TCAD Simulation and Compact Modeling of Organic Thin Film Transistors (OTFTs) for Circuit Simulation

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Abstract: In this paper we present TCAD simulation and compact modeling of OTFTs. Finite element method (FEM) based numerical simulations have been performed using density of state model and field dependent mobility model to simulate the electrical behavior of the OTFT devices. Further Universal Organic Thin Film Transistor (UOTFT) compact model has been applied for simulating the DC I-V characteristics of the device using device modeling software UTMOST-IV. TCAD simulated characteristics and compact model based simulated characteristics were compared and contrasted. Device model parameters were extracted using UOTFT model. Extracted model is applied in designing the OTFT based PMOS-like inverter and hybrid operational amplifier.

Keywords: Organic Thin Film Transistor (OTFT), Tecnology computer aided design (TCAD), Simulation, and Hybrid operational amplifier.

1. INTRODUCTION

For the last few decades flexible and transparent electronics have been studied. A key element for flexible and transparent electronics is thin-film transistor as it has wide range of responsibilities. It also has the advantage of light weight, flexibility, low cost and transparency. This technology has the opportunity to introduce the new materials, which add new mechanical properties to products, also improve the electrical performance as well as simplifying the integration process. Moreover, the cost of these devices is kept low due to the innovative use of newly created or adapted processes for large-area and flexible substrates. Typically, large-area polymeric substrates such as polypropylene (PP) or polyethylene terephthalate (PET) are used. With the advent of organic thin film transistors (OTFTs) as one of the key components of various electronic and optoelectronic applications, recent advances in organic electronics have caused researchers to refocus [1-14]. Researchers from academia and industry are considering this area as key research topic for future flexible electronics [8-11]. In this article we present numerical simulation and a simple and efficient compact modeling for organic thin film transistor (OTFT) which is useful for future flexible electronics and display applications.

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2. NUMERICAL SIMULATIONS

Since systematic cost of experimental investigation of any technology is high and it takes a lot of time therefore technology computer aided design (TCAD) is becoming very important tool to evaluate any technology. In this work TCAD simulation of pentacene based OTFT and amorphous silicon based OTFT have been performed. The pentacene based OTFT structure under consideration is shown in Figure **1** for which simulations have been performed using device simulation software ATLAS™ from Silvaco Inc. The pentacene acts as channel and its thickness is 50nm and SiO2 acts as gate dielectric and its thickness is 400nm. The Au is used for source and drain and heavily doped silicon behaves as gate. Initially physical structure of the bottom gate top contact OTFT device has been created. Further material parameters of the pentacene were defined and numerical computations have been carried out using density of states model and field dependent mobility model along with the drift diffusion model.

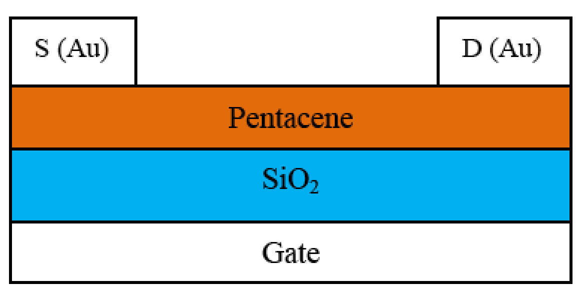

Figure 1: Structure of pentacene based OTFT.

For obtaining terminal characteristics of OTFTs fundamental equations responsible for charge transport in semiconductor devices have been solved with the help of ATLAS [8-10]

$$div\left(\varepsilon\nabla\Psi\right) = -\rho \tag{1}$$

$$\frac{\partial n}{\partial t} = \frac{1}{q} div \vec{J}_n + G_n - R_n \tag{2}$$

$$\frac{\partial p}{\partial t} = \frac{1}{q} div \vec{J}_p + G_p - R_p \tag{3}$$

Where symbols have their usual meaning.

The drift- diffusion model is given by

$$\vec{J}_n = qn\mu_n \overrightarrow{E_n} + qD_n \Delta n \tag{4}$$

$$\vec{J}_p = qp\mu_p \overrightarrow{E_p} + qD_p \Delta p \tag{5}$$

where μ=mobility, E=local electric field, and D=diffusion coefficient.

To consider the effect of trapped charge the Poisson's equation is modified by adding an additional term Q_T, as given below [8-10]

$$div\left(\varepsilon\nabla\Psi\right) = q\left(n - p - N_{tD}^{+} + N_{A}^{-}\right) - Q_T \tag{6}$$

where $Q_T == q\left(N_{tD}^{+} + N_{tA}^{-}\right)$ and $N_{tD}^{+} = density \times F_{tD}$ and $N_{tA}^{-} = density \times F_{tA}$

Here, N_{tD}^{+} and N_{tA}^{-} are ionized density of donor like trap and ionized density of accepter like traps respectively F_{tD} and F_{tA} and are probability of ionization of donor like traps and accepter like traps respectively.

The four components of density of defect states, g(E) are given as follows [8-9]

$$g_{TA}\left(E\right) = N_{TA} \exp\left[\frac{E - E_C}{W_{TA}}\right] \tag{7}$$

$$g_{TD}\left(E\right) = N_{TD} \exp\left[\frac{E_V - E}{W_{TD}}\right] \tag{8}$$

$$g_{GA}\left(E\right) = N_{GA} \exp\left[-\left[\frac{E_{GA} - E}{W_{GA}}\right]^2\right] \tag{9}$$

$$g_{GD}\left(E\right) = N_{GD} \exp\left[-\left[\frac{E - E_{GD}}{W_{GD}}\right]^2\right] \tag{10}$$

Where symbols have their usual meanings.

As pentacene in this work is a p-type semiconductor and the pentacene based OTFTs operated in the p-channel mode, we considered only the donor like states. Finally, g(E) is given as

$$g\left(E\right) = g_{TD}\left(E\right) + g_{GD}\left(E\right) \tag{11}$$

The Poole-Frenkel field dependent mobility model used in the simulations is described by equation (11) as in reference [8-10]

$$\mu\left(F\left(x\right), T\right) = \mu_o \exp\left[-\frac{\Delta}{KT_0} + \frac{\delta}{KT_0}\sqrt{F\left(x\right)}\right] \tag{12}$$

where μ_o =zero-field mobility, F =electric field intensity, Δ =activation energy δ =characteristic parameter for

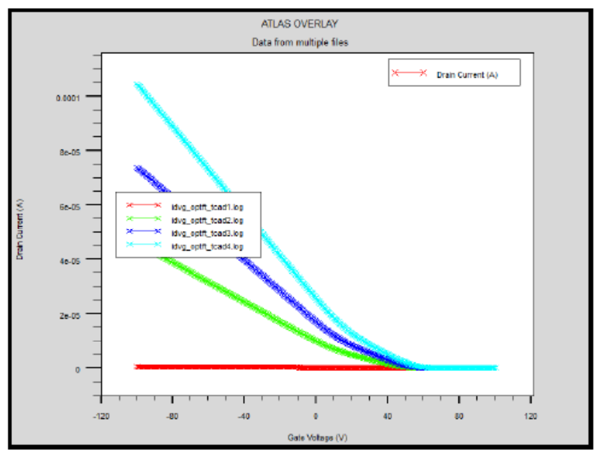

Figure 2: I_D-V_{GS} characteristics of Pentacene based TFT.

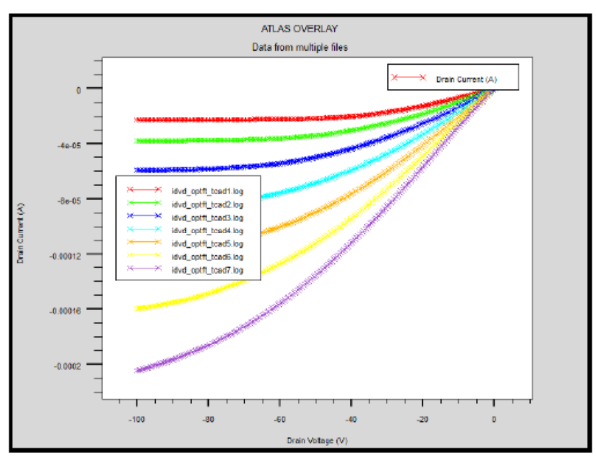

Figure 3: I_D-V_{DS} characteristics of simulated pentacene OTFT.

the field-dependence called Poole-Frenkel factor. The parameters used in simulation are given in Table **1**.

Table 1: Parameters Used in Pentacene-Based OTFT Simulation

Parameters	Values
Effective density of states in the conduction band (Nc)	2.88×10^{21} cm^3
Effective density of states in the valance band (Nv)	2.88×10^{21} cm^3
Dielectric constants (ε)	3.0
Energy gap at 300 K (Eg)	2.8 eV
N_{TD}	1.0×10^{18} cm^3/eV
W_{TD}	0.5 eV
N_{GD}	0 cm^3/eV
W_{GD}	0.15 eV
E_{GD}	0.78 eV
Accepter concentration	5.75×10^{17} cm^3
Activation energy at zero electric field for holes (deltaep.pfmob)	1.792×10^2 eV
Hole Poole–Frenkel factor (betap.pfmob)	7.758×10^5 eV(cm/V)$^{1/2}$

The simulated transfer and output characteristics of pentacene OTFT is shown in Figure **2** and Figure **3**. Further this simulated data is provided to UTMOST-IV for compact modeling.

3. COMPACT MODELING AND APPLICATION OF SPICE MODEL IN PENTACENE PTFT BASED INVERTER AND OPERATIONAL AMPLIFIER SIMULATION

Many TFT models have been reported in past [15-26]. We have used UOTFT model for spice model extraction of pentacene based OTFT. All the modeling equations can be obtained in reference [26]. The detailed explanation of the a-Si TFT and OTFT model extraction methodology can be found [15-16]. Figure **4** illustrates the output characteristics of the OTFT after optimization in UTMOST IV which is in good agreement with output characteristics of pentacene TFT obtained by numerical simulation. UOTFT model is able to reproduce the same output characteristics of OTFT as obtained from numerical simulation with mismatch error of only 1.34%. For optimization Levenberg-Marquardt algorithm was used in UTMOST IV.

The extracted spice models of the a-Si NTFT and Pentacene based PTFT are then used for circuit simulation using Gateway.

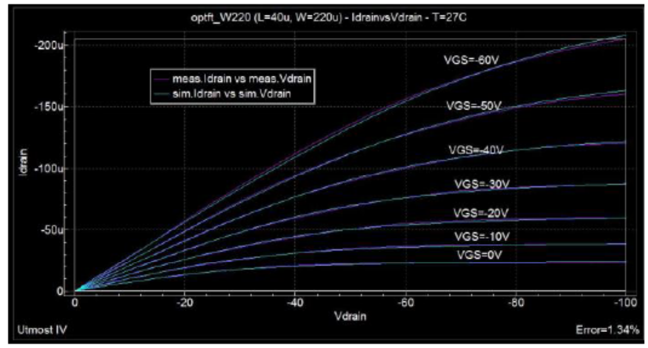

Figure 4: Output characteristics of Pentacene based TFT [9].

Circuit Simulation of Pentacene PTFT Based Inverter

Symbols for NTFT and PTFT have been created in Gateway. Figure **5** shows pentacene PTFT based inverter circuit for voltage transfer characteristics (VTC) simulation. VTC plot has been obtained with the help of extracted UOTFT model parameters for p-channel OTFT (Level=37) and extracted model parameters for n- channel A-Si TFT (Level-35). VTC plot for pentacene PTFT based inverter circuit simulated using UOTFT model parameters is shown in Figure **6**.

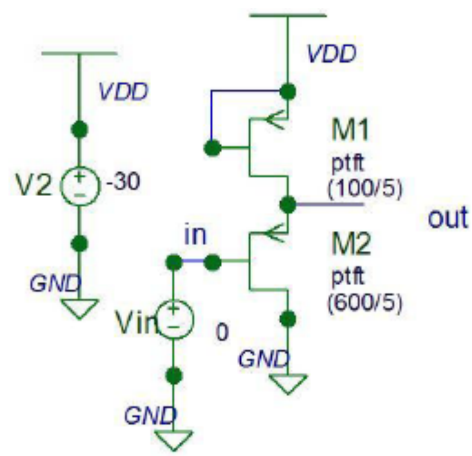

Figure 5: Pentacene PTFT based inverter circuit for VTC simulation.

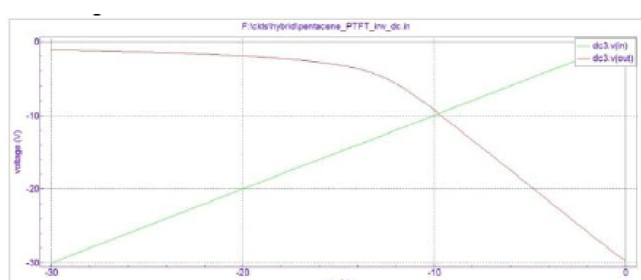

Figure 6: VTC plot for pentacene PTFT based inverter.

Circuit Simulation of Hybrid Operational Amplifier

Using the extracted model a hybrid operational amplifier has been simulated in which pentacene PTFT acts as PMOS device and A-Si NTFT acts as NMOS device. Hybrid operational amplifier circuit is shown in Figure **7** and simulated transient characteristics is shown in Figure **8**.

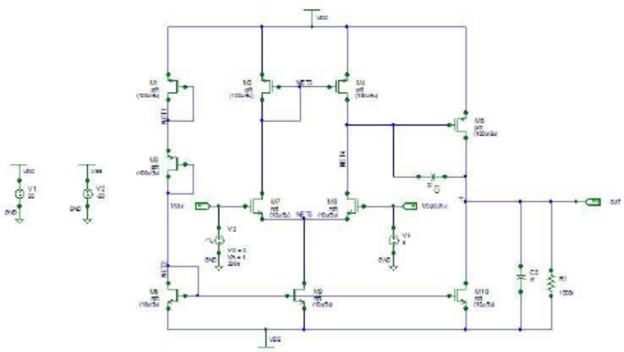

Figure7: Hybrid operational amplifier circuit.

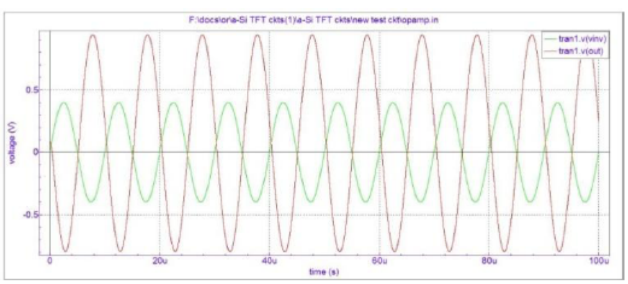

Figure 8: Input and output of hybrid operational amplifier after transient simulation.

CONCLUSIONS

In this paper we presented the technology computer aided design and simulation of pentacene based OTFT and A-Si TFT by means of 2D TCAD from Silvaco International. Compact models have been extracted for these TFTs using UTMOST-IV from Silvaco Inc. Using the extracted model, simulation of pentacene PTFT based inverter and hybrid Operational amplifier have been demonstrated successfully.

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REFERENCES

[1] Shekar BC, Lee J, Rhee S. "Organic thin film transistors: Materials, processes, and devices", Korean J Chem Engg 2004; 21(1): 267-285. https://doi.org/10.1007/BF02705409

[2] Gupta D, Katiyar M, Gupta D. "An analysis of the difference in behavior of top and bottom contact organic thin film transistors using device simulation", Org. Electron 2009; 10(5): 775-784. https://doi.org/10.1016/j.orgel.2009.03.012

[3] Cui T, Liang G. "Dual gate pentacene organic field-effect transistors based on a nanoassembled SiO2 nanoparticle thin film as the gate dielectric layer", Appl. Phys. Lett 2005; 86(6): 064102-1-064102-3. https://doi.org/10.1063/1.1861126

[4] Tate J, Rogers JA, Jones CDW, Vyas B, Murphy DW, Li W, *et al*. "Anodization and micro contact printing on electro less silver: Solution-based fabrication procedures for low-voltage electronic systems with organic active components", Langmuir 2000; 6(14): 6054-6060. https://doi.org/10.1021/la991646b

[5] Liu RL, Deng F, Yao RH, Lai PT. "Low-operating-voltage polymer thin-film transistors based on poly (3-hexylthiophene) with hafnium oxide as the gate dielectric", IEEE Trans. Device Mater. Reliab 2010; 10(2): 233-237. https://doi.org/10.1109/TDMR.2010.2042297

[6] Ortiz RP, Facchetti A, Marks TJ. "High-k organic, inorganic, and hybrid dielectrics for low-voltage organic field-effect transistors", Chem. Rev 2010; 110(1): 205-239. https://doi.org/10.1021/cr9001275

[7] Krumm J. "Printed electronics-from vision to first product", 4th European Workshop on RFID Systems and Technologies, Freiburg, Germany June 2008; 10-11.

[8] Dwivedi ADD. Rajeev Dhar Dwivedi, Raghvendra Dhar Dwivedi, Sumit Vyas and P. Chakrabarti, "Numerical simulation of P3HT based Organic Thin Film Transistors (OTFTs)" International Journal of Microelectronics and Digital integrated circuits 2015; 1(2): 13-20.

[9] Dwivedi ADD, "Numerical Simulation and Spice Modeling of Organic Thin Film Transistors (OTFTs)" International Journal of Advanced Applied Physics Research 2014; 1: 14-21. https://doi.org/10.15379/2408-977X.2014.01.02.3

[10] Pooja Kumari and Dwivedi ADD "Modeling and Simulation of Pentacene based Organic thin film transistors with Organic Gate Dielectrics. Journal of Microelectronics and Solid State Devices" 2017; 4(3): 13-18.

[11] Narendra Singh Kushwah, Dwivedi ADD "Computer Modeling of Organic Thin Film Transistors (OTFTs) using Verilog-A" Journal of Microelectronics and Solid State Devices 2018; 5(1): 1-7.

[12] Zaki T, Scheinert S, Hörselmann I, Rödel R, Letzkus F, Richter H *et al*., "Accurate capacitance modeling and characterization of organic thin-film transistors", IEEE Trans. Electr. Dev 2014; 61: 98-104. https://doi.org/10.1109/TED.2013.2292390

[13] Xiao-Hong Zhang, Shree Prakash Tiwari, Bernard Kippelen "Pentacene organic field-effect transistors with polymeric dielectric interfaces: Performance and stability", Organic Electronics 2009; 10(6): 1133-1140. https://doi.org/10.1016/j.orgel.2009.06.001

[14] Ognian Marinov, Jamal Deen M, Zschieschang Ute and Hagen Klauk, "Organic Thin-Film Transistors:Part I—Compact DC Modeling" IEEE Ttansaction on Electron Devices 2009; 56(12): 2952 - 2961. https://doi.org/10.1109/TED.2009.2033308

[15] Shur MS, Slade HC, Jacunski MD, Owusu AA and Ytterdal T. "Spice Models for Amorphous Silicon and Polysilicon Thin Film Transistors", J. Electrochemical Society 1997; 144: 2833. https://doi.org/10.1149/1.1837903

[16] Shur MS, Slade HC, Ytterdal T, Wan, Xu Z, Aflatooni K, Byun Y *et al*. "Modeling and Scaling of a-Si:H and Poly-Si Thin

Film Transistors", Material Research Society Proceedings, Amorphous and Microcrystalline Silicon Technology, 467, 1997.

[17] Benjamin Iniguez, Zheng Hu, Tor A. Fjeldly, Michael S. Shur, "Unified model for short channel poly-Si TFTs", Solid-State Electronics, 1999; 43: 1821-1831. https://doi.org/10.1016/S0038-1101(99)00142-2

[18] Dosev D, Ytterdal T, Pallares J, Marsal LF and Iniguez B. "DC SPICE Model for Nanocrystaline and Microcrystaline Silicon TFTs", IEEE Trans. Electron Device 2002; 49: 1979. https://doi.org/10.1109/TED.2002.804719

[19] Estrada M, Cerdeira A, Ortiz-Conde A, Garcia Sanches FJ and Iniguez B. "Extraction Method for polycrystaline TFT above and subthreshold model parameters", Solid-State Electronics 2002; 46: 2295. https://doi.org/10.1016/S0038-1101(02)00186-7

[20] Resendiz L, Iniguez B, Estrada M and Cerdeira A. "Modification of Amorphous Level 15 AIM SPICE Model to Include New Subthreshold Model", Proc. 24th International Conference on Microelectronics (MIEL 2004), p.291. https://doi.org/10.1109/ICMEL.2004.1314620

[21] Estrada M, Cerdeira A, Puigdollers J, Resendiz L, Pallares J, Marsal LF, Voz C and Iniguez B. "Accurate modeling and parameter extraction for organic TFTs", Solid-State Electronics 2005; 49: 1009. https://doi.org/10.1016/j.sse.2005.02.004

[22] Fjeldly A, Ytterdal T, Shur M. "Introduction to Device Modeling and Circuit Simulation", John Wiley & Sons, Inc., New York, 1998.

[23] Iniguez B, Picos R, Veksler D, Koudymov A, Shur MS, Ytterdal T, Jackson W. "Universal Compact Model for Long- and Short-Channel Thin-Film Transistors", Solid- State Electronics 2008; 52: 400. https://doi.org/10.1016/j.sse.2007.10.027

[24] Estrada M, Cerdeira A, Puigdollers J, Resendiz L, Pallares J, Marsal LF, Voz C and I-inguez B. "Accurate modeling and parameter extraction for organic TFTs", Solid-State Electronics 2005; 49: 1009. https://doi.org/10.1016/j.sse.2005.02.004

[25] Vissenberg MCJM, Matters M. "Theory of the Field-Effect Mobility in Amorphous Organic Transistors", Physical Review B 1998; 57: 12964. https://doi.org/10.1103/PhysRevB.57.12964

[26] UTMOST IV Spice models manual, Silvaco International, Santa Clara, CA, USA 2018.

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http://dx.doi.org/10.15379/2408-977X.2019.06.01.01