27]. The model explains the temperature and electric-field dependencies of charge carrier drift mobilities in disordered materials.

$$\mu(E) = \mu_0 \exp[-\frac{\Delta}{kT} + (\frac{\beta}{kT} - \gamma)\sqrt{E}]$$

where μ(E) is the field dependent mobility, μ0 is the zero field mobility, E is the electric field, Δ is the zero field activation energy, β is the electron Poole-Frenkel factor, k is the Boltzmann's constant, and T is the temperature. The Poole-Frenkel parameters extracted from the best match between simulation and experiment are Δ=0.1, β=3.58x10-5, and γ=10-5.

Figure 5 (a) shows the characteristic family of curves of pentacene TFT for gate voltages 5 – 20 volts in

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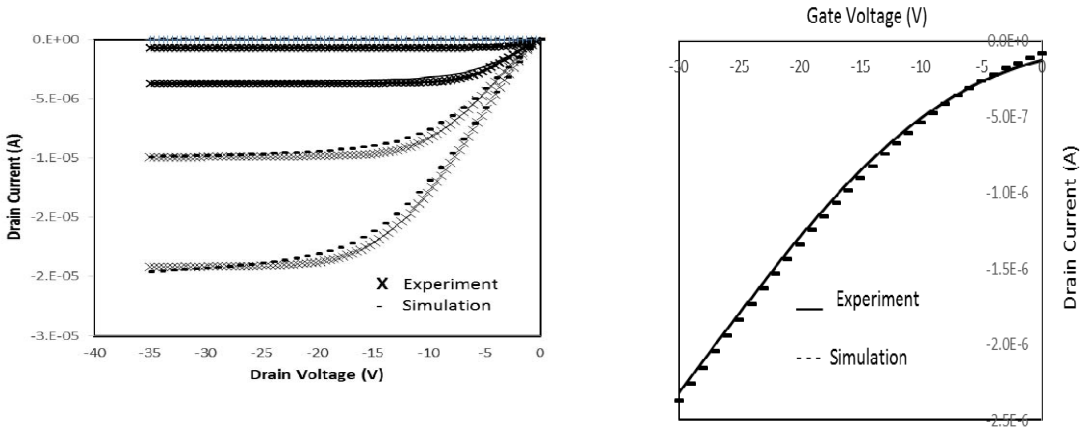
steps of 5 V. Figure 5 (b) shows transfer curves for experiment and simulations.



(a) *(b)*

Fig. 1: ID -VD plots of the transistor (a); ID -VG plots of the transistor (b)

III. Transistor Channel Parameter Simulation Results and Discussion

A top contact device (Fig. 2) with a width of 100 μm and channel length of 10 μm is used for simulation. A 30 nm pentacene active layer and a 6 nm gate dielectric is used. The thickness of gold source drain contacts is 30 nm and that of aluminum gate electrode is 20 nm

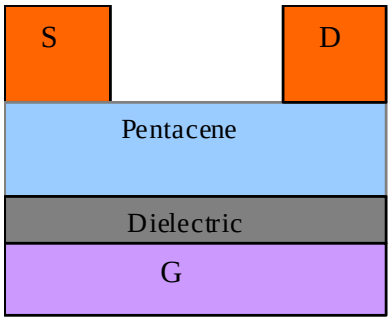


Fig. 2: Top contact device structure (not drawn to scale)

a) Impact of gate electrode work function

Fig. 3 shows drain current versus gate voltage characteristics of the device for different gate electrode work functions simulated at a drain voltage of-3 V.

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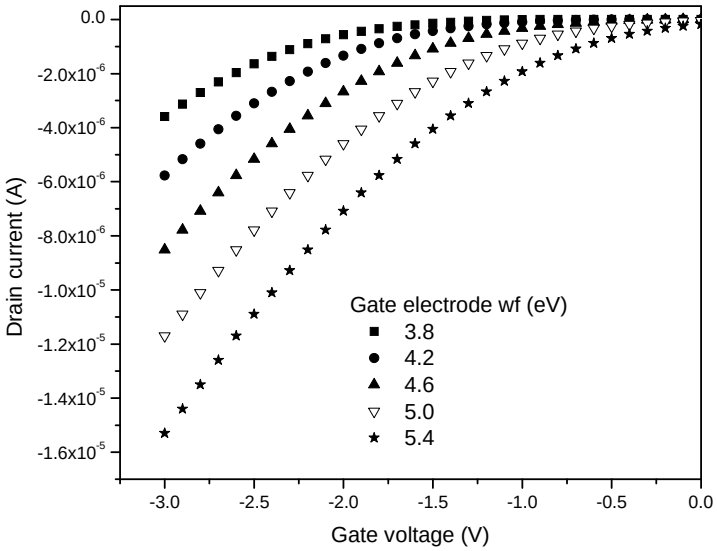

Fig. 3: Ids – Vgs characteristics of the device at different gate electrode work functions

The current increases as the work function increases which implies that there is a change in the transport channel parameters of the transistor such as the channel field and charge concentration.

The change in threshold voltage associated with change in electrode work function and change in the flat band voltage is also expected. With no charge present in the oxide or at the oxide-semiconductor interface, the flat-band voltage simply accounts for the work function difference between the semiconductor and the metal gate. As has been reported [28], the effect of gate work function is significant, particularly when the transistor is biased at accumulation. The gate work function can affect both the gate leakage current and the source drain current. As shown in Fig.3, the current increases by about a factor of 3 when the gate metal work function increases from 3.8 eV to 5.4 eV.

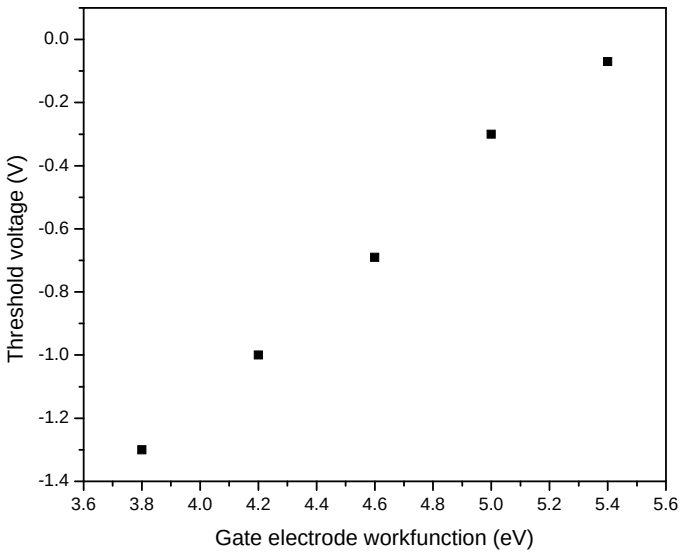

Fig. 4: Threshold voltage extracted from simulation for different gate electrode work functions

To account for this change in drain current as a function of gate metal work function, we have extracted the threshold voltage for each gate work function. The threshold voltage was extracted from the square-root of the drain current versus gate voltage curve. Fig. 4 represents the relationship between the threshold voltage of the transistor, extracted from the simulated transfer curve, and the work functions of the gate electrode. The simulations show a linear relationship between the threshold voltage and workfunction which is consistent with the relationship mentioned in the literature [17]. The gate electrode work function is one of the factors which affect the threshold voltage. The threshold voltage decreases as the work function of the gate electrode increases towards the HOMO level of pentacene. Matching the gate electrode and pentacene work functions would reduce the threshold voltage.

The effect of the work function on the electric field, which is responsible for the channel charge

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accumulation, has also been examined. We probed the electric field at the interface between the gate insulator and pentacene for fixed drain voltage (-3 V). The change in the flat band voltage or the threshold voltage is also reflected in a change on the channel electric field and channel charge concentration. As shown in Fig. 5, simulation results indicate that there exists a built in field at zero gate voltage. For each gate voltage, higher work function gate electrodes create higher channel field.

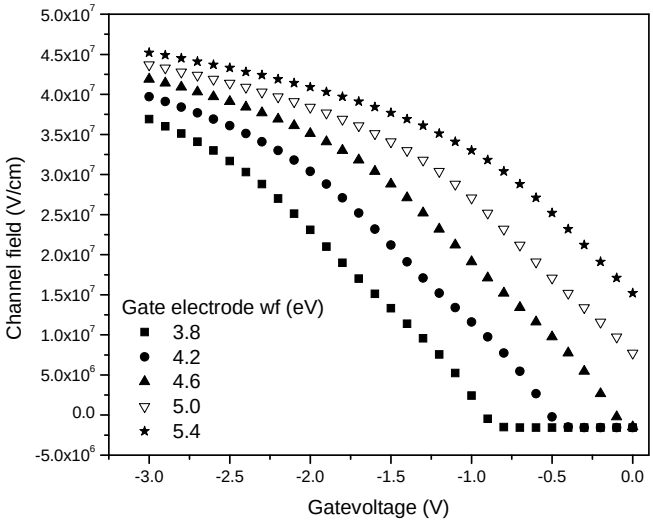

Fig. 5: Plot of extracted channel field against gate voltage for different gate electrode work functions

This field forms a channel charge at zero applied gate voltage as shown in the Fig. 6. The simulation shows about 1018 cm -2 charge concentration at zero gate voltage for 5.4 eV work function as opposed to about zero for 3.8 eV work functions. This implies that the increase seen in the drain current, as an increase in gate work function, resulted from both the field increase and threshold voltage reduction.

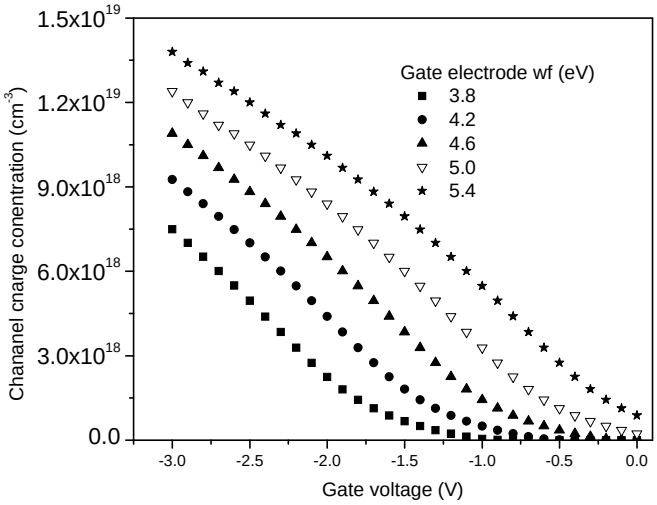

Fig. 6: Plot of extracted channel charge concentration versus gate voltage for different gate electrode work functions

We have extracted the mobility for different work functions and presented in Fig. 7. The channel mobility is also higher for higher work functions. For lower work function gate electrodes, the mobility starts at very low value at zero gate voltage and increases with gate voltage. But for the higher work function electrodes, the mobility has a higher value at zero gate voltage. This is the result of the high electric field and charge density. Experimental studies in the literature indicate that channel mobility increases when the channel field and charge concentration increases [29].

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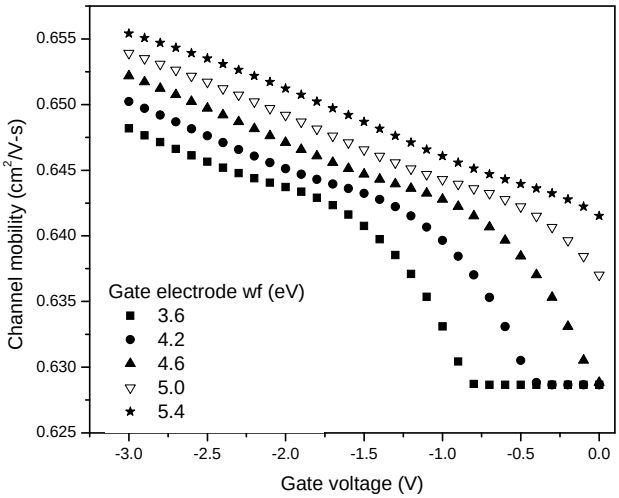

Fig. 7: Channel mobility vs gate voltage for different gate electrode work functions

To study the variation of the channel parameters the channel from the source to the drain, we have extracted the channel potential at -3V gate and drain voltages at different points along the channel. From the potential plots (Fig. 8), we can observe two important observations such as the voltage drop at the interface between the source drain electrodes and the polymer; and the nonlinearity of the channel potential. The voltage drop between the interface electrode and the semiconductor indicates a contact resistance due to different work functions plus the bulk

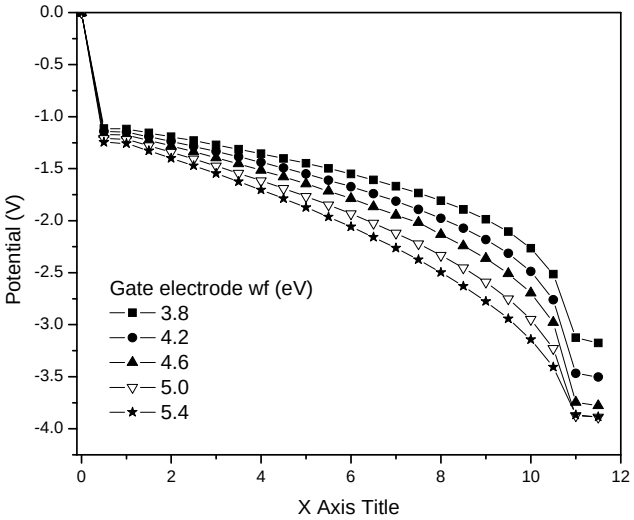

Fig. 8: Channel potential at different positions along the channel from source to drain for different gate electrode work functions

resistance of pentacene between the channel and the electrode [30]. This is attributed to low mobility or depletion near the contacts and Schottky barriers at the contacts [31,32]. The potential profiles are clearly nonlinear as seen in the figure. The nonlinearity of the potential profile is more pronounced near the drain electrode than near the source. This is due to the fact that the relative decrease of the induced charge density in the accumulation layer when going from source to drain as well as an associated decrease of the field effect mobility [33]. In going from the source (x=0) to the drain (x=12) along the channel, the potential drops fast for higher gate electrode work function. This faster drop of potential gradient is associated with the higher channel electric field we have observed at higher gate electrode work functions.

b) Impact of gate dielectric thickness

In addition to studying the impact of the work function on the channel properties, we have simulated devices at different gate insulator thicknesses to study its effect on channel field, channel charge concentration, threshold voltage, and channel charge mobility. As shown in Fig. 9 a, the field increases as the thickness of the dielectric decreases and this increase in field increases the charge accumulation in the channel (Fig. 9 b). However we haven't seen variation of the threshold voltage with thickness of the dielectric. This is because there is no variation of the flat band voltage, interface traps and charges as a function of the dielectric thickness. Fixed charge in the dielectric has not been included in our simulation model.

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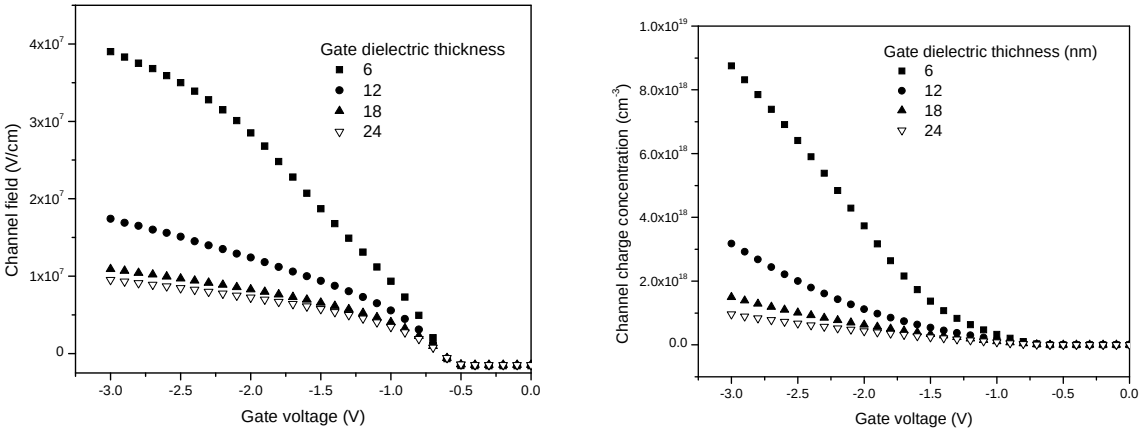

(a) (b)

Fig. 9: a) Electric field (a) and Channel charge concentration (b) probed at insulator/pentacene interface at different gate electrodes but same gate voltage (-3 V)

The change in the thickness of the dielectric has also brought the change in the channel field effect mobility. Fig. 10 shows that the mobility variation with gate voltage and thickness of the dielectric. The mobility increases as a function of electric field only up to a little over the threshold voltage. After the channel is fully formed, the mobility starts to drop as the gate voltage increases to a more negative value. The drop is significant for lower dielectric thicknesses. Increasing the gate voltage increases both the electric field and the channel charge concentration.

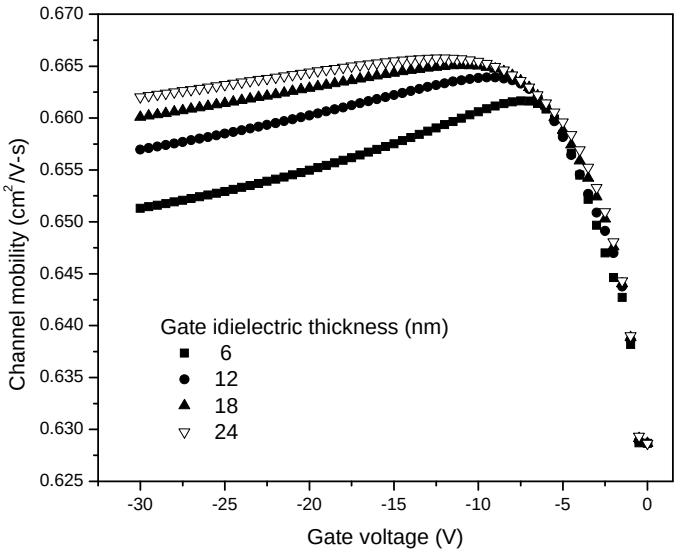

Fig. 10: Channel mobility vs gate voltage for different gate dielectric thicknesses

We have also shown this by simulating the device at a gate voltage of -3 V and dielectric thickness of 6 nm for various values of dielectric constant. The extracted mobility versus channel charge density is shown in Fig. 11. The figure shows an increase of mobility with channel charge density. So the decrease in mobility we observed in Fig. 10 at more negative gate voltages, with the decrease in dielectric thickness, should be from the high electric field strength. This is because the lower the dielectric thickness the higher the field and the higher the impact on mobility.

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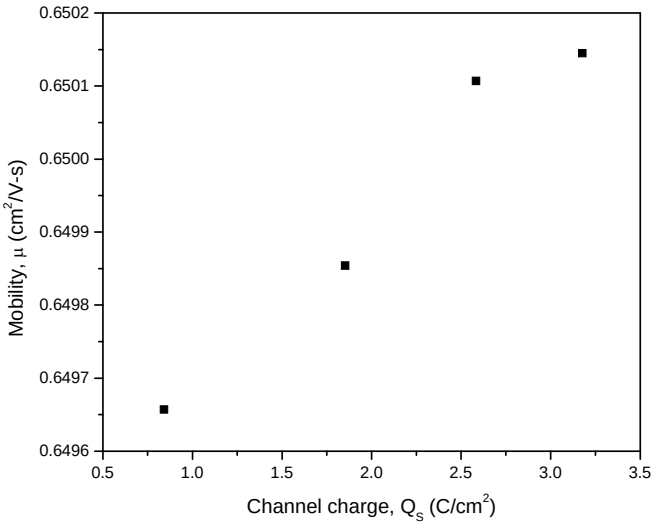

Fig. 11: Channel mobility vs channel charge concentration

IV. Conclusion

In summary, our simulation results show an impact of the gate metal work function and the gate dielectric thickness on channel field, channel potential, channel charge concentration, and mobility of the device. When the high work function gate electrode is used, there exists a built in field in the transistor channel. As the result there exist built in channel charge concentration and increased channel mobility at zero gate voltage. As expected, when the gate insulator thickness decreases the vertical electric field and the channel charge density increases. This increase in field and charge concentration slightly increases the mobility and the drain current. The field effect mobility decreases as the thickness of the dielectric decreases. The threshold voltage changes with gate electrode work function but remains the same when the thickness of the dielectric changes. The threshold voltage has changed from -1.3 V to -0.07 V by changing the work function from 3.8 eV to 5.4 eV. We also have seen a potential drop at the electrode/polymer interface and a nonlinear decrease in potential from source to drain.

V. Acknowledgments

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