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The Electrical Properties

of Au/P3HT/n-GaAs Schottky Barrier Diode

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In this study, we investigated the electrical properties of the Au/P3HT/n-GaAs Schottky diode at room temperature by using current–voltage method. The values of ideality factor and barrier height of the diode were found to be 2.45 and 0.85 eV, respectively. n ideality factor greater than unity indicates that the diode exhibits non-ideal current–voltage behavior. This behavior results from the effect of series resistance and the presence of an interfacial layer. These values were also determined from the Cheung functions and the Norde method due to the non-ideal behavior of the diode and it was seen that there was an agreement with series resistance. Also the interface states energy distribution of the diode was determined from the forward bias I-V measurements by taking into account the bias dependence of the effective barrier height. The obtained electrical parameters of the Au/P3HT/n-GaAs Schottky diode are higher than that of the conventional Au/n-GaAs Schottky diodes.

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1. Introduction

The Schottky barrier diodes are widely used in extremely important applications in electronic industry, such as microwave mixer, high-current power supplies, varistor, varactor, solarcell, photodetector, metal-based transistor, MESFET, etc. [1, 2]. Also, the Schottky diodes are often used for complicated applications in telecommunication systems, radioastronomy, radar technology, and plasma diagnostics [3].

During the last few decades, organic semiconductors have attracted increasing research interest from both academia and industry. Investigation of material properties, device structures and characteristics show that electronic and photonic devices can be successfully prepared from organic compound [4].

Conjugated polymers are recognized as organic semiconductors with electronic properties and they have found a wide application area in electronic technology [5].

It is well known that the electrical characteristics of a Schottky diode are controlled mainly by its interface properties [6]. The electrical properties of metal/semiconductor (MS) structures can be modified by introducing organic layer on semiconductor materials and have been shown to exhibit promising characteristics for diode applications [7, 8].

Over the recent decades, there have been significant advances in the scientific domain with regard to electronic devices that are based upon organic components, mainly due to that they have a number of advantages such as easy and low cost device fabrication, versatility of usage, and large area coverage [4–12]. A common thiophone–based donor material is poly(3-hexylthiophene) or P3HT. P3HT appears to be one of the best materials to date for such devices. It combines the commercial availability with sufficient solubility, a low bandgap relative to the most conjugated polymers and a high degree of intermolecular order leading to high charge carrier mobilities ($\mu_{hole} \approx 0.1-0.2 \text{ cm}^2/(\text{V s})$ measured in field effect transistor geometries) [13]. It is a stable polymer. It is soluble in several organic solvents, which makes it compatible with low-cost solution processing [14]. P3HT organic polymer is electron rich material that can be oxidized fairly readily, having high-energy HOMO level, and is typically hole conducting material [15].

In this study, P3HT thin interfacial polymer layer was deposited on n-GaAs using spin coating system to obtain as a new structure Au/poly(3-hexylthiophene) P3HT/n-GaAs Schottky barrier diode. The electronic parameters of the diode were determined by using current–voltage measurements at room temperature.

2. Experimental procedures

The substrate used in this study is *n*-GaAs semiconductor wafer with (100) orientation, 400 μ m thickness and 50.8 mm diameter. Before making contacts the wafer was chemically cleaned using the RCA cleaning procedure (i.e. 10 min boiling in H₂SO₄+H₂O₂ followed by a 10 min HCl + H₂O₂ + 6H₂O at 60 °C). It was immersed in diluted 20% HF for 60 s. The wafer was rinsed in de-ionized water of resistivity 18 M Ω cm with ultrasonic cleaning in each step. After that, the sample was dried in the high-purity nitrogen stream and inserted into the deposition chamber. There were used Au (88%) and Ge (12%) for ohmic contact [1]. The ohmic contact with a thickness of ≈1875 Å was made by evaporating 99.995% purity Au metal and germanium on the back of the surface wafer in a thermal evaporator unit

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at 10^{-6} Torr. Then it was annealed at 450 °C for 5 min in flowing N₂ in a quartz tube furnace. Front surface of samples were coated with a conducting polymer P3HT (Fig. 1) film by spin coating (VTC-100) with 1200 rpm for 60 s. After that rectifier the Schottky contacts were formed on the other faces by evaporating ≈ 1000 Å thick Au. All evaporation processes were carried out in a vacuum coating unit at about 5.1×10^{-6} Torr. Thus, Au/P3HT/*n*-GaAs/Au sandwich Schottky barrier type diode was fabricated. The *I*–*V* measurements were performed using a Keithley 6517A electrometer. All measurements were controlled by a computer via an IEEE-488 standard interface so that the data collecting, processing and plotting could be accomplished automatically.



Fig. 1. Molecular structure of P3HT.

3. Result and discussion

The morphology properties of the P3HT film deposited on n-GaAs substrate were investigated by scanning electron microscopy (SEM). The surface morphology of a P3HT thin film spin-coated onto n-GaAs substrate is shown in Fig. 2. As seen in Fig. 2, the structure of the film is consisted of P3HT which are distributed almost homogeneously on semiconductor surface.



Fig. 2. SEM images of P3HT thin film onto $n\text{-}\mathrm{GaAs}$ substrate.

Figure 3 shows the forward and reverse bias current–voltage characteristics of the Au/P3HT/n-GaAs Schottky barrier diode.

According to the thermionic emission theory the current–voltage (I-V) characteristics of a Schottky diode is given as follows [16, 17]:

$$I = I_0 \exp\left(\frac{qV}{nkT}\right) \left[1 - \exp\left(-\frac{qV}{kT}\right)\right],\tag{1}$$

where



Fig. 3. Current versus voltage characteristic of the Au/P3HT/n-GaAs at room temperatures.

$$I_0 = AA^*T^2 \exp\left(-\frac{q\,\Phi_{\rm b0}}{kT}\right) \tag{2}$$

is the saturation current, $\Phi_{\rm b0}(I-V)$ is the zero bias barrier height, A^* is the Richardson constant and equals to 8.16 A cm⁻²K⁻² for *n*-GaAs [2, 18], where *q* is the electron charge, *V* is the bias voltage, *A* is the effective diode area, *k* is the Boltzmann constant, *T* is the temperature in K, *n* is the ideality factor. From Eq. (1), ideality factor *n* can be written as

$$n = \frac{q}{kT} \left(\frac{\mathrm{d}V}{\mathrm{d}(\ln I)} \right). \tag{3}$$

 Φ_{b0} is the zero-bias barrier height (BH), which can be obtained from the following equation:

$$\Phi_{\rm b0} = \frac{kT}{q} \ln\left(\frac{AA^*T^2}{I_0}\right). \tag{4}$$

Figure 3 presents the semilog-forward and reverse bias current–voltage (I-V) characteristics of the Au/P3HT/*n*-GaAs/Au structure. The values of the barrier height and ideality factor were calculated as $\Phi_{b0} =$ 0.85 eV from the experimental saturation current I_0 , and n = 2.45 from the slope of the linear region of the semilog-forward bias I-V characteristics indicating that the effect of series resistance in this region was not important, respectively, by using Eqs. (3) and (4). For an ideal Schottky barrier diode n = 1. Our *n* ideality factor value is considerably larger. The high values in the ideality factor are caused possibly by various effects such as inhomogeneities of P3HT film thickness, non-uniformity of the interfacial charges and series resistance [1, 3, 17].

At high currents there is forever a deviation which has been clearly shown to depend on parameters such as the interfacial layer thickness, the interface states density and series resistance, as one would expect [19]. The series resistance R_s is an important parameter, affecting the electrical characteristics of the Schottky barrier contacts. The Schottky diode parameters such as the barrier height, the ideality factor and the series resistance can also be obtained using a method developed by Cheung et al. [20]. The values of the series resistance can be determined by the following functions:

$$\frac{\mathrm{d}V}{\mathrm{d}\left(\ln I\right)} = IR_{\mathrm{s}} + n\left(\frac{kT}{q}\right),\tag{5}$$

$$H(I) = V - n\left(\frac{kT}{q}\right) \ln\left(\frac{I}{AA * T^2}\right),\tag{6}$$

and H(I) is given as follows:

$$H\left(I\right) = IR_{\rm s} + n\Phi_{\rm b0}.\tag{7}$$

The plot of $dV/d(\ln I)$ versus I in Fig. 4 and H(I)versus I is shown in Fig. 5, respectively. The $dV/d(\ln I)$ plot is a straight line region where the series resistance dominates. According to Eqs. (5) and (7), in the plot of $dV/d(\ln I)$ versus I and H(I) versus I, their slope gives the series resistances while their intercept with yaxis gives n(kT/q) and $n * \Phi_{b0}$, respectively. The ideality factor and series resistance values of the diode were calculated from Fig. 4 and found to be n = 251 and $R_{\rm s} = 217 \ \Omega$, respectively. The ideality factor obtained from $dV/d(\ln I)-I$ plot is seen to be greater than that obtained from $\ln I - V$ characteristic. The difference between the values of the ideality factors can be attributed to the fact that the first one is only under the effect of the interfacial properties and the second one is under the effect of both the interfacial properties and the series resistance [8]. In addition, the $R_{\rm s}$ and $\Phi_{\rm b0}$ values were calculated from the slope and intercept of H(I) versus Iplot and were found to be 206 Ω and 0.85 eV, respectively. The values of series resistance obtained by applying the Cheung functions show a good consistency with each other.



Fig. 4. Plot of ${\rm d}V/{\rm d}\ln I$ vs. I for the Au/n-GaAs/P3HT/Au diode.



Fig. 5. Plot of H(I) vs. I for the Au/n-GaAs/P3HT/Au diode.

Alternatively, we have used the Norde functions [4, 21] to obtain junction parameters of the diode. The Norde function is given as

$$F(V) = \frac{V}{\gamma} - \left(\frac{kT}{q}\right) \ln\left(\frac{I}{AA*T^2}\right),\tag{8}$$

where γ is a dimensionless integer greater than ideality factor. That is, according to our results, the value of γ is 3. If the minimum of the F(V) versus V plot is determined, the value of barrier height can be obtained by using the following equation:

$$\Phi_{\rm b} = F\left(V_0\right) + \frac{V_0}{\gamma} - \frac{kT}{q},\tag{9}$$

where F(V) is the minimum point of F(V), and V is the corresponding voltage. The Norde plot for device is shown in Fig. 6.



Fig. 6. Plot of F(V) versus V of the Au/n-GaAs/P3HT/Au Schottky diode.

The value of the series resistance has been calculated from the Norde function for device by using the following relation:

$$R = \frac{kT(\gamma - n)}{qI_0}.$$
(10)

The some parameters of the device from the F-V plot have been determined as $\Phi_{\rm b} = 1.05$ eV and $R_{\rm s} = 214 \ \Omega$, respectively. It is seen that there is a agreement between the values of the series resistance obtained from the Cheung and Norde plots. There is a difference in the values of $\Phi_{\rm b}$ obtained from the forward-bias $\ln I-V$, Cheung functions and Norde functions. The discrepancy between different methods may result from such causes as contamination in the interface, an intervening insulating layer, edge leakage current, or deep impurity levels [17].

The interface state density affects the electronic parameters of the diode. Therefore we investigated interface state density. The density of the interface state of the diode can be obtained from the forward bias I-V characteristics at room temperature by the following relation [22]:

$$n(V) = 1 + \frac{\delta}{\varepsilon_{\rm i}} \left(\frac{\varepsilon_{\rm s}}{W_{\rm d}} + qN_{\rm ss} \right). \tag{11}$$

Thus, according to Eq. (11), the interface state density can be obtained as below

$$N_{\rm ss}\left(V\right) = \frac{1}{q} \left\{ \frac{\varepsilon_{\rm i}}{\delta} \left[n\left(V\right) - 1 \right] - \frac{\varepsilon_{\rm s}}{W_{\rm d}} \right\},\tag{12}$$

where W_d is the depletion width, δ is the thickness of the interfacial layer, $N_{\rm ss}$ is the density of the interface states, $\varepsilon_{\rm s}(13.1\varepsilon)$ [18] and $\varepsilon_{\rm i}(4.4\varepsilon)$ [23] are the permittivity of the

semiconductor and interfacial layer, respectively. In n-type semiconductors, the energy of the interface states with respect to the bottom of the conduction band at the surface of the semiconductor is given by [24]:

$$E_{\rm c} - E_{\rm ss} = q(\Phi_{\rm e} - V), \tag{13}$$

where V is the applied drop across the depletion layer and $\Phi_{\rm e}$ is the effective barrier height and $E_{\rm ss}$ is the energy corresponding to the bottom of the conduction band at the surface of the semiconductor. The relationship between effective barrier height, applied voltage V and the ideality factor n in given by

$$\Phi_{\rm e} = \Phi_{\rm b0} + \left(1 - \frac{1}{n}\right)V. \tag{14}$$

Thus, the energy distribution profile of $N_{\rm ss}$ as a function $(E_{\rm c} - E_{\rm ss})$ for Au/P3HT/*n*-GaAs/Au was obtained from the forward bias *I*–V measurements by taking the bias dependence of the effective barrier height ($\Phi_{\rm e}$) into account by using Eqs. (12), (13) and (14). The interface state density versus ($E_{\rm c} - E_{\rm ss}$) curve of the diode is given in Fig. 7. As can be seen from Fig. 7, the calculated interface states density varies from 6.56×10^{11} cm⁻² eV⁻¹ in ($E_{\rm c} - 0.378$) eV to 4.26×10^{10} cm⁻² eV⁻¹ in ($E_{\rm c} -$ 0.414) eV. That is, there is an exponential decrease from bottom of conduction band towards to midgap of GaAs. This confirms that the density of interface states changes with applied bias and each of applied biases corresponds to a different position in the GaAs band gap.



Fig. 7. Energy distribution of interface state density of the Au/P3HT/*n*-GaAs/Au Schottky diode.

4. Conclusion

In this study, we have fabricated as a new structure Au/P3HT/n-GaAs Schottky diode. The electrical properties of the diode have been investigated at room temperature by using current–voltage method. The values of ideality factor and barrier height of the diode were found to be 2.45 and 0.85 eV, respectively. The values of the ideality factor, series resistance and barrier height were also determined from the Cheung and Norde functions due to the non-ideal behaviour of the diode. It was seen that there was agreement with series resistance. This diode showed a rectifying behavior and yielded different barrier height and ideality factor in

comparison to conventional GaAs diode. Also, the energy of interface states were determined from the forward bias I-V measurements by taking the bias dependence of the effective barrier height ($\Phi_{\rm e}$) into account. The interface state density decreases exponentially with bias from 6.56×10^{11} cm⁻² eV⁻¹ in (E_c - 0.378) eV to 4.26×10^{10} cm⁻² eV⁻¹ in ($E_{\rm c} - 0.414$) eV.

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