COMPUTATIONAL RESEARCH PROGRESS IN APPLIED SCIENCE & ENGINEERING (CRPASE)

CRPASE: TRANSACTIONS OF APPLIED SCIENCES

Journal homepage: http://www.crpase.com

CRPASE: Transactions of Applied Sciences, Vol. 06(03), 216-219, September 2020 ISSN 2423-4591

Research Article

Diffusion Currents in Hole Devices Organic Polymers Semiconductors

Muhammad Ammar Khan[1,2*], Bilal Ahmad[3], Amr S. Zalhaf[4]

[1] *Department of Physical and Numerical Science, Qurtuba University of Science & Information Technology, D.I.Khan, Pakistan*
[2] *University of Electronic Science and Technology of China, Chengdu, P.R.China.*
[3] *Department of Electrical Engineering, University of Poonch Rawalakot, AJ&K, Pakistan*
[4] *Electrical Power and Machines Engineering Department, Tanta University, Tanta 31511,Egypt.*

Keywords

Organic diode,
Mobility,
Charge transport,
Electronic devices,
New density of state (DOS).

Abstract

The transport model of improved J-V formula based on the work by Ammar and Sun[1] is now applied to hole only devices (MEH-PPV), and (PF-TAA) of different thickness with various temperatures. The obtained results are strongly agree with complete numerical solution and experimental data. From this study it is verified that this formula base charge transport model is accurate, precise, and covers a large number of materials. These theoretical result are opening an interesting prospects in near future.

1. Introduction

Charge transport models developed for disordered organic semiconductors[2]-[4], and semiconductor is inserted between two metal electrodes is called a MIM (metal-insulator-metal) diode. The MIM diodes are typically fabricated from aluminum, chromium, and niobium. These types of diodes are used for the rectification of high frequency electromagnetic radiation, the development of nantenna, and MIM-TFD technology. The current in organic diodes is space charge limited (SCL)[1]. We are very familiar that space charge limited current in organic polymers MIMs diode can be described by solving drift-diffusion equations by using formulae of density dependent mobility in exponential density of states. We have observed in literature[5], the description of diffusion current for insulators in MIM diodes in which mobility has been taken as constant, which is not suitable for wide voltage ranges. When mobility is taken as a constant these equations are difficult to solve.

Different theories and models [6-15] have been developed, which is used to describe the carrier transport in organic semiconductor, and space charge limited (SCL). A new density of state (DOS) mobility model with non-degenerate holes and degenerate trapped holes is proposed and verified by Ammar et al [8]. The results show that the new DOS is far better than the Gaussian DOS. Some of exponential models [16-18] gives good description for typical diodes as compare to model of Bruyn et al [5] in which mobility has been taken as constant.

2. Mathematical Description

We have drift-diffusion equation for holes as

$$J_p(x) = -q\mu_p(x)p(x)\frac{\partial\varphi}{\partial x} - KT\mu_p(x)\frac{\partial p(x)}{\partial x} \qquad (1)$$

Applying bounderies [5], [11] non-symmetric contacts with low and high potential to devices $P(l)=N_f\ exp\ (-V_l/KT)$, $P(h)=N_f\ exp\ (-V_h/KT)$. Taking the value of band-bending parameter in Bruyn et al[5] approximation and with Poisson equation [6-8],[10],[11], the diffusion current with built potential V_{lh} is given by

$$b = \frac{KT}{q}\left[ln\left(\frac{q^2N_vL^2}{2KT\varepsilon}\right)-2\right] \qquad (2)$$

$$J = \frac{qN_v\mu(V_{lh}-V)\left[exp\left(\frac{qV}{KT}\right)-1\right]}{Lexp\left(\frac{qb}{KT}\right)\left[exp\left(\frac{qV_{lh}}{KT}\right)-exp\left(\frac{qV}{KT}\right)\right]} \qquad (3)$$

So the complete equation for drift diffusion current for hole and electrons devices with the

---

[*] Corresponding Author: Muhammad Ammar Khan
E-mail address: ammarkhan18@yahoo.com

Received: 12 May 2020; Revised: 10 June 2020; Accepted: 14 June 2020

Please cite this article as: M. A. Khan, B. Ahmad, A.S. Zalhaf, Diffusion Currents in Hole Devices Organic Polymers Semiconductors, Computational Research Progress in Applied Science & Engineering, CRPASE: Transactions of Applied Sciences 6 (2020) 216–219.

extension of parameter γ which is the linear dependence between γ, and $1/T$ is

$$\gamma = B\left(\frac{1}{K_BT} - \frac{1}{K_BT_0}\right) \tag{4}$$

$$J_p = \frac{qN_f\mu_p(0)(V-V_{th})\left[\exp\left(\frac{qV}{KT}\right)-1\right]\exp\left[\gamma\sqrt{\frac{V-V_{th}}{L}}\right]}{L\exp\left(\frac{qb}{KT}\right)\left[\exp\left(\frac{qV_{th}}{KT}\right)-\exp\left(\frac{qV}{KT}\right)\right]} \tag{5}$$

Moreover in this case E_F-E_v>>kT, trapped charge, and free charge treated as degenerate, and non-degenerate respectively. E_v is the center energy, and E_f is the quasi-Fermi energy which satisfy the non-degenerate condition. So the density of holes is

$$n = N_0 exp\left[\frac{E_v - E_f}{KT}\right] exp\left[\frac{\sigma^2}{2K^2T^2}\right] exp\left[\frac{-q\varphi(x)}{KT}\right] \tag{6}$$

The thermally activated behavior[17] as

$$\mu(0) = \mu_0 \exp\left(\frac{-\Delta}{K_BT}\right) \tag{7}$$

And the analytic expression for the mobility at zero field[1] is given below

$$\mu_p(F) = \mu_p(0)\exp\left(\gamma\sqrt{F}\right) \tag{8}$$

3. Application to Device

Eq. (5) based transpose model apply to poly(2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene)(MEH-PPV) diode with thickness 100nm[19] at different temperatures. From Eq. (1) and Eq. (5), we analysis the numerical solutions and then calculated the J-V curves. The excellent agreement between the theoretical results and experimental data as depicted in Figure 1.

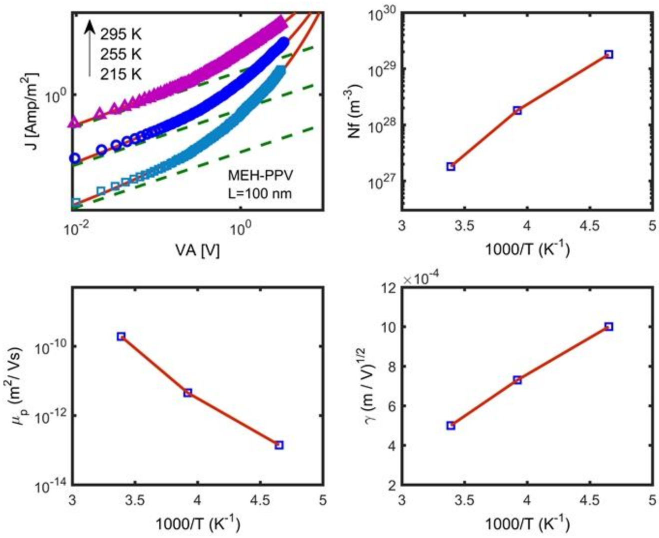

Figure 1. (color online) Comparison of calculated J-V curves by using modified model with experimental data[19] for MEH-PPV) diode with 100 nm thickness of organic layer at three different temperature. (solid lines: $\gamma\neq0$; dashed lines: $\gamma=0$), and Variations of $\gamma(T)$, $Nf(T)$, & $\mu_p(0)$, with temperature lines are smoothed curves by using (4) , (6), (7) respectively.

By using Eq. (6), the variations of $N_f = N_0 exp\left[\frac{E_v-E_f}{KT}\right] exp\left[\frac{\sigma^2}{2K^2T^2}\right]$ with temperature has been analyzed here with optimized points, and also show variations of parameters μp by Eq. (7), and γ with temperature by Eq. (4) in Figure 1.

This mobility model also apply to poly(fluorene-triarylamine) FP-TAA with different layer thicknesses at 170K. The comparison of theoretical results with experimental data as depicted in Figure 2 is an excellent agreement. Figures 1, and 2 also indicate the importance of parameter γ in Eq. (5) data at low and high voltage. When taking the value of γ as zero, then calculated curves and the experimental points are not agree with each other. This means that γ plays an important role in excellent fittings for J-V curves.

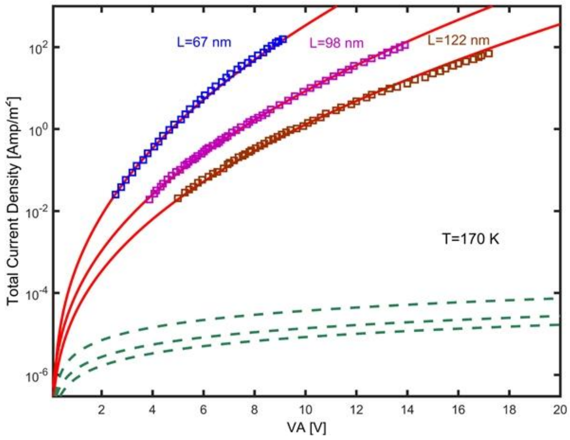

Figure 2. (color online) Comparison of calculated J-V curves with experimental data[20][21]for hole-only J(V) curves for poly(fluorene-triarylamine) PF-TAA based devices copolymer different layer thicknesses at 170 K (solid lines: $\gamma\neq0$; dashed lines: $\gamma=0$).

The potential barriers for materials (MEH-PPV), and (FP-TAA at different thickness) are listed in table1, and Table 2 respectively which shows that $V_h > V_l$. The larger value of V_h shows positive built potentials. In Table 1 we see that mobility is the increasing function of temperature which is fine and reasonable. Table 2 also represent the parameters of hole-only device poly(fluorene-triarylamine) PF-TAA at different thickness. By comparing the results of Figure 1 and Figure 2 it is clear that results obtained from improved JV formula[1] is far better than[19]-[21].

Table 1. V_l *(eV)*, V_h *(eV)* and Temperature-dependent parameters N_f, μ_p, and γ optimized by fitting J–V data for MEH hole only 100nm[19]

	V_l (eV)	V_h (eV)	T(K)	215	255	295
MEH			N_f (m^{-3})	1.8E29	1.8E28	1.8E27
(100nm)	0.286	0.288	$\mu_p(0)(m^2/Vs)$	1.4E-13	4.5E-12	1.9E-10
			$\gamma(m/V)^{1/2}$	0.001	0.00073	0.0005

Table 2. V_l *(eV)*, V_h *(eV)* and Temperature-dependent parameters with constant values of N_f, μ_p, and γ optimized by fitting J–V data for poly(fluorene-triarylamine) FP-TAA with different layer thicknesses at 170K [20][21]

	T(K)	Thickness (nm)	$\mu_p(0)(m^2/Vs)$	$\gamma(m/V)^{1/2}$	N_f (m^{-3})	V_h (eV)	V_l *(eV)*
	170	67	4.5E-8	0.00132	5.6E21	0.388	0.277
PF-TAA	170	98	4.5E-8	0.00132	5.6E21	0.305	0.286
	170	122	4.5E-8	0.00132	5.6E21	0.308	0.290

4. Conclusions

In this work, the *J-V* formula based transport model is applied to hole only devices of different thickness at different temperature. The obtained results are strongly agree with complete numerical solution and experimental data. This formula is more accurate and now it is confirm that this formula based charge transport model covers a large number of materials. We expact that this transport model also covers an electron only devices for all thickness.

Conflict of Interest Statement

The authors declare no conflict of interest.

References

[1] M. A. Khan and S. Jiu-Xun, Improved model for diffusion-limited current in organic metal-insulator-metal diodes, RSC Advances 5 (2014) 18720–18724.

[2] O. Simonetti and L. Giraudet, Transport models in disordered organic semiconductors and their application to the simulation of thin-film transistors, Polymer International 68 (2019) 620–636.

[3] N. I. Craciun, J. Wildeman, and P. W. M. Blom, Universal arrhenius temperature activated charge transport in diodes from disordered organic semiconductors, Physical Review Letters 100 (2008) 056601.

[4] W. Kaiser, T. Albes, and A. Gagliardi, Charge carrier mobility of disordered organic semiconductors with correlated energetic and spatial disorder, Physical Chemistry Chemical Physics 20 (2018) 8897–8908.

[5] P. De Bruyn, A. H. P. Van Rest, G. A. H. Wetzelaer, D. M. De Leeuw, and P. W. M. Blom, Diffusion-limited current in organic metal-insulator-metal diodes, Physical Review Letters 111 (2013) 186801

[6] C. Krellner, S. Haas, C. Goldmann, K. P. Pernstich, D. J. Gundlach, and B. Batlogg, Density of bulk trap states in organic semiconductor crystals: Discrete levels induced by oxygen in rubrene, Physical Review B - Condensed Matter and Materials Physics 75 (2007) 245115.

[7] J. Dacuña, A. Salleo, Modeling space-charge-limited currents in organic semiconductors: Extracting trap density and mobility, Physical Review B - Condensed Matter and Materials Physics 84 (2011) 195209.

[8] M. A. Khan and J. X. Sun, Improvement of mobility edge model by using new density of states with exponential tail for organic diode, Chinese Physics B, 24 (2015) 047203.

[9] S. V. Yampolskii, Y. A. Genenko, C. Melzer, and H. von Seggern, Self-consistent model of unipolar transport in organic semiconductor diodes: accounting for a realistic density-of-states distribution, Journal of Applied Physics 109 (2011) 073722.

[10] M. Z. Szymanski, I. Kulszewicz-Bajer, J. Faure-Vincent, and D. Djurado, Comparison of simulations to experiment for a detailed analysis of space-charge-limited transient current measurements in organic semiconductors, Physical Review B - Condensed Matter and Materials Physics. 85 (2012) 195205.

[11] M. A. Khan, S. Jiu-Xun, J. Ke, C. Ling-Cang, and W. Qiang, Consistent double Gaussian model with non-symmetric potential barriers at contacts for organic diodes, RSC Advances. 5 (2015) 3113–3121.

[12] M. A. Khan and S. Jiu-Xun, Modified transport model for organic diodes considering the neutral condition and two types of density of state, Chinese Journal of Physics53 (2015) 1–16.

[13] A.Y.Sosorev, Simple charge transport model for efficient search of high-mobility organic semiconductor crystals', Materials and Design 192 (2020) 108730.

[14] S. L. M. Van Mensfoort and R. Coehoorn, Effect of Gaussian disorder on the voltage dependence of the current density in sandwich-type devices based on organic semiconductors, Physical Review B - Condensed Matter and Materials Physics 78 (2008) 085207.

[15] L. Jun, S. Jiu-Xun, and C. Zhao, Improved expression of charge-carrier mobility in disordered semiconducting polymers considering dependence on temperature, electric field and charge-carrier density, Synthetic Metals 159 (2009) 1915–1921.

[16] D. H. Dunlap, P. E. Parris, and V. M. Kenkre, Charge-dipole model for the universal field dependence of mobilities in molecularly doped polymers', Physical Review Letters 77 (1996) 542–545.

[17] P. Blom, M. de Jong, and M. van Munster, Electric-field and temperature dependence of the hole mobility in poly (p-phenylene vinylene), Physical Review B - Condensed Matter and Materials Physics 55 (1997) R656–R659.

[18] C.-X. Zhou, J.-X. Sun, Z.-J. Deng, and S. Zhou, Study of applicability of Boltzmann-statistics and two mobility models for organic semiconductors, Semiconductors 47 (2013) 1351–1357.

[19] G. A. H. Wetzelaer and P. W. M. Blom, ‘Ohmic current in organic metal-insulator-metal diodes revisited’, Physical Review B - Condensed Matter and Materials Physics 89 (2014) 241201.

[20] R. Coehoorn and P. A. Bobbert, Effects of Gaussian disorder on charge carrier transport and recombination in organic semiconductors, physica status solidi (a) 209 (2012) 2354–2377.

[21] S. L. M. Van Mensfoort, S. I. E. Vulto, R. A. J. Janssen, and R. Coehoorn, ‘Hole transport in polyfluorene-based sandwich-type devices: Quantitative analysis of the role of energetic disorder’, Physical Review B - Condensed Matter and Materials Physics 78 (2008) 085208.