

THE EFFECTS OF N-GAAS SUBSTRATE ORIENTATIONS ON THE ELECTRICAL PERFORMANCE OF PANI/N-GAAS HYBRID SOLAR CELL DEVICES

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ABSTRACT:

This paper reports the fabrication and electrical characterization of hybrid organic-inorganic solar cell based on the deposition of polyaniline (PANI) on n-type GaAs substrate with three different crystal orientations namely Au/PANI/(100) n-GaAs/(Ni-Au), Au/PANI/(110) n-GaAs/(Ni-Au), and Au/PANI/(311)B n-GaAs/(Ni-Au) using spin coating technique. The effect of crystallographic orientation of n-GaAs on solar cell efficiency of the hybrid solar cell devices has been studied utilizing current density-voltage (J - V) measurements under illumination conditions. Additionally, the influence of planes of n-GaAs on the diode parameters of the same devices has been investigated by employing current-voltage (I - V) characteristics in the dark conditions at room temperature. The experimental observations showed that the best performance was obtained for solar cells fabricated with the structure of Au/PANI/(311)B n-GaAs/(Ni-Au). The open-circuit voltage (V_{oc}), short circuit current density (J_{sc}), and solar cell efficiency (η) of the same device were shown the values of 342 mV, 0.294 mAcm⁻², 0.0196%, respectively under illuminated condition. All the solar cell characteristics were carried out under standard AM 1.5 at room temperature. Also, diode parameters of PANI/(311)B n-GaAs heterostructures were calculated from the dark I - V measurements revealed the lower reverse saturation current (I_0) of 3.0×10^{-9} A, higher barrier height (ϕ_b) of 0.79 eV and lower ideality factor (n) of 3.16.

KEYWORDS: (100) GaAs, (110) GaAs, (311)B GaAs, PANI, IV curve, Hybrid device.

1. INTRODUCTION

Currently, a lot of attention has been paid to the fabrication of hybrid solar cells based on inorganic n-type GaAs and organic p-type Polyaniline (PANI). The organic materials have the advantages of a high absorption coefficient over the inorganic ones with a comparatively thin layer of about (100-200) nm (Marinova et al., 2017). There are many reports in the literature about the growth of films on conventional (100) GaAs substrate (Patanè et al., 1999). Fabrication of hybrid organic-inorganic photovoltaic device was carried out by Halliday et al. (1999) using the growth of PANI film on n-type, p-type, and undoped epitaxial GaAs substrate. They proposed that the presence of surface states on GaAs film controls the interfacial electrical and optical characteristics of the PANI/GaAs interface (Halliday et al., 1999). Henini et al. (1999) used atomic force microscopy and photoluminescence to study the optical characteristic of In_{0.5}Ga_{0.5}As/GaAs heterostructure with three different GaAs substrate orientations (100), (311)A, and (311)B, respectively. The authors found that the two-dimensional or three-dimensional transition growth mode is intensely affected by substrate orientation (Henini et al., 1999). On the other hand, semiconductor structure which was grown on the high index GaAs substrate for instance (311)A and (311)B showed higher optical absorption, anisotropy, and hole mobility compared to the same structure grown on the conventional (100) GaAs substrate (Jameel et al., 2016; Li & Niewczas, 2007; Wang et al., 2009). Yan & You (2013) reported the lower short-circuit current for device structure of

polymer/(100) GaAs as compared to the polymer/(111)B GaAs device structure. They have shown that (111)B GaAs substrate orientation creates lower surface state density and recombination rate at the polymer/GaAs interface (Yan & You, 2013). The same group systematically investigated the hybrid solar cell through the deposition of different polymers on n-type GaAs and the obtained PCEs were very low in the range of 0.02% up to 2.75%. The electrical properties of spin-coated p-type PANI on (100), (311)A, and (311)B n-type GaAs substrates were reported by Jameel et al. (2015). Their study indicated that the crystallographic orientation of GaAs affects the electrical properties of the device. Furthermore, the most recent study about the hybrid photovoltaic device based on n-GaAs and conducting polymer PANI was carried out in 2018 by Salehi et al. (2018). This research group has investigated the effect of employing two different metals (Al or Ag) on the efficiency of the solar cells. The achieved efficiencies for (PEDOT: PSS) and (PANI) were 4.41% and 1.4%, respectively (Salehi et al., 2018). In this work, the fabrication and electrical properties of Au/PANI/n-type GaAs hybrids solar cell grown on (100), (311)A, and (311)B n-type GaAs are presented. The impact of the substrate plane on the solar efficiency and electrical properties such as reverse saturation current, barrier height, ideality factor series resistance, and shunt resistance have been investigated using Current-Voltage (I-V) measurements under light and dark conditions.

2. SAMPLES FABRICATION

In this report, n-type GaAs wafers with different orientations of (100), (110), and (311) B have been used as an inorganic

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substrate for depositing the PANI thin film. For producing a device more properly it is important to have a general idea about the orientation of crystal structure. The information about the orientation of the crystal can be obtained via studying the Millar indices of a plane. Generally, there are two main indexes with crystal planes: the planes that consist of only 0's and 1's having cubic crystal structure are called low index planes such as (100), (110), and (111). Its surface is exhibiting various reforms whose structures are commonly determined previously. The surface of (110) exhibits the simplest construction. The unit cell involving one of both threefold coordinated Ga and threefold coordinated As atoms (Li & Niewczas, 2007). However, high index planes are consisting greater values for instance (n11) where n has a value larger than one for example (211)B, (311)A, (311)B, and (511)B. The substrates (100), (110), and (311)B were doped with a silicon (Si) doping concentration of $2 \times 10^{18} \text{ cm}^{-3}$. Before the deposition process, the substrates were cleaned using methanol and acetone and consequently rinsed with deionized water and dried with the stream of argon gas. Then, a backside Ohmic contact of nickel (Ni)-gold (Au) was deposited by thermal evaporation employing an auto BOC Edwards 306 vacuum system. For more details see the deposition method expressed in Felix et al. (2011) and Jameel et al. (2015). This was followed by a deposition of the polyaniline thin film, prepared by chemical synthesis process, onto (100), (110), and (311)B n-GaAs substrates utilizing spin coating technique. Finally, circular electrical contacts of gold (Au) were deposited via thermal evaporation method at a chamber pressure of around 10^{-5} mbar on top of the PANI films with the area of 0.025 cm^2 to create Au/PANI/(100) n-GaAs/(Ni-Au), Au/PANI/(110) n-GaAs/(Ni-Au) and Au/PANI/(311)B n-GaAs/(Ni-Au) heterojunctions device structures. The current-voltage (I-V) characteristics of the fabricated devices have been carried out under both illumination and dark conditions using I-V source-meter (model Keithley 2450).

3. RESULTS AND DISCUSSION

To investigate the effect of crystallographic orientation of n-GaAs substrates on the efficiency of solar cell for hybrid organic/inorganic semiconductor devices, the current density-voltage (*J-V*) measurements at room temperature and under illuminated conditions were performed on the PANI samples grown on (100), (110) and (311)B n-GaAs substrates. Figure 1(a-c) shows the current density against the applied voltage (*J-V*) curve of all the three devices under the light condition with the intensity of 100 mW/cm^2 (AM 1.5). Important cell parameters such as open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (*FF*), and solar cell efficiency (η) can be extracted under illumination conditions. Table 1, summarize the results of the three fabricated solar cells.

Table 1. Photovoltaic performances of the PANI samples deposited on (100), (110), and (311) B n-GaAs substrates under the illumination of 100 mW/cm^2 .

Sample ID	V_{oc} (mV)	J_{sc} ($\times 10^{-3} \text{ mA/cm}^2$)	<i>FF</i>	η ($\times 10^{-3} \%$)
(100)	216	3.92	0.26	0.22
(110)	100	0.74	0.25	0.01
(311)B	342	294	0.19	19.60

V_{oc} and J_{sc} values for the sample with (110) crystal orientation are substantially smaller comparing to (100) and (311)B for the same conditions. Fill factor *FF* has the values of 0.26, 0.25, and 0.199 for PANI/(100), (110), and (311)B n-GaAs samples, respectively. Series resistance is the summation of semiconductor device resistance and

conductance resistance in direction of current flow (Rebaoui et al., 2017). Therefore, contact resistance cause to increase in the value of series resistance which in turn decreases V_{oc} and efficiency of the solar cell. Shunt resistance originated from generation and recombination also causes a low fill factor. The efficiency η value is calculated by using Equation 1 to be $2.2 \times 10^{-4} \%$ for PANI/(100) n-GaAs, $1.85 \times 10^{-5} \%$ for PANI/(110) n-GaAs and $19.65 \times 10^{-3} \%$ for PANI/(311)B n-GaAs heterojunction devices. η value of the PANI deposited on (311)B n-GaAs plane is higher than that of PANI deposited on (100) and (110) n-GaAs planes. These values are presented in Table 1, where it can be noted that the value of η increases as the orientation of n-GaAs substrate is changed from (110) to (100) and (311)B n-GaAs. This investigation confirms the effect of substrate orientation on solar cell efficiency.

$$\eta (\%) = \left(\frac{V_{oc} J_{sc} FF}{P_{in}} \right) \times 100\% \quad (1)$$

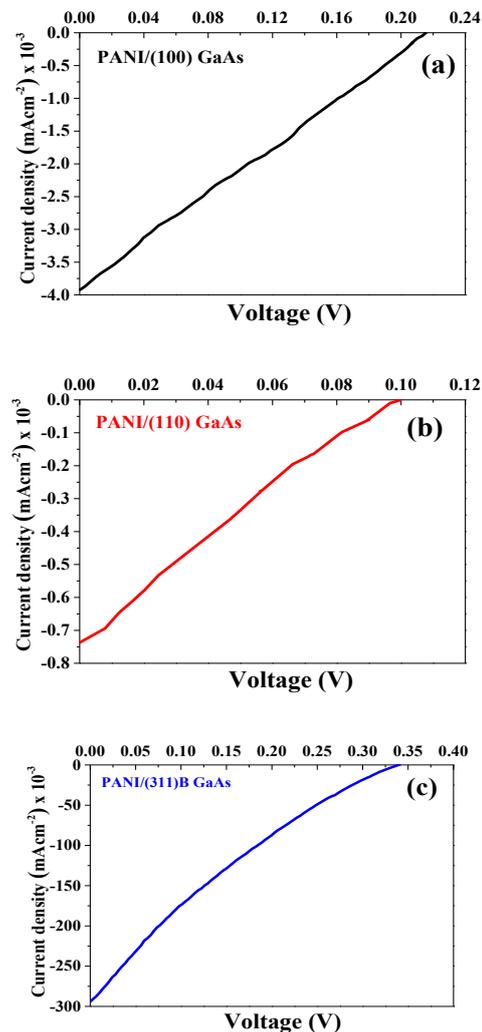


Figure 1. *J-V* characteristics under the illuminated condition and room temperature of (a) PANI/(100) n-GaAs hybrid solar cells device (black color), (b) PANI/(110) n-GaAs hybrid solar cells device (red color), and (c) PANI/(311)B n-GaAs hybrid solar cells device (blue color).

To study further the effect of GaAs substrate orientation on the electrical properties of the organic/inorganic semiconductor devices, the dark current-voltage (*I-V*) measurements were carried out at room temperature (300 K) on the PANI film samples coated on n-type GaAs substrate with three different crystal orientations of (100), (110), (311)B, respectively, as shown in Figure 2.

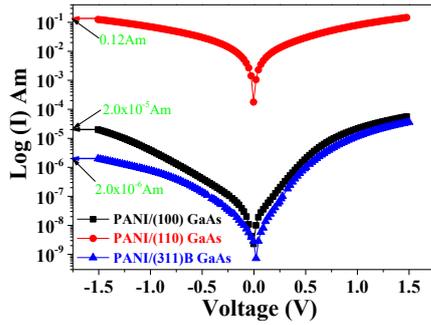


Figure 2. Semi-logarithmic plots of I - V characteristics under the dark conditions of PANI/(100) n-GaAs, PANI/(110) n-GaAs, and PANI/(311)B n-GaAs hybrid solar cell devices at room temperature.

It can be observed from Figure 2 that at -1.5 V reverse bias, the lower leakage current was obtained in PANI/(311)B n-GaAs devices (2.0×10^{-6} A) compared to the PANI/(100) n-GaAs (2.0×10^{-5} A) and PANI/(110) n-GaAs (0.12 A) devices. The increase or decrease in the leakage current, which could be due to an increase or decrease in the number of natural or manufacturing defects (Al Saqri et al., 2017; Jameel et al., 2019). The leakage current values of the fabricated devices in this work are lower than those achieved by Halliday et al. (1999) and Jameel et al. (2015). Additionally, it can be seen from Figure 2 that, for all three devices, the forward bias I - V measurements deviate significantly from linearity with increasing voltage. This could be related to the effects of series resistance (Rebaoui et al., 2017). Moreover, from Figure 2 at the applied voltage of ± 1 V, it was observed that the values of diode rectification ratio (which can be determined by dividing the forward current (I_F) to the reverse current (I_R)) for PANI/(100) n-GaAs, PANI/(110) n-GaAs and PANI/(311)B n-GaAs devices are 5.35, 1.13 and 15.23, respectively as exhibited in Table 2. The ohmic behavior of the Au/PANI/Au/glass structure is obtained from the dark I - V curve as illustrated in Figure 3. The linear straight-line of the obtained I - V curve is sufficient evidence to verify that the PANI is making ohmic contact with Au.

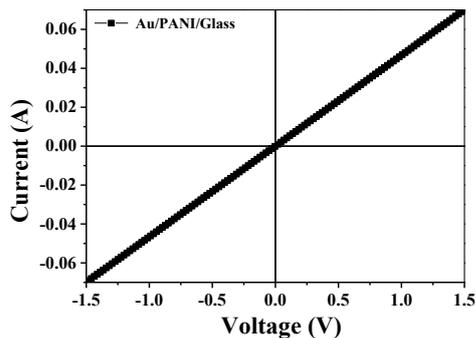


Figure 3. Shows the Ohmic behavior between gold contact and conducting polymer (PANI).

The turn-on voltage (V_{on}) of the three samples is determined from the linear I - V curve as demonstrated in Figure 4. The turn-on voltages were found by the extrapolation of the straight-line through the forward region of the I - V curve to the zero-current value. It was noted from Figure 4 that the

Table 2. Summary of solar cell parameters for PANI/(100), (110), and (311)B n-GaAs devices at room temperature and under dark conditions.

Sample ID	I_F/I_R	V_{on} (V)	R_s (K Ω)	R_{sh} (K Ω)	I_o ($\times 10^{-7}$ A)	n	ϕ_b (eV)
(100)	5.35	0.53	51.6	71.0	0.16	3.95	0.75
(110)	1.13	0.07	0.009	0.012	15000	4.42	0.45
(311)B	15.23	0.67	18.4	77.2	0.03	3.16	0.79

sample with (311)B crystal orientation has a higher V_{on} value of 0.67 V as compared to 0.53 V and 0.07 V achieved for the (100) and (110) crystal orientation, respectively as displayed in Table 2. This could be one of the reasons for obtaining high efficiency for the PANI/(311)B n-GaAs devices.

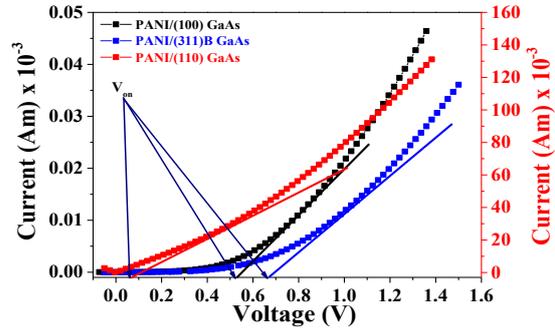


Figure 4. The turn-on voltage (V_{on}) values of PANI deposited on (100), (110), and (311)B n-GaAs substrates.

The diode parameters such as reverse saturation current (I_o), barrier height (ϕ_b), ideality factor (n) and series resistance (R_s) were determined using thermionic emission equation which is expressed by (Coskun et al., 2003; Sze, 2002):

$$I = I_o \left[\exp\left(\frac{q(V - IR_s)}{nkT}\right) - 1 \right] \quad (2)$$

Where

$$I_o = A^*ST^2 \exp\left(\frac{-q\phi_{b0}}{kT}\right) \quad (3)$$

The values of I_o were calculated by extrapolating the straight-line portion in the $\ln(I)$ versus V plot (see Figure 5).

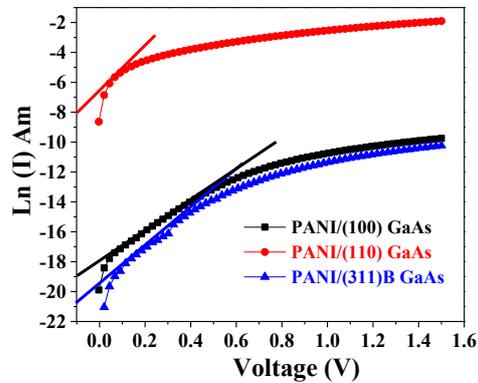


Figure 5. Dark $\ln(I)$ versus forwarding bias voltage (V) characteristics of PANI/(100) n-GaAs, PANI/(110) n-GaAs, and PANI/(311)B n-GaAs hybrid solar cell devices at room temperature.

When I_o is obtained, the zero-bias barrier height ϕ_b can be determined utilizing the following equation (Salehi et al., 2006):

$$\phi_b = \frac{kT}{q} \ln\left(\frac{SA^*T^2}{I_o}\right) \quad (4)$$

The ideality factor (n), which is a measure of diode conformity behavior to pure thermionic emission, can be found using the plot $\ln I$ versus V (Figure 5) and with the Equation 5

$$n = \frac{q}{kT} \left(\frac{dV}{d \ln I} \right) \quad (5)$$

In the above equations, V is the forward-bias voltage, q is the electronic charge, T is the absolute temperature, k is the Boltzmann constant, A^* is the effective Richardson constant of $8.16 \text{ A.cm}^{-2}.\text{k}^{-2}$ for n-type GaAs and S is the effective diode area.

The natural log-linear I - V curves and summary of solar cell parameters under the dark condition of the fabricated device with three different structures of Au/PANI/(100) n-GaAs/(Ni-Au), Au/PANI/(110) n-GaAs/(Ni-Au), Au/PANI/(311)B n-GaAs/(Ni-Au) are illustrated in Figure 5 and Table 2.

According to the thermionic emission theory, the saturation current I_0 , for all three devices at room temperature and in dark, is obtained from intercepts of the plot of forward-bias $\ln(I)$ versus V (Figure 5). The value of I_0 is calculated to be $1.6 \times 10^{-8} \text{ A}$ for the PANI/(100) n-GaAs, $1.5 \times 10^{-3} \text{ A}$ for PANI/(110) n-GaAs, and $3.0 \times 10^{-9} \text{ A}$ for PANI/(311)B n-GaAs heterojunctions. I_0 of PANI grown on (311)B n-GaAs orientation is higher than that of PANI grown on (100) and (110) n-GaAs substrates. Additionally, the barrier height ϕ_b measured employing Equation 4 have shown the values of 0.75 eV, 0.45 eV, and 0.79 eV for the PANI grown on (100), (110), and (311)B n-GaAs planes, respectively, as displayed in Table 2. The ϕ_b value of PANI fabricated on (311)B n-GaAs is higher than those of (100) and (110) devices. This value is also higher than those ϕ_b values reported by Halliday et al. (1999) and Jameel et al. (2015). Taking into consideration these values are also better than those values determined by Zaidan et al. (2011). The low value of I_0 yields the high value of ϕ_b for PANI/(311)B n-GaAs device. The high value of saturation current I_0 is probably due to defects that play as trapping or recombination centers (Jameel et al., 2015). Therefore, one can infer that the PANI/(311)B n-GaAs sample has low defects which indicates low recombination as compared with PANI/(100) n-GaAs and PANI/(110) n-GaAs samples. This resulted in a high value of ϕ_b and subsequently increases the efficiency of the solar cell and device performance. However, the ideality factor n can be extracted from slope of the forward natural log-linear I - V curve (Figure 5) using Equation 5. The lowest value of the n (3.16) was achieved for (311)B sample as compared to n (4.42) and n (3.95) of PANI samples deposited on (100) and (110) n-GaAs substrates, as exhibited in Table 2. Taking into account the fact that the n value is equal to 1 for an ideal diode, it is found that for all the three samples the n values are higher than unity, but the PANI/(311)B n-GaAs heterostructures show the closest result to the ideal case. It is important to point out that the higher ϕ_b and lower n values for the PANI samples grown on (311)B n-GaAs substrate are the strong evidence of its better electrical properties when compared with PANI/(100) n-GaAs and PANI/(110) n-GaAs heterojunctions. It can also be noted that the electrical properties of the PANI/(100) n-GaAs solar devices are better than those of the PANI/(110) n-GaAs solar devices. As a result, the substrate orientation has a significant effect on the optical and electrical properties of the solar cell devices. Comparing the results presented in Tables I and II it is observed that the PANI/(311)B n-GaAs solar device has the highest efficiency, the highest barrier height, which means higher V_{oc} , and the lowest reverse saturation current as well as the lowest ideality factor. The value of series resistance (R_s) and Shunt resistance (R_{sh}) was calculated from the dark I - V measurements. The value of R_s is calculated to be 51.6 k Ω , 0.009 k Ω , and 18.4 k Ω for the PANI sample deposited on (100), (110), and (311)B, respectively. Whereas R_{sh} value for PANI/(100) n-GaAs, PANI/(110) n-GaAs and PANI/(311)B n-GaAs devices is found to be 71.0 k Ω , 0.012

k Ω , and 77.2 k Ω , respectively. Samples with (110) crystal orientation have significantly lower values of R_s , R_{sh} , and barrier height (ϕ_b) comparing with (100) and (311)B as shown in Table 2. These results indicate that the PANI sample fabricated on (110) n-GaAs substrate has almost ohmic behavior which means no rectification as well. As described above and indicated in Tables I and II, the crystal orientation affects strongly the solar cell efficiency and junction parameters. These considerable differences are could be due to recombination of photo-generated charge carriers resulted from the weak built-in potential or narrow depletion width between conducting polymer (PANI) and inorganic semiconductor n-GaAs (Jameel et al., 2015).

4. CONCLUSION

In this paper spin coating method has been used for deposition of conducting polymer (PANI) on three n-GaAs substrates with (100), (110), and (311)B crystal orientations. The solar cell and diode junction parameters have been investigated through measuring J - V and I - V measurements under light and dark conditions, respectively. The J - V results of the three samples revealed that the value of the efficiency (η) of ($19.6 \times 10^{-3} \%$) for PANI/(311)B n-GaAs hybrid photovoltaic devices is higher than of ($2.2 \times 10^{-4} \%$) for PANI/(100) n-GaAs and of ($1.85 \times 10^{-5} \%$) for PANI/(110) n-GaAs heterostructure solar cell devices. Moreover, a higher leakage current and lower turn-on voltage (V_{on}) values in the PANI sample deposited on (110) and (100) n-GaAs could be attributed to more recombination than in the PANI/(311)B n-GaAs heterostructure device. The low value of saturation current (I_0) and the high value of barrier height (ϕ_b) for PANI fabricated on (311)B n-GaAs plane also confirm that the substrate orientation of n-GaAs results in an increase of efficiency and electrical performance. This is also confirmed by the lower value of ideality factor n obtained in the PANI/(311)B n-GaAs hybrid devices (3.16) compared to the PANI/(100) n-GaAs (3.95) and PANI/(110) n-GaAs (4.42) devices. Therefore, the crystal orientation of the n-GaAs substrate strongly affects the electrical performance of PANI/n-GaAs hybrid photovoltaic devices.

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