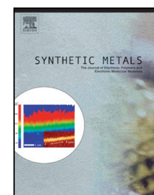
Synthetic Metals 206 (2015) 120–123

Contents lists available at ScienceDirect

Synthetic Metals

journal homepage: www.elsevier.com/locate/synmet



Electrostatic interface recombination in the system of disordered materials characterized by different permittivities

Jędrzej Szmytkowski *

Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Narutowicza 11/12, 80-233 Gdańsk, Poland

ARTICLE INFO

Article history:
Received 28 January 2015
Received in revised form 30 April 2015
Accepted 3 May 2015
Available online 26 May 2015

PACS:
72.20.Jv
72.40.+w
72.80.Le
73.50.Gr
73.50.Pz
85.65.+h

Keywords:
Disordered materials
Polymers and organics
Organic electronics
Recombination

ABSTRACT

We report on the analysis of an electrostatic interface recombination in a system consisting of disordered organic materials. This process is a consequence of the polarization effect which takes place at the interface of two phases characterized by different permittivities. In this paper, the impact of tail and deep localized states on the recombination order is demonstrated. We also discuss the influence of temperature on this process.

© 2015 Elsevier B.V. All rights reserved.

Nowadays, we observe an extensive progress of organic electronics. Electronic devices based on molecular semiconductors attract a great attention due to such attractive features like low cost production, low temperature processing, large area and flexibility. Organic photovoltaic cells (OPV), organic light emitting diodes (OLED) and organic thin-film transistors (OTFT) are typically made from at least two materials. The presence of boundaries between used compounds causes that many physical phenomena take place at the interfaces, including a recombination of charge carriers [1] and a dissociation of excitons into separated electrons and holes [2]. It is obvious that a full explanation of all interfacial effects is needed to construct more effective devices.

In general, organic semiconductors are treated as amorphous materials characterized by an energetic disorder originating from a different environment of molecules. The charge transport in such systems can be explained by hopping between disordered localized energy states [3]. The distribution of them is described by the density of states (DOS). There is a general consensus that a shape of the DOS in organic semiconductors is well modeled by a Gaussian function [4] or an exponential function [5].

In this work, we analyze an influence of the localized states at tail and deep energies on the interface recombination process which occurs at the boundary between two organic materials characterized by different dielectric constants. As to our knowledge, this problem is reported for the first time in literature.

Let us consider a system consisting of two materials characterized by permittivities ε_1 and ε_2 ($\varepsilon_1 < \varepsilon_2$). If a charge carrier e is located near the boundary between these compounds, then two image charges are induced as a consequence of the electrostatic polarization effect [6]. When we assume that e is situated in a material with lower permittivity ε_1 and taking into account a planar interface, we obtain that the first image charge $e' = e(\varepsilon_1 - \varepsilon_2)/(\varepsilon_1 + \varepsilon_2)$ is placed in a material with ε_2 and the second image charge carrier $e'' = 2e\varepsilon_2/(\varepsilon_1 + \varepsilon_2)$ is exactly in the position of e. This effect causes that e is attracted to the boundary between both phases. The interface of two different materials can be treated as a structural defect, so also as a recombination center for electrons and holes which reach the interface. Recently, we have analyzed

* Tel.: +48 583471650.
E-mail address: jedrek@mif.pg.gda.pl

http://dx.doi.org/10.1016/j.synthmet.2015.05.001
0379-6779/© 2015 Elsevier B.V. All rights reserved.

this type of recombination and derived the interface recombination coefficient in the form [7]

$$\gamma_I = \left|\frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2}\right| \frac{e\mu}{\varepsilon_0 \varepsilon_1}, \tag{1}$$

where ε_0 is a permittivity of vacuum and μ describes a mobility of charge carriers in the material with permittivity ε_1. We have demonstrated that the effect of electrostatic interface recombination is able to explain the reduced nongeminate recombination coefficient, which has been experimentally observed for organic donor–acceptor bulk heterojunction solar cells [7–9].

The recombination rate is given by [7]

$$R = \gamma_I n^2, \tag{2}$$

where n is a concentration of charge carriers. In general, a mobility of charge carriers is concentration-dependent. It gives that γ_I is also a function of n. Thus we can write the power law relation

$$R \sim n^{\delta}, \tag{3}$$

where $\delta \geq 2$. The exponent δ is called an order of recombination. If γ_I does not depend on the concentration, then δ = 2. The overall mobility for charge carriers of one sign can be defined using the Matthiessen's rule

$$\frac{1}{\mu} = \frac{1}{\mu_t} + \frac{1}{\mu_d}, \tag{4}$$

where μ_t is a tail states mobility and μ_d is a deep states mobility.

For a system with a double-exponential DOS, which is often considered for organic semiconductors, we can use analytical formulas for the mobilities μ_t and μ_d. The tail states mobility μ_t can be described by the Vissenberg–Matters equation [5]

$$\mu_t = \frac{\sigma_0}{e}\left[\frac{(T_t/T)^4 \sin(\pi(T/T_t))}{(2\alpha)^3 B_c}\right]^{(T_t/T)} n_t^{(T_t/T)-1} \tag{5}$$

and the deep states mobility is given by the formula derived by Toricelli [10]

$$\mu_d = \frac{\sigma_0}{e}\left[\frac{\pi N_t T_t^3}{(2\alpha)^3 B_c T^3}\right]^{(T_t/T)} \left[\frac{\sin(\pi(T/T_d))}{\pi(T/T_d) N_d}\right]^{(T_d/T)} n_d^{(T_d/T)-1}. \tag{6}$$

In Eqs. (5) and (6), the parameter σ_0 is a conductivity prefactor, T represents a temperature, T_t and T_d are characteristic temperatures associated with the distribution of tail and deep states, respectively, n_t and n_d are carrier concentrations from tail and deep states, respectively, N_t and N_d are total numbers per unit volume of tail and deep states, respectively. We should notice about the inequalities $T_d > T_t$ and $N_d \ll N_t$ which are valid for organic semiconductors [10–12]. The parameter B_c represents a critical percolation factor. For the case of 3–D amorphous solids, B_c = 2.8 [13]. The physical sense of the parameter α is that its reciprocal (α^{-1}) represents overlap parameter between localized states. We can write $\alpha = 10/a$, where a describes a distance between the localized states and may be defined as $a = 1/\sqrt[3]{N_t}$.

The total concentration of charge carriers n is a sum of n_t and n_d. Both concentrations n_t and n_d may be written in the form [10]

$$n_{t,d} = N_{t,d}\left[\frac{\pi T/T_{t,d}}{\sin(\pi T/T_{t,d})}\right] exp\left(\frac{\Delta E_F}{kT_{t,d}}\right), \tag{7}$$

where k represents the Boltzmann constant, ΔE_F is an energy difference between the energy of a quasi-Fermi level and E_{LUMO} (for electrons) or E_{HOMO} (for holes).

The static dielectric constant is approximately 3 for most organic semiconductors [7], thus the permittivities ε_1 = 3 and ε_2 = 3.5 have been chosen for the analysis. We assume here that the dielectric constants are temperature independent.

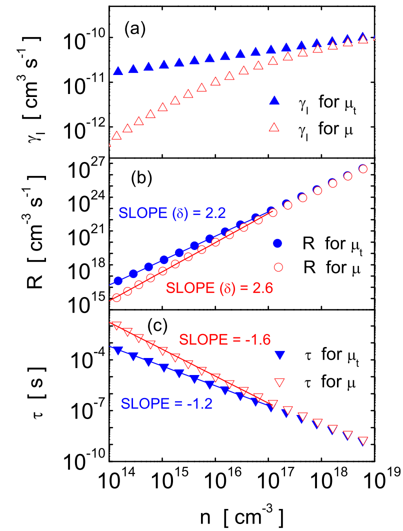


Fig. 1. (a) Interface recombination coefficient γ_I versus n calculated for tail states mobility μ_t and overall mobility μ. (b) Concentration dependence of recombination rate R for both mobilities μ_t and μ. Lines represent fits to calculated data below concentration 10^{17} cm^{-3}. The slopes indicate orders of recombination δ. (c) Recombination time τ versus n calculated for tail states mobility and overall mobility. Lines represent fits to calculated data below concentration 10^{17} cm^{-3}. Parameters are the same for all figures: T = 300 K, T_t = 350 K, T_d = 600 K, $N_t = 10^{20}$ cm^{-3}, $N_d = 10^{18}$ cm^{-3}, $\sigma_0 = 10^3$ S cm^{-1}, B_c = 2.8, ε_1 = 3, ε_2 = 3.5.

Fig. 1 consists of three panels drawn for the same parameters which allow to obtain a typical room temperature mobility of the order of magnitude 10^{-4} cm^2 V^{-1} s^{-1} for concentration $\sim 10^{16}$ cm^{-3}. It is known that the presence of deep states decreases a mobility for lower charge carrier concentrations [10]. This fact should lead to a similar tendency of the interface recombination coefficient γ_I. In Fig. 1(a) we compare two interface recombination coefficients calculated for a tail states mobility μ_t and an overall mobility μ. It is clearly visible that the coefficient γ_I calculated for μ_t is larger than γ_I obtained for μ for lower densities n. Fig. 1(b) illustrates the concentration dependence of the recombination rate R obtained from Eq. (2). We can see that R is linear for the tail states mobility μ_t with slope (recombination order δ) which exceeds 2 in the whole concentration range (10^{14}–10^{19} cm^{-3}). When deep states are taken into account, then δ increases for concentrations below 10^{17} cm^{-3} and reaches the same value as δ obtained for μ_t for higher n. It confirms that the presence of deep localized states causes the increasing of recombination order for lower carrier densities. In order to present a physical explanation of this tendency, we should note that the recombination rate R is mobility-dependent. It is evident from Eq. (4) that the lowest mobility between tail and deep states gives the largest contribution to the overall mobility μ. The role of tail or deep states is associated with a position of the quasi-Fermi level E_F [10]. If the position of E_F is near the band edge, then there are more tail states than the deep ones and $n \simeq n_t$. The mobility is inversely proportional to concentration, so it gives that $\mu_t \ll \mu_d$ and the overall mobility μ is approximately equal to μ_t. For this case, the R rises, so the recombination order δ decreases. The time of recombination τ calculated from the expression $\tau = (\gamma_I n)^{-1}$ is presented versus n in Fig. 1(c). We can see that τ decreases with a concentration of charge carriers for both mobilities μ_t and μ. The comparison demonstrates that τ calculated for overall mobility is larger than τ obtained for μ_t in the range of lower concentrations. Lines represent fits to data below $n = 10^{17}$ cm^{-3}. Their slopes (−1.2 and −1.6) agree well with the relation $\tau \sim n^{-(\delta-1)}$ [14]. Recently, we have reported a similar dependence for recombination time using other model of recombination where excitons annihilate on the electron–hole Langevin

Download English Version:

https://daneshyari.com/en/article/1440627

Download Persian Version:

https://daneshyari.com/article/1440627

Daneshyari.com