Disorder effect on carrier mobility in Fullerene organic semiconductor

N Mendil¹, M Daoudi², Z Berkai³ and A Belghachi⁴
¹,²,³,⁴ Laboratory of semiconductor device physics, University of Tahri Mohamed Bechar, P.O.B n°417 Bechar 08000, Algeria.
mendil_nesrine@yahoo.com

Abstract. The critical factor that limits the efficiencies of organic electronic devices is the low charge carrier mobility which is attributed to disorder in organic films. In this context, we have studied the effects of disorder on carrier mobility in organic Schottky diode of electrons for the fullerene (C₆₀). Our results show that the mobility is sensitive probes of structural phase transitions and order-disorder underlying C₆₀. Where it is one reason behind the low mobility which it take as value 1.4x10⁻² cm²/V.s above critical temperature Tc =289K.

1. Introduction

Over the years, the world’s industries and research organization have shown their interest in the renewable energy resources due to the limited fossil fuel reserves, which emit tons of carbon dioxide and other pollution every second. The efficient use of sunlight to produce the domestic electricity by means of solar cell devices is the perfect way to deal with the limitation of the reserve fossil fuel [1]. The recent growing demand for cost-effective renewable energy has generated considerable interest in the field of organic solar cells. Organic photovoltaic (OPV) cells have the potential to substantially lower costs for solar energy conversion, given their expected low materials and fabrication costs. Since fullerene (C₆₀) organic semiconductor was discovered, it has drawn the attention of physicists and chemists alike, which much work has been done on its physical and chemical properties. At ambient conditions the C₆₀ molecules are centered on sites of a face-centered-cubic (fcc) with a=1.42nm and energy gap about 1.5eV [2]. The order-disorder transition in C₆₀ occurs around 289K at ambient pressure. At this transition freely rotating molecules get orientation ordered in a simple cubic lattice (sc) and below 90K the occupation of the nearly degenerate states does not change, so this temperature is identified with the quenching disorder transition [3-4]. In this work, we use a single active-layer OPV cell, where we have studied the effects of disorder on carrier mobility, conductivity and resistivity in C₆₀ organic Schottky diode which it is the most frequently used as electron acceptor organic semiconductor due to its unique physical and chemical characteristics[5].
2. Theoretical model

Charge transport mechanisms in organic semiconductors have a great importance since they are the basis for a new class of electronic and optoelectronic devices. In this context, the transport properties of charge carriers in the organic material have been investigated by using a mathematical simulation taking into account the effect of disorder, where the mobility ($\mu$) varies depending on the temperature ($T$), the applied voltage ($V$) and the energetic disorder ($\delta$), it can take 0.03eV ($T<289$K) and 0.06eV ($T>289$K) [6]. The charge carrier mobility is given by the following equation[7]:

$$\mu = \mu_{\infty} \exp \left[ - \left( \frac{3\delta}{5K_B T} \right)^2 + 0.78 \left( \frac{\delta}{K_B T} \right)^{1.5} - 2 \right] \sqrt{\frac{eV}{\delta d}}$$  \hspace{1cm} (1)

where $\mu_{\infty} = 0.03 \text{ cm}^2/\text{V.s}$, the mobility as the temperature is going to infinity and $K_B$ is the Boltzmann constant [eV/K].

In the absence of traps the space charge limited the current density ($J$) can be written as a function of the applied voltage as[8]:

$$J = \frac{9}{8} \varepsilon_r \varepsilon_0 \mu \frac{V^2}{d^3}$$  \hspace{1cm} (2)

where $\varepsilon_r$=4 relative dielectric constant [7], $d$ is the organic film thickness [cm].

The electrical resistivity of electron in C$_{60}$ is expressed as follows:

$$\rho = \frac{V}{dJ}$$  \hspace{1cm} (3)

3. Result and discussion

The temperature dependence of mobility is an important topic to understand the charge transport mechanism in organic materials, so in these figures 1 (a) and (b), we can see that the electron mobility decrease with increasing of temperature and lattice parameter.

In figure 1 (a), for the low temperature (T=50K - 100K) the electron mobility has a sufficient decrease from $3.5\times10^{-2}$ cm$^2$/Vs up to $2.5\times10^{-2}$ cm$^2$/Vs however when the temperature increase from 150K to 250K the electron mobility decrease from $2.1\times10^{-2}$ cm$^2$/Vs to $1.7\times10^{-2}$ cm$^2$/Vs and it remains constant. In figure 1 (b), the mobility continues to decrease from $1.55\times10^{-2}$ cm$^2$/Vs to $1.4\times10^{-2}$ cm$^2$/Vs and it remains constant. If we compare the carrier mobility of amorphous silicon, which it is about
The conductivity of the C\textsubscript{60} single crystal is $17 \times 10^{-8} \text{ (}{\Omega} \cdot \text{cm})^{-1}$ and the activation energy is 0.581 eV. However, for the poly-crystalline films, the conductivity and activation energy are reported to be $10^{-6}$ to $10^{-8} \text{ (}{\Omega} \cdot \text{cm})^{-1}$ and 0.3-0.6 eV, respectively [10]. For amorphous films, these values are within the intervals $10^{-7}$-$10^{-10} \text{ (}{\Omega} \cdot \text{cm})^{-1}$ and 0.5-1.1 eV. With improving the crystallinity of C\textsubscript{60} films, their conductivity increases, and the activation energy fall [11]. So the conductivity of the crystalline C\textsubscript{60} is obviously higher than that of the C\textsubscript{60} amorphous films. So, we can conclude that C\textsubscript{60} takes a behavior of poly-crystalline form when the temperature is in range of 50K-125K and amorphous form when T is in range of 125K-250K.

4. CONCLUSION
In this paper we have discussed the impact of energetic disorder on the charge carrier mobility, conductivity and resistivity. It was shown that the disorder is one of the key parameters to explain the transport in organic semiconductors. More specifically, increasing the disorder energy push the mobility decreases and it will be less temperature dependent.

ACKNOWLEDGEMENT
This work is partly supported by Algerian ministry of higher education and research (CNEPRU) project N° D03820140006
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