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Traps density and temperature effects on the performance of organic rectifying diode based on pentacene

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ABSTRACT

In this paper, we present an approach to determinate the traps density in pentacene semiconductor. The influences of both traps distribution (exponential, gaussian) and temper-ature have been investigated. The defects density associated with pentacene was extracted by fitting the simulated and experimental curves. Current-voltage characteristics are performed using a physically based device simulator. Simulation results show a good agreement with experimental.

1. Introduction

Recently, organic semiconductors have received a great interest for their low-cost manufacturing, easy processing and Flexible property [1], which make them promising for divers electronic applications.

such as solar cells [2], Light-Emitting Diode [3] and organic field-effect transistor [4]. In addition, another important application is organic rectifying diodes used in radio-frequency identification tags (RFID) to convert an alternating current (AC) into a direct current (DC) [5].

Pentacene, belonging to the polyacenes family, is one of the most organic semiconductor used widely.

for fabrication of organic devices, in particular organic rectifying diode operates in high frequency [6,7]. However, most intrinsic organic semiconductors present a significant defects which can affect the performances of devices.

In this context, the present study aimed to investigate the influences of traps density and temperature on electrical behavior of an organic device via numerical simulation using Technology Computer Aided Design (TCAD) software. Furthermore, simulation is used to extract the density of traps through comparison between simulated and experimental I-V characteristics. The device under study consist of two organic thin layers sandwiched between two metallic contacts, A good agreement with experiment results, reported in Ref. [8], was found.

2. Device structure

The device under investigation, shown in Fig. 1 is based on two organic layers: 160 nm of Pentacene followed by 30 nm of PEDOT:PSS (Poly (3,4 ethylenedioxythiophene): poly (styrene-sulfonate))), sandwiched between an anode (gold) and cathode (aluminum) electrodes. The area of this structure was fixed as 170 μm × 10 μm.

The deposition of PEDOT:PSS thin layer is known to provide a qualified electron injection between gold electrode (Au) and pentacene layer.

Table 1 summarizes the main physical parameters of pentacene, PEDOT:PSS and electrodes used in electrical simulation.

The energy diagram of our organic diode is shown in Fig. 2. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of pentacene are, respectively, at about 5 and 3 eV from the vacuum level and the work functions of gold

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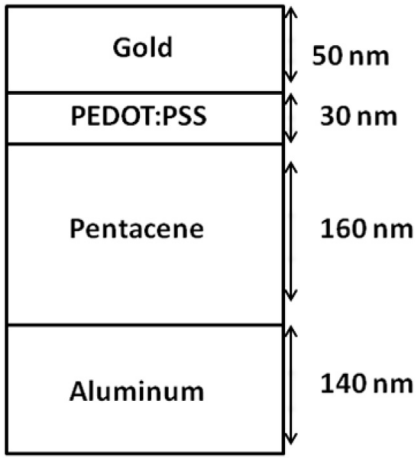

Fig. 1. Schematic devise structure.

Table 1
Main physical parameters of materials.

Materials	Parameter	Value	Unite
Pentacene	Affinity	3	eV
	Band gap	2	eV
	Density of conduction Band	10^{21}	cm^{-3}
	Permittivity	3	
	Density of valence Band	10^{21}	cm^{-3}
Aluminum	Work function	4.2	eV
Gold	Work function	5.1	eV
Pedot:pss	Work function	5	eV

(Au), PEDOT:PSS and aluminum (Al) are around 5.1, 5, and 4.2 eV, respectively, which are the reported values in the literature [9,10].

With low energy barrier from pentacene HOMO, PEDOT:PSS and gold work function the holes carriers will be injected easily into pentacene when forward bias is applied while, holes are difficulty injected from aluminum electrode to pentacene layer when diode is in reverse bias.

2.1. Equations and physicals models

2.1.1. Basic equations

Numerical simulation can be very helpful to reduce experimental characterization cost and to predict the electrical characteristics. In this context, current-voltage (I–V) simulation have been made by solving Poisson's equation relates variations in the electrostatic potential to the space charge density, continuity equations for charge carrier and drift-diffusion model derived from the Boltzmann transport equation.

These equations are given below:

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

where Ψ is the electrostatic potential, ε is the local permittivity, and ρ is the local space charge density. The reference potential can be defined in various ways. The local space charge density is the sum of contributions from all mobile and fixed charges, including electrons, holes, and ionized impurities.

$$\frac{\partial n}{\partial t} = \frac{1}{q}\mathrm{div}\,\vec{Jn} + Gn - Rn \tag{2}$$

$$\frac{\partial p}{\partial t} = \frac{1}{q}\mathrm{div}\,\vec{Jp} + Gp - Rp \tag{3}$$

where n and p are the electron and hole concen-tration, $\vec{Jn}$ and $\vec{Jp}$ are the electron and hole current densitie, *Gn* and *Gp* are the generation rates for electrons and holes, *Rn* and *Rp* are the recombination rates for electrons and holes, and q is the magnitude of the charge on an electron.

$$\overrightarrow{Jn} = qn\mu n\ \vec{E} + \ qDn\ \Delta n \tag{4}$$

$$\vec{Jp} = qp\mu p\ \vec{E} + \ qDp\ \Delta p \tag{5}$$

where q is used to indicate the absolute value of the electronic charge, $\vec{E}$ the electric field, μ_n and μ_p are electron and hole motilities, n and p are the electron and hole concentrations.

D_n and D_p are Einstein diffusion constants expressed as follow:

$$Dn = \mu n\ \ \frac{k\,T}{q} \tag{6}$$

$$Dp = \mu p\ \ \frac{k\,T}{q} \tag{7}$$

where k is Boltzmann's constant and T is the temperature.

2.1.2. Poole frenkel mobility

In most organic materials mobility depends strongly on electric fields, mobility increase with increasing electric field, this relationship can be presented by the Poole-Frenkel equation as follow:

$$\mu(E) = \mu 0\ \ \exp\left[-\ \frac{\Delta}{kT} + \left(\frac{\beta}{kT} - \alpha \right)\sqrt{E} \right] \tag{8}$$

where $\mu(E)$ is the Poole-Frenkel mobility, μ_0 the zero field mobility, Δ the activation energy at zero electric field, E, k, T and β are, respectively, the electric field, boltzmann constant, temperature, and hole Poole-Frenkel factor and α is used as a fitting parameter.

2.1.3. Defect model

In organic semiconductors the energetic distribution of traps is generally defined as an Exponential eq. (9) or Gaussian eq. (10) density of states (DOS) near the transport band edges.

$$GD(E)\ = \frac{Nt}{kTc}\ \exp\left[\frac{Ev\ - E}{kTc}\right] \tag{9}$$

where, N_t is the total density of traps, E the energy, E_v the energy of the valence band edge, k the boltzmann constant and Tc the

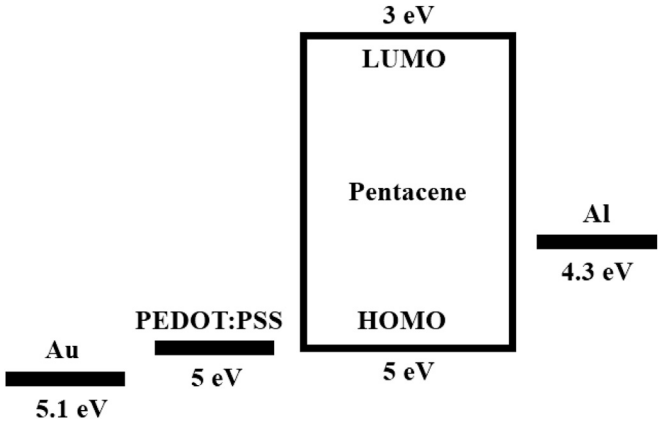

Fig. 2. Schematic of energy diagram.

characteristic temperature.

$$GD(E) = \frac{NID}{\sqrt{2\pi}\ \sigma}\exp\left[\frac{(Ev - E)^2}{2\,\sigma^2}\right] \quad (10)$$

where, NID is the total density of traps and σ is the gaussian width traps.

The trapped state concentration is given by the following equation:

$$PD = \int_{Ev}^{Ec} GD(E)\ \ ftD(E, n, p)dE \quad (11)$$

where f_{tD} (E,n,p) is the donor probability of occupation.

The Probability of occupation is defined by:

$$ftD = \frac{vp\ SIGDH.p + vn\ SIGDE\ ni\ exp\left(\frac{E-Ei}{kT}\right)}{vn\ SIGDE\left(n + niexp\left[\frac{E-Ei}{kT}\right]\right) + vp\ SIGDH\left(p + ni\ exp\left[\frac{Ei-E}{kT}\right]\right)} \quad (12)$$

where v_n is the electron thermal velocity, v_p the hole thermal velocity, n_i the intrinsic carrier concentration, the hole concentration, SIGDE and SIGDH are the donor electron and hole capture cross sections.

3. Results and discussions

Simulators based on analytical model have been showed an exceptional efficiency in characterize-ation and optimization of devices before an actual fabrication as well as in validation and extraction of parameters. In this respect a two-dimensional numerical simulation of an organic diode, shown in Fig. 1, based on pentacene semiconductor was carried out using ATLAS software.

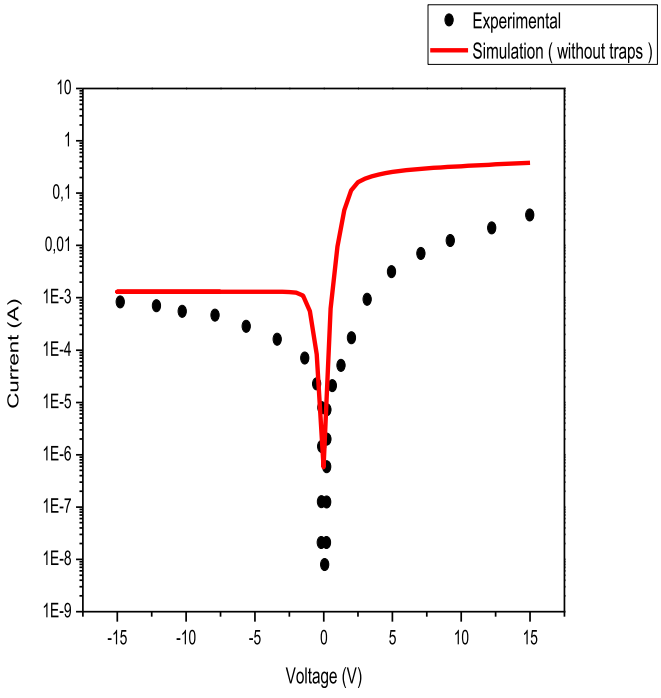

Fig. 3. Comparison between simulation (without traps) and experimental I-V characteristics.

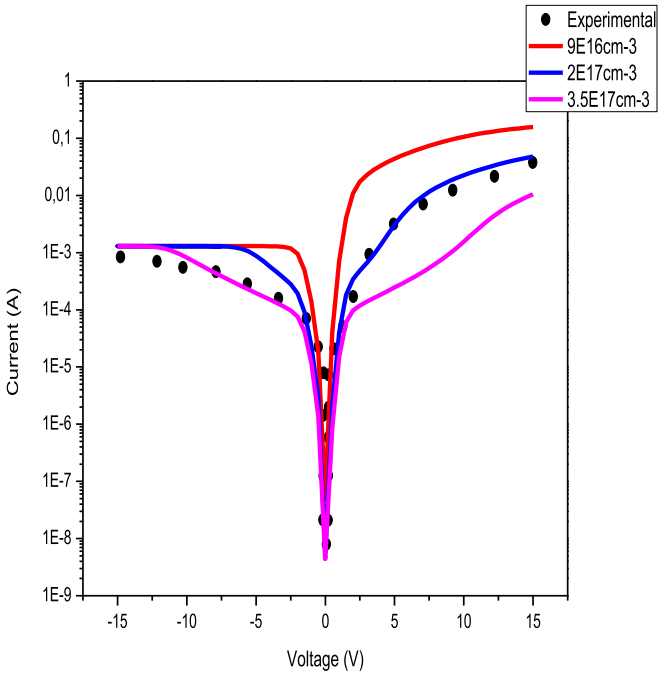

Fig. 4. Effect of exponential traps density on I-V characteristics.

3.1. Trap dependence

In order to validate the structure simulated, traps density of pentacene has been inserted into simulation to fit the experimental results reported in literature [8], The simulated current-voltage curve without traps is shown in Fig. 3 and compared with I-V character-istic find experimentally.

Fig. 4 and Fig. 5 presents the semi logarithmic plots of simulated and experimental I-V curves as function of traps concentrations for exponential and gaussian trap distribution. As expected, by increase-ing traps density current decrease.

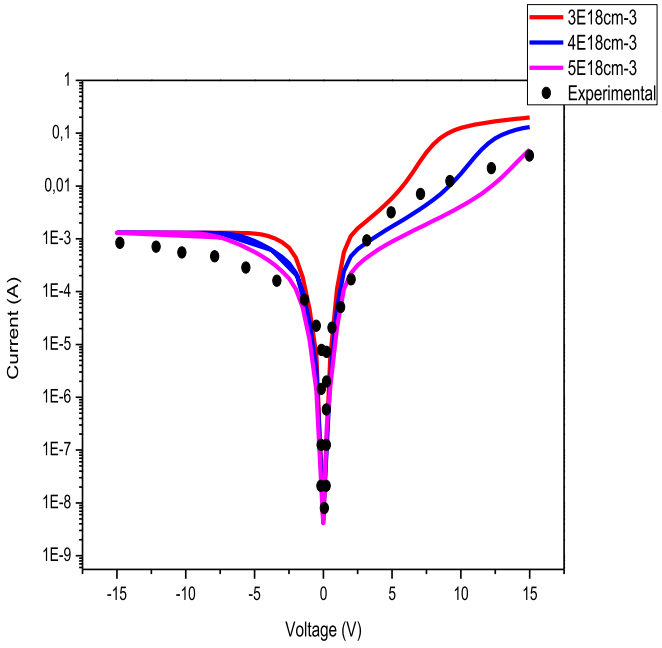

Fig. 5. Effect of gaussian traps density on I-V characteristics.

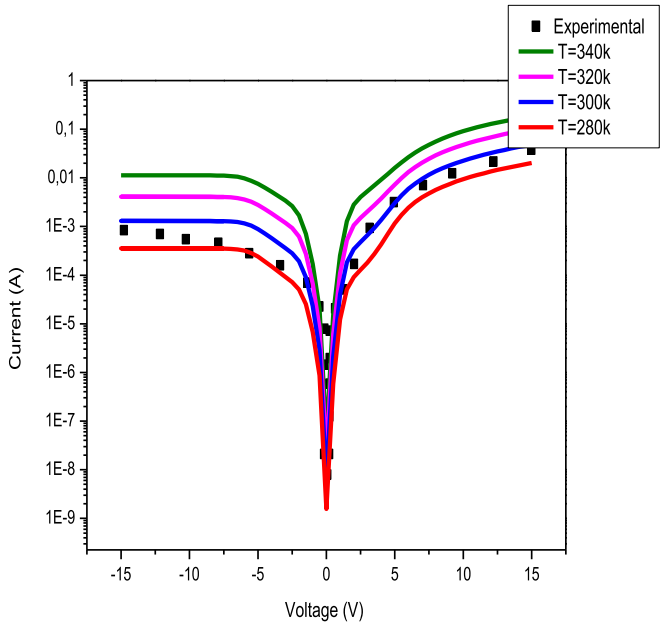

Fig. 6. Effect of temperature on Current–voltage characteristics.

Traps within most organic semiconductors are caused by structural defects or chemical impurities.

At high traps density, the majority of charges carriers are trapped which reducing considerably the current. However at low traps density, only a portion of the carriers are necessary to fill all the traps and the others participate in conduction which increasing the current.

We note that the best agreement between the simulated and experimental I–V characteristics has been obtained for an exponential trap distribution with a density equal to 2.10^{17} cm^{-3} which close to other experimental results [11].

In literature, many researchers propose an exponential trap distribution in organic diode based on pentacene [12], which is in good agreement with our work as can be seen by comparing Figs. 4 and 5, which are the simulated curves with exponential and gaussian trap distribution, respect-tively.

Simulation shows that with an exponential trap distribution, simulated curves fit better, with exper-imental data, than. gaussian trap distribution.

3.2. Temperature dependence

The forward and reverse bias I-V characteristics of Al/pentacene/PEDOT:PSS/Au structure measured at different temperatures are summarized in Fig. 6. obviously, similar to those reported in Ref. [13], the curves was influenced by changing temperature, current increases as temperature increases.

By increasing temperature, charge carriers trapped will be thermally released from its traps states. These freed carriers will directly participate in conduction mechanism which will generate an increasing in current.

The increase of the current with temperature not just caused by thermally released trapped charges, it is also caused by the increase of the Pool-Frenkel mobility. Indeed, Mobilities are taken to be field dependent with the Poole Frenkel effect and by the presence of an electric field, trap barrier decreases, making it easier for carriers to escape the trap by thermal emission, Consequently, carriers number responsible for enhancing the current is increased and the Pool-Frenkel mobility in pentacene can be enhanced.

Higher temperatures enhance transport by affording the energy needed to overcome the trap.

4. Conclusion

In summary, an organic diode, based on pentacene semiconductor, have been simulated using physic-cally based device simulator Atlas/Silvaco. The process of simulation is based on solving the differential equations describing the transport mechanism in organic semiconductor.

As a result, we proved that current is affected by pentacene traps density and temperature. Furthermore, we can state that our approach to determinate the traps density has shown great efficiency since a good agreement with experim-ental and literature was found.

Acknowledgments

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