Simulation Standard

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Two-Dimensional *ATLAS* Device Simulation of Pentacene Organic Thin-film Transistors

1. Introduction

Recent years has seen rapid acceleration in the research and development of organic thin film transistors (OTFTs) as key components for active matrix displays, radio frequency identification tags, and many other small scale integrated circuits. There are many advantages to OTFTs, such as the flexibility of the plastic fabrication substrate and the potential cost savings to manufacturers that adopt a solution process and / or ink-jet printing process.

One of the most widely studied organic semiconductor materials used for OTFTs is Pentacene. Pentacene-based OTFTs have a typical field effect mobility of around 1 [cm^2 / (V sec)]. This is of comparable value to hydrogenated amorphous silicon. OTFTs on lightweight flexible substrates are expected to eventually replace hydrogenated amorphous silicon TFT applications on glass substrates.

As need to understand basic device operation, to optimize device structures, and to consider novel device structures grows, the importance of numerical device simulation is rising as well.

2. The Device Structure and Models

In order to simulate I-V characteristics of OTFTs, it is important to consider how carrier transport in organic semiconductors is described. In many cases, the space-charge limited current (SCLC) model is successful in explaining the conduction current of organic semiconductors. This is especially true in devices such as organic light-emitting diodes (OLEDs) and OTFTs. Fortunately, the SCLC model is suited for use in conjunction with more conventional carrier drift and diffusion type device simulators like ***ATLAS***.

In the SCLC model, the carriers are self-trapped. In addition, one of the most determinant factors for carrier transport characteristics are the energy distributions of density of states (DOS) within the bandgap. The TFT module in ***ATLAS*** is able to define these density of state distributions.

In this article, a Pentacene TFT reported by Lin, et al. [1] is simulated with ***ATLAS*** and then compared to their experimental ID-VD curves.

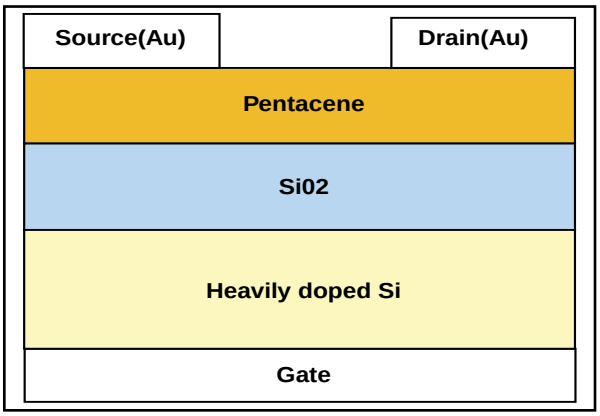

Figure 1. A cross-section of a pentacene organic thin-film transistor.

The device structure is shown in Figure 1. A staggered inverted structure is adopted. The thickness of the oxide layer is 400 [nm] and the Pentacene active layer is 50[nm]. The channel length and width are 20 [um] and 220 [um], respectively. The extracted field-effect mobility is 0.62 [cm2 / (Vsec)].

For the purpose of numerical simulation, the energy band gap of Pentacene is defined 2.8 [eV] from an optical bandgap data of Pentacene [2]. Figure 2 shows energy distribution of DOSs assumed. The acceptor tail DOS is important and is expressed by an exponential function of energy.

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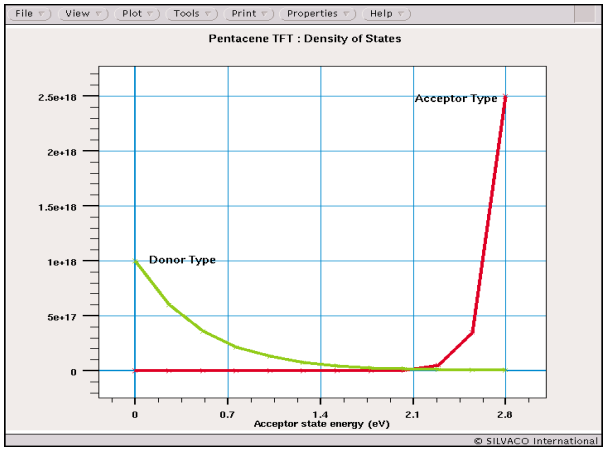

Figure 2. Energy distribution and DOS used within the ***ATLAS*** simulations.

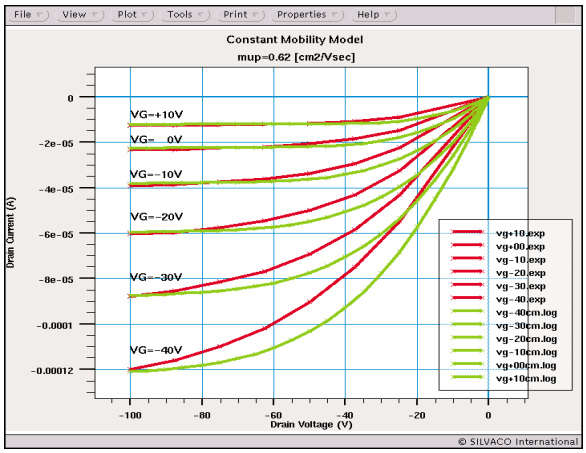

Figure 3. Simulated (green) ID-VD curves using a constant mobility model and the experimental (red) curve.

3. Simulation Results and Discussion

Figure 3 shows the simulation results (green lines) compared with the experimental data (red lines). The gate bias-dependent saturation drain currents appear to agree with the experiment, but the currents in transition regions, from linear to saturate, are still different.

Though a constant mobility model is used in the case illustrated in Figure 3, most organic semiconductor materials have electric field-dependent carrier drift mobility. An often-used mobility model has the square root dependence of a Pool-Frenkel electric field. Such mobility is expressed as the following:.

$$\mu = \mu_0 \exp\left(-\frac{E_0}{k_B T}\right)\exp\left[\sqrt{E}\left(\frac{\beta}{T}-\gamma\right)\right]$$

Where β and γ are fitting parameters. User defined mobility models are easily consolidated into ***ATLAS*** by means of the ***ATLAS C-Interpreter*** option module. Figure 4 shows the results of using this mobility model. The results agree with the experimental data.

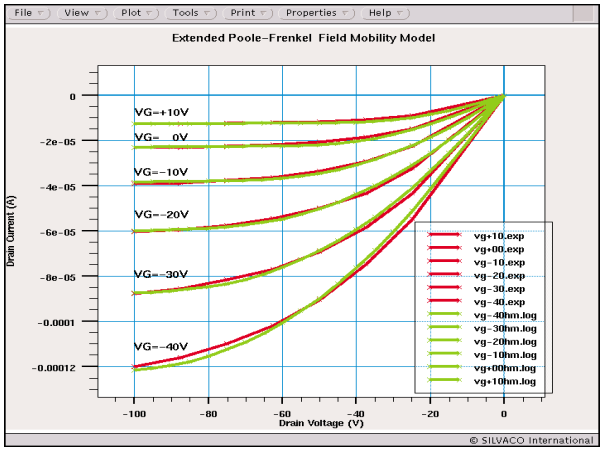

Figure 4. Simulated ID-VD (green) curves using field dependent mobility model and the experimental (red) curves.

Figure 5 shows a hole concentration distribution and current flow lines at VD=-100V and VG=-40V. This illustrates basic device operation and the evaluation of physical quantities in the device.

4. Conclusion

The experimental ID-VD curve of a Pentacene OTFT is numerically well simulated by ***ATLAS*** using the SCLC model and a field-dependent mobility model. These numerical simulations are helpful in understanding OTFT's basic device operation, an accurate physical quantity evaluation, and the optimization of device structures.

References

[1] Y.Lin, D.J.Gundlach, S.F.Nelson, and T.N.Jackson, IEEE ED., Vol.44, No.8, 1325(1997).

[2] I,Kymissis, C.D.Dimitrakopoulos, and S.Purushothaman, IEEE ED., Vol.48, No,6, 1060(2001).

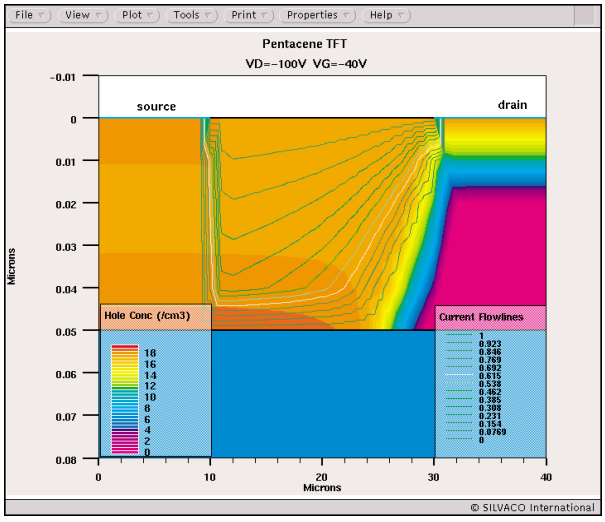

Figure 5. Hole concentration distribution and current flow lines in the OTFT device.