Estimation of Electrical Parameters of OD Organic Semiconductor Diode from Measured I-V Characteristics

Syed Abdul Moiz, Mansoor M. Ahmed, and Kh. S. Karimov

In this paper the effect of temperature on the electrical properties of organic semiconductor disperse orange dye 25 (OD) have been examined. Thin films of OD have been deposited on In_2O_3 substrates using a centrifugal machine. DC current-voltage (I-V) characteristics of the fabricated devices (Al/OD/In_2O_3) have been evaluated at varying temperatures ranging from 40 to 60°C. A rectification behavior in these devices has been observed such that the rectifying ratio increases as a function of temperature. I-V characteristics observed in Al/OD/In_2O_3 devices have been classified as low temperature (≤ 50°C) and high temperature characteristics (approximately 60°C). Low temperature characteristics have been explained on the basis of the charge transport mechanism associated with free carriers available in OD, whereas high temperature characteristics have been explained on the basis of the trapped space-charge-limited current. Different electrical parameters such as traps factor, free carrier density, trapped carrier density, trap density of states, and effective mobility have been determined from the observed temperature dependent I-V characteristics. It has been shown that the traps factor, effective mobility, and free carrier density increase with increasing values of temperature, whilst no significant change has been observed in the trap density of states.

Keywords: Organic semiconductor, I-V characteristics, orange dye, trap factor, space charge limited current.

Manuscript received June 22, 2004; revised May 2, 2005.

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I. Introduction

A number of potential applications of organic semiconductor materials for use in electronics and optoelectronics devices such as sensors, plastic batteries, solar cells, field effect transistors, optical data storage, organic electroluminescent devices, and so on have been found [1]. However, degradation of these devices with respect to temperature and the aging effect are still some serious concerns. To improve stability together with improved performance, it is very important to have a good understanding of the physical phenomena taking place in polymer-based devices such as charge transport, density of traps, mobility, and other factors with respect to temperature and aging [2].

Disperse Orange Dye 25 (OD) is a promising organic semiconductor material [3]. Karimov and coworkers have already reported I-V characteristics of OD films grown at different gravity conditions [4]. OD has attracted research attention due to its ease of synthesis and good environmental stability. Furthermore, its high degree of response to humidity makes it a good candidate for humidity sensors and related applications [3]. However, a very limited amount of information is available in scientific literature about the electrical properties of OD, especially as a function of temperature.

To explain their electrical behavior, the charge transport mechanism in organic semiconductor materials is a controversial topic, and no unified theory is available to explain the experimental results under different conditions to an acceptable degree of accuracy [5]. Various models have been put forward to explain the charge transport mechanism in these materials. Among them, two models have been used most frequently to explain the I-V characteristics [6]: (a) the trapping model with a space-charge-limited current and (b) the field dependent mobility model.

The trapping model assumes that there is a certain distribution of traps, called localized states, in the energy space where the free charge carriers can be trapped. These trapped carriers may be released after some specific period due to either temperature or any other excitation, and eventually they take part in the electrical response of a polymer. Most frequently, an exponential distribution of traps in the energy band is assumed. Whereas in the field dependent mobility model, which assumes exponential dependence of mobility μ_p on the square root of electric field F over a wide range of field defined by the Poole-Frenkel (PF) law, μ_p can be expressed as in [7]:

$$\mu_p = \mu_o \exp\left(\sqrt{\frac{F}{F_0}}\right). \tag{1}$$

Here, μ_o is the mobility at F_o and its value is sample dependent.

The exponential trap distribution model with constant mobility was first proposed by Mark and Helfrich [8]. It was assumed that the free carrier concentration p_o is much less than the trapped carrier concentration p_t, and the trap distribution h as a function of energy E is given as:

$$h(E) = \frac{N_t}{E_c} \exp\left(-\frac{E_n}{E_c}\right), \tag{2}$$

where N_t is the density of traps and E_c is the characteristic constant of the distribution, also often expressed as characteristics temperature, T_c, such that $E_c = kT_c$, where k is the Boltzmann constant. Traps are locations arising from disorders, dangling bonds, impurities, etc, and are called localized states that very often capture free charge carriers, playing a very important role in the conduction process of a polymer [9]. Based on the exponentially distributed traps theory, the current density J of a polymer having thickness d, relative permittivity ε_s, and density of states in the valance band N_v is given [10] by

$$J = q^{1-l} \mu_p N_v \left(\frac{2l+1}{l+1}\right)^{l+1} \left(\frac{l\varepsilon_s}{(l+1)N_t}\right)^{l} \frac{V^{l+1}}{d^{2l+1}}, \tag{3}$$

where $l = T_c / T$ and T is the absolute temperature.

Equation (3) shows that the J-V characteristics may be predicted by a power law of the form J–V^m, where $m = l+1$. Thus, the experimental I-V characteristics may be used to determine the electrical parameters of a conducting polymer by employing (3) to its different regions of operation [11].

In this study, Al/OD/In_2O_3 junctions were fabricated and characterized as a function of temperature, and the observed characteristics were explained on the basis of the trapped space charge limited current model, see (3), by assuming that the traps are exponentially distributed within the energy band gap of the OD. An attempt has been made to estimate the density of traps, free and trapped carrier concentrations, traps factor, and their variation as a function of temperature in OD films.

II. Experiment

In this work, a highly pure form of commercially available orange color OD having chemical formula $C_{17}H_{17}N_5O_2$ was used for the fabrication of films. Figure 1 represents the molecular structure of OD. The molecular weight of OD was 323 gm/mole with a density of 0.9 gm/cm^3. A 10% by weight OD as a solute in distilled water was used at room temperature to prepare the solution. Thin films of OD were grown in a spin coater on In_2O_3 substrates at an angular speed of 10,000 rpm. The thickness of OD films was estimated by optical measurements and by knowing the mass of deposited matter with its density and deposited area; it was found to be approximately 3 µm. Optical examination showed that the structures of films were like a mosaic. The nature of OD films was characterized by the hot probe method and observed as a p-type semiconductor. A thin film of Al was vacuum

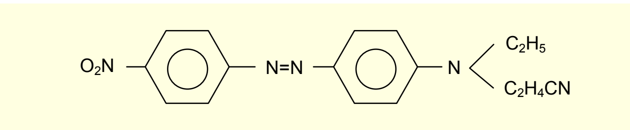

Fig. 1. Molecular structure of disperse orange dye 25 (OD).

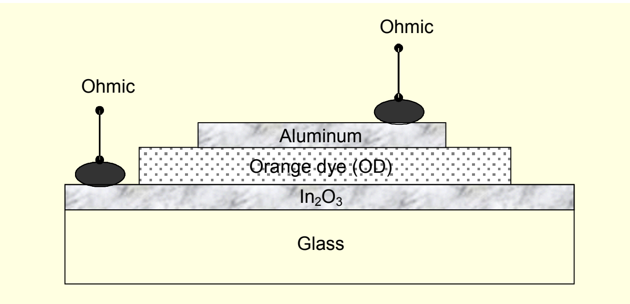

Fig. 2. A cross-sectional view of an Al/OD/In_2O_3 diode fabricated by depositing OD onto an In_2O_3 substrate. Two Ga metal electrodes are used to provide ohmic contacts.

evaporated on OD and liquid Ga metal was then used to fabricate ohmic contacts with In_2O_3 and Al both. A cross-sectional view of a finished device is shown in Fig. 2.

DC I-V characteristics were evaluated for varying temperatures ranging from 40 to 60°C with a conventional measurement system of good accuracy, the details of which is given elsewhere [12]. The temperature of the device was varied with a tungsten filament in a specially designed jar using an *in situ* temperature measurement facility. Temperature was measured with an error of ± 0.5°C. In DC measurements, it was observed that the device took about 1 minute to give a stabilized output whenever there was a change in the applied potential. Thus, sufficient time was given to allow the system to attain the stable values. As a result, the reported I-V characteristics are under steady state conditions and are therefore fully reproducible.

III. Characterization

I-V characteristics as a function of temperature for an Al/OD/In_2O_3 device are shown in Fig. 3. The plot shows that the device has diode-like characteristics. Furthermore, it is evident from the figure that the observed electrical response varies as a function of temperature. In Region-1, a negligible amount of current is flowing, and a zoomed view of this region showed that the characteristics are almost linear, though with a very nominal slope. At higher voltage, the current varies as $I \propto V^n$. When $n \geq 3$, it is referred to as Region-III, and the current in that region increases exponentially. Whereas in Region-II, the current varies with voltage as $I \propto V^2$ (i.e., it follows the square law), indicating the presence of space charge limited conduction.

Lamperts theory of space charge limited current predicts that valuable information can be obtained from I-V characteristics of amorphous materials while operated in Region-II [13]. For this region, (3) is reduced to

$$J = \frac{9}{8}\varepsilon_s \theta \mu_p \frac{V^2}{d^3}, \tag{4}$$

where θ represents the traps factor defined as the ratio of free hole/electron carrier density, p_o/n_o to the total carrier density, $(p_o + p_t)$ or $(n_o + n_t)$, and for a *p*-type polymer film

$$\theta = \frac{p_o}{p_o + p_t}. \tag{5}$$

Experimentally, the value of traps factor θ can be calculated from the ratio of current density, J_1 and J_2 at the beginning and end of square law region, respectively [9]. Figure 4 shows the variation of traps factor with temperature. It is evident from the figure that the value of θ increases gradually and there is then a steep increase in its value with increasing values of temperature. This may be attributed to the fact that at higher temperature more trapped charge carriers are released from their localized states and play a role with free carriers in the conduction process for OD films.

Using (4) and assuming θ = 1, the variation in μ_p as a function of temperature has been evaluated from the observed characteristics and plotted in Fig. 5. The figure also shows the variation in effective mobility that has been plotted by incorporating the traps factor. Examination of the figure reveals that the effective mobility, which included the traps factor, is somehow less than the mobility of a pristine (trap free) organic semiconductor OD, the difference becoming prominent when

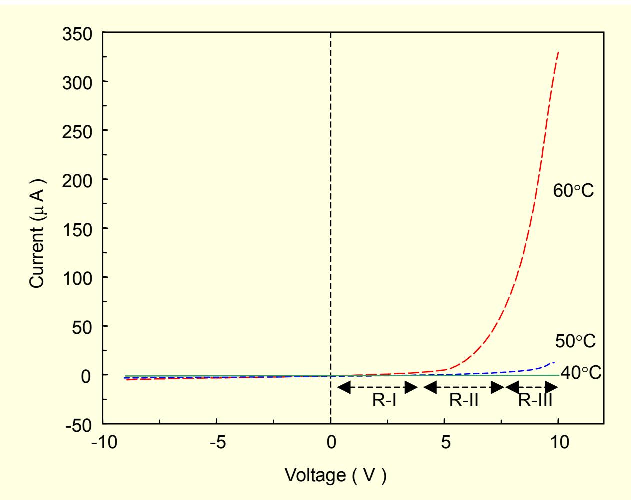

Fig. 3. Current voltage characteristics of an Al/OD/In_2O_3 organic semiconductor diode at 40°C, 50°C, and 60°C.

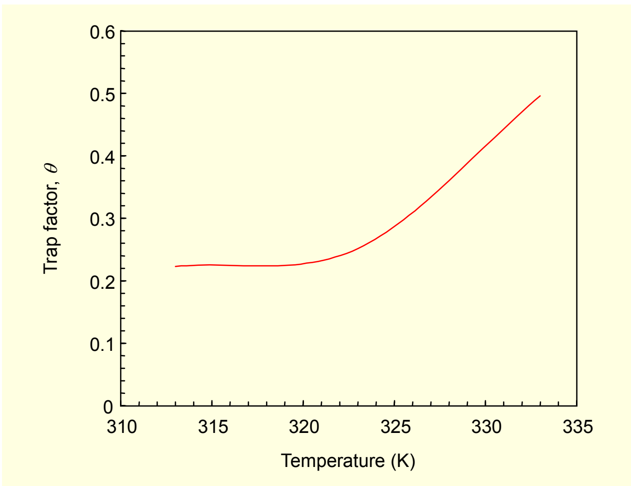

Fig. 4. Variation of trap factor (θ) with temperature for an Al/OD/In_2O_3 device.

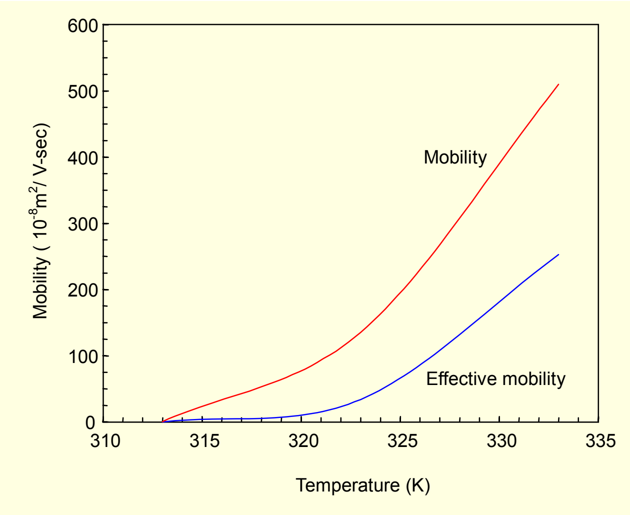

Fig. 5. Variation of effective mobility and trap-free mobility with respect to temperature for OD film.

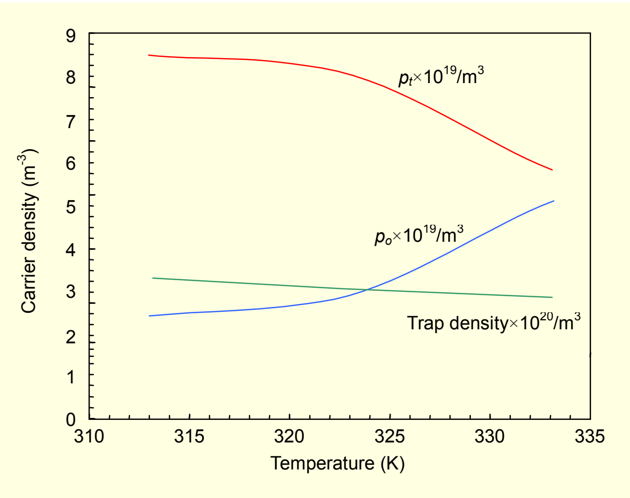

Fig. 6. Variation in free carrier density, p_o; trapped carrier density, p_t; and trap density of states, N_t, for OD film as a function of temperature.

the sample is heated at higher temperatures. Effective mobility can be expressed [10] as

$$\mu_{eff} = \mu_p \ \theta = \mu_p \left[\frac{p_0}{p_0 + p_t} \right]. \tag{6}$$

Figure 6 shows the variation of p_o, p_t and N_t as a function of temperature. These variables have been calculated using the variation in the observed current as a function of temperature in the square law region of Fig. 3. Figure 6 illustrates that the magnitude of N_t remains almost constant, whereas p_0 is increasing while p_t is decreasing as a function of temperature. Trap-filled limited voltage, V_{TFL}, may be defined as the voltage at which all traps as localized states are filled and is given by

$$V_{TFL} = \frac{qN_t d^2}{2\varepsilon_s}. \tag{7}$$

Any increase in the applied voltage beyond V_{TFL} will generate excess injected carriers causing a steep rise in the current, preceded by the square law region as shown by Region-III.

Region-I, shown in the I-V characteristics of Fig. 3, is mainly associated with p_0 and thus behaves as a liner region. The current in that region is, therefore, defined by taking $l = 0$ in (3), which reduces to

$$J = q\mu_p \ p_o \frac{V}{d} = q\mu_p \ p_o E. \tag{8}$$

IV. Discussion

Examining the plots shown in Figs. 3 through 6, it is evident that the electrical response of OD films for a temperature range of 40 to 60°C can be divided into two categories called a) low temperature response and b) high temperature response. At a relatively high temperature (approximately 60°C), the current increases sharply as shown in Fig. 3, whereas at a low temperature (≤ 50°C), the observed change in the current magnitude is very small. Thus, the charge transport mechanism taking place at these two temperatures, to explain the observed response, will be different.

Different conduction mechanisms may arise because of the energy states available in the conjugate organic semiconductors. It is a well reported fact that the charge transport mechanism in organic semiconductor materials and devices depends upon localized as well as extended states [11], [14]. Both of these states are involved in defining the charge flow in organic semiconductors. Owing to the availability of local and extended energy states, an organic semiconductor material may be seen as an inorganic amorphous semiconductor material.

At higher temperature, the free carries trapped by the localized energy states may acquire sufficient energy to leave the localized traps and enter into the extended energy states, thus contributing into the flow of the current. As seen in Fig. 6, the concentration of free carriers increases considerably at higher temperatures resulting in a corresponding decrease in trapped carrier concentration in the localized states. This explains the observed high current at higher temperatures in OD films.

Figure (7) shows a band diagram of an Al/OD/In_2O_3 device where the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO), which act like valance and conduction bands respectively in an inorganic semiconductor, are 2.73 eV apart [3], [15]. The band diagram shows that there is a nonlinear contact between In_2O_3 and OD, whereas it is defining almost a linear contact between OD and Al. This nonlinear junction between In_2O_3/OD is responsible for the observed nonlinear characteristics shown in Fig. 3.

The charge transport in organic semiconductors is mainly determined by a hopping process between two localized molecular states, as is seen in amorphous semiconductors [11]. However, the traps, which could be present due to impurity, distortion, structural defects, or other reasons, would tend to restrict the charges inside the energy band gap, and hence affecting the overall hopping process. When temperature increases, it is assumed that the charges become excited and may jump from a localized state to an extended sate. This gives an increase magnitude of the current at higher temperatures as depicted in Fig. 3. As the traps factor is a ratio between p_0 and $(p_0 + p_t)$, it therefore also increases by increasing temperature as shown in Fig. 4. This model, which is based on the presence of traps and the extended states, explains reasonably well the observed characteristics of Al/OD/In_2O_3 devices as a function of temperature.

Moreover, the mobility of free carriers reduces in the presence of traps. The effective mobility will, therefore, be smaller than the ideal case mobility for a given organic material. The effective mobility of OD calculated from the observed characteristics is shown in Fig. 5. The figure shows that the mobility for OD-based devices increases by increasing the temperature, and this increase in the mobility may be associated to the energy of the carriers, which is now considered high enough to allow them to move without falling into a trap of relatively lower energy. As trapped density is a material-related phenomenon, for a finished OD-based device there may not be a significant change in the trap density by increasing the temperature to approximately 60°C. Thus, almost a constant line, as shown in Fig. 6, is observed for the trap density for OD when plotted as a function of temperature.

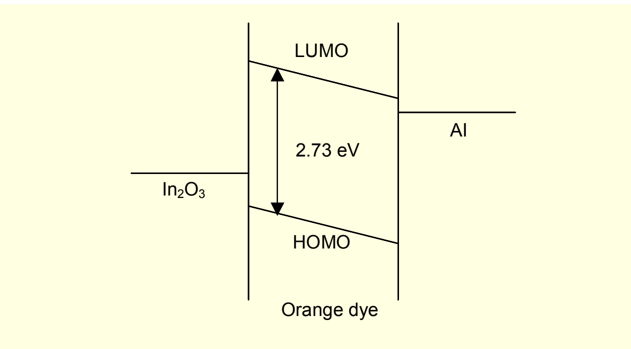

Fig. 7. Band structure of an Al/OD/In_2O_3 device showing a nonlinear junction.

V. Conclusion

Thin films of OD were deposited on In_2O_3 substrates by a spin coater, and current voltage (I-V) characteristics of Al/OD/In_2O_3 devices were measured for a temperature interval of 40 to 60°C. It has been observed that these devices are nonlinear in their electrical response with diode-like characteristics. Measured I-V characteristics were explained by assuming a hopping of free carriers from localized to extended energy states present in OD films. By applying the trapped space charge limited current model on the observed I-V characteristics, different electrical parameters such as traps factor, effective mobility, free carrier density, trapped carrier density, and trap density of states have been determined and their variation as a function of temperature has been shown. The evaluated data shows that traps factor and free carrier density both increase with temperature, whereas trapped carrier density decreases as a function of temperature. It has been observed that the effective mobility of free carriers increases with temperature which may be attributed to the increased thermal energy of the carriers, which is assumed to be high enough to allow them to move without encountering a trap of relatively lower energy available in OD films.

Acknowledgements

The authors are thankful to GIK Institute of Engineering Sciences and Technology for its supports for this work and the facilities used.

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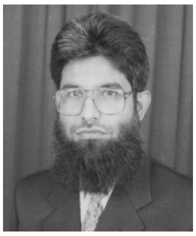

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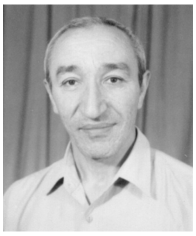

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