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Electrical characteristics of Au/Ti/n-GaAs contacts over a wide measurement temperature range

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Abstract
We have fabricated Au/Ti/n-GaAs/In Schottky barrier diodes using the magnetron dc sputter technique. The capacitance–temperature (C–T) measurements with bias voltage as a parameter and the current–voltage (I–V) and capacitance–voltage (C–V) measurements have been made in the temperature range of 60–300 K. The temperature-dependent capacitance measurements have been made at 1.0 MHz. The capacitance versus temperature curve at each bias voltage has four regions with slopes different from each other. The capacitance decreases with a decrease in temperature at each bias voltage. Such a temperature-dependent behavior could be attributed to modulation of the space charge region caused by the emission of deep-level impurities or interface states. The carrier concentration calculated in the $-1.0$ to $-2.0$ V range of $C^{-2}$–$V$ plots was close to the value of $7.43 \times 10^{15}$ cm$^{-3}$ given by the manufacturer around room temperature. The ideality factor value from the $I$–$V$ characteristics has remained almost unchanged between 1.07 and 1.10 in the temperature range of 150–300 K, indicating that the current across the device obeys the thermionic emission current model quite well over the whole bias range at temperatures above 150 K. Therefore, the conventional Richardson plot in this temperature range has given a Richardson constant of $8.21$ A (cm K)$^{-2}$, within experimental error, which is in very close agreement with the theoretical value of $8.16$ A (cm K)$^{-2}$ for n-type GaAs. Again, it has been seen that the ideality factor with the values of 1.10 at 150 K and 1.22 at 60 K does not show a considerable decrease. The experimental parameters show that the Au(90 nm)/Ti(10 nm)/n-GaAs contact is a good candidate for electronic device applications.

Keywords: metal semiconductor contacts, GaAs semiconductor, thermionic emission

(Some figures may appear in colour only in the online journal)

1. Introduction

Metal–semiconductor (MS) rectifying or ohmic contacts are of great importance for device applications such as organic photovoltaic solar cells, p–n junctions, bipolar transistors, metal–semiconductor field effect transistors (MESFETs) and high-electron mobility transistors (HEMTs) [1–3]. The MS contact theory serves as the foundation of the physics of semiconductor devices in modern electronic applications and in understanding other semiconductor devices [1–7]. The
refractory metal gate technology has been used for the fabrication of high-speed MESFETs to reduce the parasitic overlap capacitances between gate and source and series resistance and thus to improve the speed–power performance [5–9]. The occupancy of substrate traps is affected by temperature variations, illumination, or irradiation, and this is true of the space charge region. For this reason, the variation of device parameters over a wafer may arise from the nonuniform distribution of traps in the wafer as well as the interface states [1–7].

Schottky contacts play an important role in controlling the electrical performance of devices. Sehgal et al [10, 11] have investigated the thermal stability of Au/Pt/Ti Schottky contacts on n-GaAs with Ti films of 0–60 nm. They have found [10, 11] that by introducing the Ti film between GaAs and Au/Pt the interdiffusion of Pt and Au is also prevented. These results are useful for reducing the gate metallization resistance of MESFET transistors, and these contacts can next be used to fabricate submicrometer gate length GaAs MESFETs. Arulkumaran et al [12] have analyzed silicon doped Ti/n-GaAs Schottky barrier diodes (SBDs) formed by the evaporation method and obtained a barrier height (BH) of 0.78 eV for these diodes at room temperature. Dio et al [13] have reported forward and reverse current–voltage (I–V) characteristics for Ti/GaAs diodes prepared by ion beam sputtering, and they have shown [13] that the I–V analysis in the temperature range of 100–360 K indicates that the thermionic emission (TE) is the main transport mechanism for all the samples, although there are deviations from this behavior at low temperature. They have obtained [13] an average of 0.81 eV for Ti/n-GaAs diodes prepared at different sputtering voltages and currents, and have interpreted the departure from ideal conditions as a direct effect of BH inhomogeneities at the metal–semiconductor interface. Therefore, the performance of GaAs based devices especially depends on the surface and interface defect density, series resistance, temperature and applied bias voltage [1–9].

We have investigated measurement temperature capacitance–voltage (C–V) and I–V characteristics of Au/Ti/n-GaAs/In SBDs in the temperature measurement range of 60–300 K. We have fabricated the Au/Ti/n-GaAs/In diodes using the magnetron dc sputter technique. The Au thin films have been used as a top layer to protect the Ti metallic layer on the GaAs substrate [14]. As mentioned by Forment et al [15], gallium arsenide is an important semiconductor for optoelectronics, fast computers and microwave applications and Ti/n-GaAs yields a high barrier. As is well known, if the following current in a Schottky barrier obeys the thermionic emission current model quite well in a given temperature range, the experimental conventional Richardson plot of the saturation currents in this temperature range should give an expected Richardson constant (RC) value for the semiconductor substrate which is in very close agreement with the theoretical value within experimental error. Our purpose is to investigate whether the experimental conventional RC value of the semiconductor substrate used in the fabrication of such a Schottky diode really is in very close agreement with the theoretical RC value or not, and moreover to show experimentally how the device capacitance under the bias voltage changes with the temperature.

**Experimental details**

The Au/Ti/n-GaAs SBDs structures were fabricated using an n-type single crystal GaAs wafer with (100) surface orientation, having 400 nm thickness, 2 inch diameter, 7.43 × 10^{15} cm^{-3} carrier concentration and 1.2 Ω cm resistivity (given by the manufacturer). Then, the wafer was rinsed in DI water of 18 MΩ cm resistivity for an extended time and dried under N2 flow. After surface cleaning of the n-GaAs, high purity (99.999%) indium with a thickness of about 2000 Å was coated with at a pressure of about 10^{-6} Torr in a high vacuum system. To form a good ohmic contact, the n-GaAs wafer with the ohmic contact was annealed at 385 °C for 3 min under N2 atmosphere. For the Schottky contacts, the n-GaAs wafer was placed on a rotating table. Ti(10 nm) Schottky contacts are made using the magnetron dc sputter technique, and Au(90 nm) was evaporated as a top layer on the Ti/n-GaAs structure to protect the Ti metallic layer in high vacuum system of 10^{-6} Torr. Ti and Au Schottky contacts were squares with 0.01 cm² area. After the fabrication process, the I–V characteristics of the Au/Ti/n-GaAs were measured using a Keithley 2400 SourceMeter. All measurements were made in the temperature range of 60–300 K using a temperature controlled Janis vpf-475 cryostat, which enables us to make measurements in the temperature range of 20–450 K. The sample temperature was always monitored by use of a copper–constantan thermocouple close to the sample and measured with a Keithley model 199 DMM scanner and Lakeshore model 321 auto-tuning temperature controller with sensitivity better than ±0.1 K.
2. Results and discussion

Figure 1 shows the experimental capacitance versus temperature curves for the Au/Ti/n-GaAs SBD, where the capacitance is a function of the measurement temperature with the bias voltage as a parameter at 1.0 MHz. The capacitance decreases with a decrease in temperature at each voltage. It can be seen from figure 1 that there are four regions with different slopes from 60 to 300 K at each bias voltage. It can be said that the deep level or interface states with different densities and energies affect each region. The slopes decrease with bias voltage decreasing from +0.20 to −2.0 V. That is, the slopes at −2.0 V are lower than those at +0.20 V, depending on the measurement temperature. Such a temperature-dependent behavior of the capacitance could be attributed to modulation of the space charge region caused by the emission of more carriers from the required levels such as deep-level impurities or interface states [2, 3, 16]. As is well known, a C–V plot in the idealized case should show an increase in capacitance with increasing forward voltage independent of temperature and frequency. However, the experimental results had shown that the capacitance in the C–V plot might be influenced by the nonidealities [2, 3, 17–23]. Figure 2 shows the C–V characteristics of the Au/Ti/n-GaAs SBD at 1.0 MHz in the temperature range of 60–300 K with steps of 10 K. The C–V characteristics were measured in +0.20 to −2.0 V range at each temperature, where the forward bias branch ranges from 0.00 to 0.20 V, and the reverse bias branch ranges from 0.00 to −2.0 V. As can be seen from figure 2, the decrease in capacitance in the reverse bias from 0.00 to −2.0 V implies an increase in the semiconductor depletion width. Since the charge neutrality condition at the interface should be satisfied, widening of the depletion width in the reverse bias C–V characteristics results from a reduction of the ionized donor concentration.

Figure 3 shows the reverse and forward bias C–2–V curves from the data in the temperature range of 60–300 K in figure 2. The C–2–V curves show two linear regions separated by a transition segment, especially from 300 to 130 K. That is, the curves have two slopes in the temperature range of 130–300 K and then trend approximately to have a single slope over the whole voltage range with decreasing temperature. The constant slope yields a uniform doping concentration. This behavior may be due to a change of the carrier concentration profile depending on the sample temperature. The straight line intercepts of the C–2–V plots with the voltage axis were obtained from both linear regions at each temperature. The C–V BH and carrier concentration values are determined from intercepts and slopes of the straight lines in the C–2–V plots for each temperature. These values are given in figures 3 and 4.

Figure 4 shows the carrier concentrations calculated from the two present slopes at each temperature in figure 2. As seen from figure 4, the difference between the carrier concentrations for the two regions decreases with decreasing temperature. It can be said that the carrier concentration has almost the same value from 60 to 120 K. For example, the carrier concentration is 3.21 × 10^{15} and 3.10 × 10^{15} cm^{-3} at 60 K while it is 7.48 × 10^{15} and 4.53 × 10^{15} cm^{-3} at 300 K for the two mentioned regions in figure 3. Furthermore, the carrier concentration decreases with a decrease in temperature because more electrons may be frozen at the required state levels in the freeze-out region, and it remains almost constant from 60 to 120 K. Moreover, the value of 7.48 × 10^{15} cm^{-3}
from the slope in the −1.0 to −2.0 V range at 300 K is in close agreement with the value of 7.43 × 10^{15} cm\(^{-3}\) given by the manufacturer. Thus, when these values and figure 3 are considered, it can be said that the slope in the −1.0–0.0 V range becomes more pronounced with increasing temperature. That is, it can be said that the bulk deep levels or interface states are more effective and they lead to reduction of the carrier concentration in about the −1.0–0.0 V range at each temperature above 120 K. In addition to these, it was found by Vandenbroucke [22] that a large density of donor-like defects for the diodes with a sputter-deposited metal contact is present in the near-surface region, together with a region of decreasing density deeper into the semiconductor. These donor-like states in the surface region, induced during bombardment of the substrate, are believed to be responsible for the observed electrical behavior [3]. The carrier concentration remains almost constant as the temperature is decreased from 60 to 120 K. More electrons may be frozen at the donor level in the freeze-out region.

As mentioned above, figure 5 shows the obtained C–V BH values (open triangles) from the C\(^{-2}\)–V plots for each temperature. The BH value has linearly increased from 0.81 eV at 300 K to 0.89 eV at 120 K, and has deviated from linearity at temperatures below 120 K. The temperature coefficient of the BH can be determined from this plot. The temperature dependence of the BH is expressed as \(\Phi(T) = \Phi(T = 0) − \alpha T\). According to the equation, the slope of the straight line yields a value of \(\alpha = −0.54 \text{ meV K}^{-1}\), called the temperature coefficient value of the BH. Passler [23], Thurmond [24] and Lautenschlager et al. [25] indicated the values of −0.472, −0.5405 and −0.55 meV K\(^{-1}\) for the temperature coefficient of the energy band gap of n-type GaAs, respectively. The variation of the BH value with temperature is normally explained within the frame of the Fermi level pinning concept due to the temperature dependent variation in the band gap [24, 25]. The temperature coefficient of the BH obtained by us is approximately equal to the temperature coefficient of the energy gap of n-type GaAs.
Figure 6 shows the semi-log current–voltage curves of the Au/Ti/n-GaAs Schottky barrier diode in the temperature range of 60–300 K. The experimental values of the ideality factor and SBH have been calculated from the intercept and slope of the linear portion of the forward-bias ln $I$–$V$ plot at each temperature in figure 6. The intercept of the linear portion corresponds to the saturation current at $V = 0$ volts.

Figure 7 shows the SBH versus measurement temperature plot for the device in the temperature range of 60–300 K. The SBH value has increased from 0.77 eV at 300 K to 0.81 eV at 180 K with a slope of $-0.24 \text{ mV K}^{-1}$, and has remained almost at the same value as 0.81 eV in the 130–180 K range. The dashed straight line in figure 7 shows a fit to experimental data in the 130–300 K range. Again, the BH value has sharply decreased from 0.82 eV at 130 K to 0.48 eV at 60 K. The decrease of the BH in the 60–130 K range is in very close agreement with the results obtained in [26–29]. It has been mentioned in [26] that the BH is not temperature dependent but rather the current transport mechanisms. In fact, the current processes are temperature dependent and consequently the extraction of the BH indicates that the BH changes with temperature [26]. When varying the temperature different current mechanism changes too [26].

The ideality factor value of the device has remained almost unchanged between 1.07 and 1.10 in the temperature range of 150–300 K, and has decreased from 1.10 at 150 K to 1.22 at 60 K. These values are given in table 1. Göksu et al [9] obtained the BH and ideality factor values of 0.62 and 1.61 (at 60 K) and 0.91 and 1.02 (at 320 K) for Ti/n-GaAs SBDs without an Au layer prepared by magnetron DC sputtering, respectively. Arulkumaran et al [12] have obtained a BH of 0.78 eV at room temperature for Ti/n-GaAs SBDs formed by the evaporation method. Dio et al [13] have obtained an average of 0.81 eV for Ti/n-GaAs diodes prepared at different sputtering voltages and currents. The values of the ideality factor near unity indicate that the experimental $I$–$V$ data obey the TE current model quite well over the whole

![Figure 7. Barrier height versus measurement temperature plot for Au/Ti/n-GaAs structure in the temperature range of 60–300 K. The dashed straight line shows a fit to experimental data in the 130–300 K range.](image)

![Figure 8. $nT$ versus $T$ plot showing the $T_0$ anomaly for the Au/Ti/n-GaAs structure in the temperature range of 60–300 K. The solid line is ideal Schottky diode behavior given as ideality factor $n = 1$; the dashed straight line shows a fit to experimental data.](image)

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>$\Phi_b$ (eV)</th>
<th>$n$</th>
<th>$I_0$</th>
</tr>
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<tr>
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<td>0.770</td>
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<tr>
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<td>180</td>
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<td>0.475</td>
<td>2.221</td>
<td>$3.30 \times 10^{-38}$</td>
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</table>
bias range at temperatures above 150 K. The values of the SBH and ideality factor have been calculated using equation (1) and (2), called the TE current relationships, given in [1–3]. The case can be seen more clearly in figure 8, which shows the nT versus T plot for Au/Ti/n-GaAs in the temperature range of 60–300 K. This is called the T0 anomaly plot determining the temperature dependence of the ideality factor n. The solid line in figure 8 is ideal Schottky diode behavior given as n=1, which goes through the origin. The dashed straight line fitted to experimental data for information about the T0 effect should be parallel to the ideal Schottky line. A value of T0=11.28 K was obtained from the experimental plot. As can be seen from figure 8, the dashed straight line significantly deviates from linearity below 120 or 130 K. It has been pointed out in [27–33] that the change at low temperatures may be ascribed to the current flow through small regions, so-called ‘patches’, with low BH. The conventional Richardson ln(I0/T^2) versus (kT)^{-1} plot in the temperature range of 60–300 K in figure 9 is linear in the 120–300 K range, where I0 is the saturation current in the TE current expression [1–3]. Therefore, it has given an RC of 8.21 Α (cm K)^{-2} from the conventional Richardson plot (figure 9), within experimental error. This value is in very close agreement with the theoretical value of 8.16 Α (cm K)^{-2} for n-type GaAs. Thus, it can be said that the I–V characteristics of the device obey the TE current model in the 120–300 K range [34–41].

As is well known, when the MS Schottky diodes are characterized by I–V and C–V data, the BH calculated from the C–V data is higher than the BH value extracted from the saturation current of the semi-log forward bias characteristics and gives an average value of the BHs of the patches present in the Schottky contact. The mentioned saturation current is the intercept of the linear portion of the semi-log forward bias curve. Osvald [33] says that the I–V and C–V measurement techniques are differently sensitive to possible occurrence in the inhomogeneous Schottky contacts at especially low temperatures. Because the current of the Schottky diode depends exponentially on the BH, the inhomogeneities and small patches with lower BH in the contact strongly influence the resulting apparent BH [28–41].

The BH of the Au/Ti/n-GaAs/In can be also calculated by Norde’s method [42], because the device shows an ideal behavior. A function F(V) was derived from the TE current expression by Norde [40]:

\[ F(V) = \frac{V}{\gamma} - \frac{kT}{q} \ln \left( \frac{I(V)}{A^* A_0 T^2} \right) \]

where the current I(V) is obtained from the I–V curves at each temperature in figure 6. This function can be used to determine the BH [42]. Figure 10 shows the F(V) versus V plots obtained using the experimental I–V data in equation (1). The BH relation is given as follows [38]:

\[ \Phi(T) = F(V_{min}) + \frac{V_{min}}{2} - \frac{kT}{q} \]

where F(V_{min}) is the minimum value of F(V) and the corresponding voltage and current are V_{min} and I_{min}, respectively. The BH values from the F(V)–V curves are given as a function of temperature in figure 4 (indicated by open squares). The expressions (1) and (2), which are called Norde’s functions, are based on the TE current mechanism [2, 3, 42, 43].

The BH value has linearly increased from 0.81 eV at 300 K to 0.89 eV at 120 K, and deviates from linearity at temperatures below 120 K. As can be seen from figure 5, the BH values calculated by Norde’s method and C–V characteristics coincide with each other in the temperature range of 120–300 K, but not at low temperatures below 120 K. As
indicated above, the BH values calculated from the C−V data give an average value of the BHs of patches present in the Schottky contact. Thus, it can be said that Norde’s method used to calculate the BH value in the ideal Schottky diodes gives approximately an average value of the BHs at each temperatures except for low temperatures [28, 42, 43]. The temperature coefficient of the BH can be also determined from this plot. The fitting to the $\Phi(T)$ data equation above yields a straight line with the slope of $\alpha = -0.51$ meV K$^{-1}$ called the temperature coefficient value of the BH. This result has been also confirmed by the temperature coefficient value (open triangles) of $\alpha = -0.54$ meV K$^{-1}$ from $C^{-2}$−V curves in figure 4.

In conclusion, the I−V characteristics of the device have almost given the diode parameters independent of the measurement temperature at temperatures above 130 K. It can be said that the Au/Ti/n-GaAs/In diodes fabricated by the magnetron DC sputter technique are a candidate for electronic device applications. The BH value from the I−V data of the device has increased from 0.77 eV at 300 K to 0.82 eV at 180 K, and has remained at almost the same value in the 130−180 K range. Furthermore, it has been found that the experimental conventional RC value of the semiconductor substrate used in the fabrication of the Schottky diode is really in very close agreement with the theoretical RC value, because the I−V characteristics of the device obey the TE current mechanism in the 120−300 K range. The capacitance versus temperature curves plotted as a function of the bias voltage characteristics have given four regions with different slopes at each bias voltage, and the slopes decrease with decreasing voltage from 0.20 to −2.0 V. A carrier concentration value of $7.43 \times 10^{15}$ cm$^{-3}$ was calculated from the $C^{-2}$−V plots around room temperature, which is close to the value given by the manufacturer.

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