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Temperature dependent ideality factor and barrier height of Ni/*n*-GaAs/In Schottky diodes

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ABSTRACT

Temperature-dependent current–voltage (*I–V*) characteristics of Ni/*n*-GaAs/In Schottky diodes which are fabricated by magnetron DC sputtering system have been studied. The zero-bias barrier height (BH) versus temperature plot involves two distinct regions. At low temperatures, the zero-bias BH increases with increasing temperature due to lateral distribution of the barrier height. Werner and Güttler's model has been employed to analyze the temperature dependence of barrier height and ideality factor at low temperatures. The standard deviation of the zero-bias BH was calculated as 64 mV and the voltage coefficients of the barrier height were determined as $\rho_2 = -6.94 \times 10^{-4}$ and $\rho_3 = -5.73$ mV. At high temperatures, the zero-bias BH decreases with increasing temperature because of the temperature dependence of semiconductor band gap. The non-linearity has been observed in the Richardson plot due to temperature dependence of the zero-bias BH. Furthermore, the T_0 effect and the temperature dependence of flat band BH of the diodes were investigated.

1. Introduction

It is well known that the quality of metal-semiconductor contacts plays an important role in the performance of various semiconductor devices and integrated circuits [1–5]. Especially, Schottky (i.e. rectifying) barrier contacts can be used for a wide variety of device applications such as MESFET's, switching, photovoltaic [6]. Besides different device and circuit applications, Schottky contacts can also be used as test vehicles for exploring the physical and electrical properties of a semiconductor material and its surface [1,7].

Much of our comprehension of metal-semiconductor contacts is reached by interpreting the electrical characterization of Schottky barrier contacts [8]. According to the classical model of Schottky barrier contact, the barrier height value does not vary from region to region and the metal-semiconductor interface is abrupt [9,10]. However, such a description fails to account for an abnormal decrease of the zero-bias barrier height and an increase in the ideality factor which are usually observed with decrease in temperature (T). In Schottky diodes when current–voltage (*I–V*) data are analyzed in terms of thermionic emission (TE) theory [9,11–14]. In recent years, the existence of a strong dependence of the experimentally observed Schottky barrier heights (SBHs) and ideality factor on the temperature is attributed to lateral inhomogeneities in the SBH [10,15–17]. Several authors have described lateral inhomogeneities in the SBH with a Gaussian distribution [9,10,17]. Werner and Güttler who assume the inhomogeneity of SBH has a Gaussian distribution have tried to explain the transport properties of inhomogeneous Schottky contacts [17]. They have showed that the transport properties of inhomogeneous Schottky contacts are strongly affected by spatial fluctuations in the BH. Their model has been successfully applied by several authors to analyze the temperature-dependent *I–V* data of Schottky barrier contacts [10,13,18–21].

III–V compound semiconductors are of great importance due to their applications in various electro-optic devices [2]. In particular, metal-semiconductor contacts formed by metal deposition on GaAs are employed in light detectors, solar cells, microwave communication devices, and high-speed microelectronic applications [2,22]. Furthermore, GaAs devices can be used in high frequency applications because of its unique properties such as high electron mobility and high saturated electron velocity [23]. Therefore, it is essential to obtain better understanding of the fundamental physical and electrical properties of the metal-GaAs Schottky barrier contacts so that the performance of the GaAs devices can be improved [1].

In this study, we have investigated the *I–V* data of Ni/*n*-GaAs/In Schottky diodes in a wide temperature range of 60–320 K which are fabricated by magnetron DC sputtering system. The data have been analyzed by utilizing the very well known analytical tools. At low temperatures, the temperature dependence of barrier height and ideality factor of the Ni/n-GaAs/In Schottky diodes has been interpreted by means of potential fluctuations model developed by Werner and Güttler [17].

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2. Experimental procedure

The Schottky diodes have been prepared by using cleaned and polished n-GaAs with (1 0 0) orientation and 1.46×10^{16} cm^{-3} carrier concentration. Before making contacts, the wafer was degreased consecutively in trichloroethylene, acetone, and methanol for 3 min and all metals were cleaned in acetone and methanol. After this process, the wafer and metals were rinsed in deionized water with 18 MΩ resistivity. The n-GaAs wafer was dipped in a $5H_2SO_4$:-H_2O_2:H_2O solution for 1.0 min to remove any layers with surface damage and undesirable impurities, and then in a H_2O:HCl solution followed by rinsing with the deionized water. The wafer was then dried with high-purity nitrogen and inserted into the deposition chamber immediately after the etching process. For ohmic contacts, in was evaporated on the back of the wafer in the vacuum-coating unit at 10^{-5} Torr. Then a low resistance ohmic contact was formed by thermal annealing at 380 °C for 3 min in flowing N_2 in a quartz tube furnace. The Schottky metallization of Ni was deposited by magnetron DC sputtering, and their shape was a circular dot with a diameter of 1.5 mm. The thickness of Ni was approximately 50 nm. Thus, Ni/n-GaAs/In Schottky diodes have been fabricated. The temperature dependence of the I–V characteristics was measured in the temperature range of 60–320 K using a Leybold Heraeus closed-cycle helium cryostat that enables us to make measurements in the temperature range of 10–340 K, and a Keithley Model 2400 SourceMeter in the dark. The sample temperature was always monitored by a copper constantan thermocouple and a Windaus MD850 electronic thermometer with sensitivity better than ±0.1 K.

3. Results and discussions

3.1. I–V Characteristics

When the current flow through a Schottky diode can be described by thermionic emission theory, the I–V relationship of Schottky diode is given by [3].

$$I = AA*T^2 \exp\left(-\frac{q\Phi_b^{eff}}{kT}\right)\left[\exp\left(\frac{q(V-IR_s)}{kT}\right)-1\right], \quad (1)$$

where A is the area of the diodes (cm^2), $A*$ is the effective Richardson constant (8.16 A/cm^{2}K^2 for n-GaAs), T is the temperature (K), q is the electronic charge (C), k is the Boltzmann's constant (J/K), $\phi_b{}^{eff}$ is the effective BH at a given bias (eV), and R_s is the series resistance (Ω). The effect of the series resistance can be neglected in the low current region where the semilog I–V characteristic is linear.

In general, the existence of deviations from thermionic emission theory and the voltage dependence of the barrier height are represented by addition of ideality factor (n) to Eq. (1). The relationship between $\Phi_b{}^{eff}$ and n is given by the following expression [3,24],

$$\Phi_b^{eff} = \Phi_{bo} + (1-\frac{1}{n})V \quad (2)$$

Here Φ_{b0} is the zero bias barrier height. The thermionic emission equation for moderate forward bias (where $V - IR_s > 3kT/q$) can be written by using Eqs. (1) and (2) as,

$$I = I_0 \exp(\frac{qV}{nkT}) \quad (3)$$

$$I_0 = AA*T^2 \exp(-\frac{q\Phi_{b0}}{kT}) \quad (4)$$

The saturation current (I_0) can be determined by extrapolating the forward bias semilog I–V characteristic to zero applied voltage. The slope of the linear portion of semilog I–V characteristic yields the value of ideality factor.

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

The semilog plots of the forward bias I–V characteristics of Ni Schottky diodes on n-GaAs (1 0 0) at various temperatures are shown in Fig. 1. The plots are linear over a wide range of current values. If the current transport across a Schottky contact is dominated by thermionic emission, the gradual shift of the I–V curves towards a higher voltage will be observed with decrease in temperature in accordance with Eq. (1) [13]. Fig. 1 reveals the current transport across the Ni/n-GaAs/In Schottky diodes is governed by the thermionic emission. For each temperature, the semilog forward bias I–V curves at high voltage are not linear and depict saturation behavior due to the existence of the series resistance [20,25].

The zero-bias BH and the ideality factor values calculated by using Eqs. (4) and (5) were plotted versus temperature in Fig. 2. As can be seen from the figure, the ideality factor decreases with the increasing temperature as in references [5,9,12–14,26–28]. The zero bias barrier height increases with the temperature up to 180 K and does not significantly change between 180 and 240 K. Then, it decreases slowly with the temperature up to 320 K. Similar result has been reported for Au/n-GaAs Schottky diodes [19].

If we consider that the temperature dependence of the zero bias barrier height is linear, the slope of the ϕ_{b0} vs. T plot will be large and positive in the range of 60–180 K. Conversely, the slope will be small and negative in the range of 240–320 K. In the light of above discussions, the temperature dependence of the zero bias barrier height between 240 and 320 K can be explained by the variation of the semiconductor band gap (E_g) with the temperature. In accordance with the temperature dependence of the GaAs band gap, the zero bias barrier height should increase as the temperature decreases [13]. It is worth noting that the zero-bias BH at low temperatures has shown strong temperature dependence and has opposite sign of the semiconductor band gap temperature coefficient [5,28,29]. Therefore, the temperature dependence of ϕ_{b0} is not attributed to the variation of the semiconductor band gap with temperature.

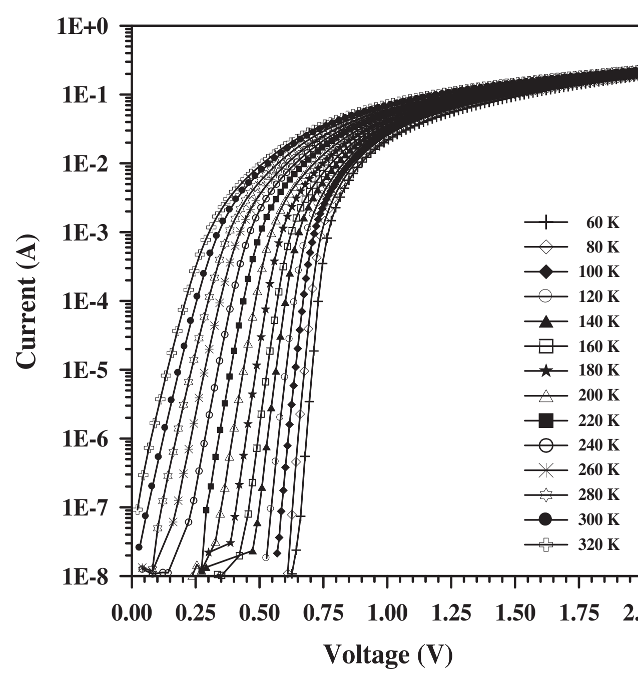

Fig. 1. Forward bias current–voltage characteristics of Ni/n-GaAs/In Schottky diodes at different temperatures in the range 60–320 K.

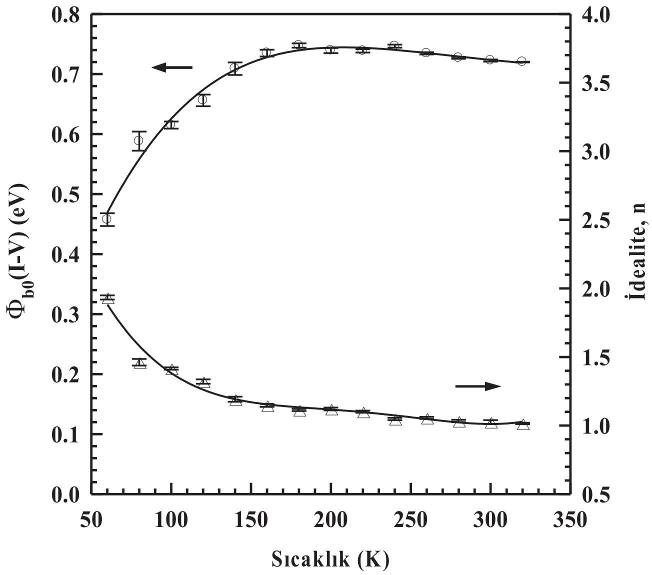

Fig. 2. Variation of zero bias barrier height and ideality factor with temperature for Ni/n-GaAs/In Schottky diodes.

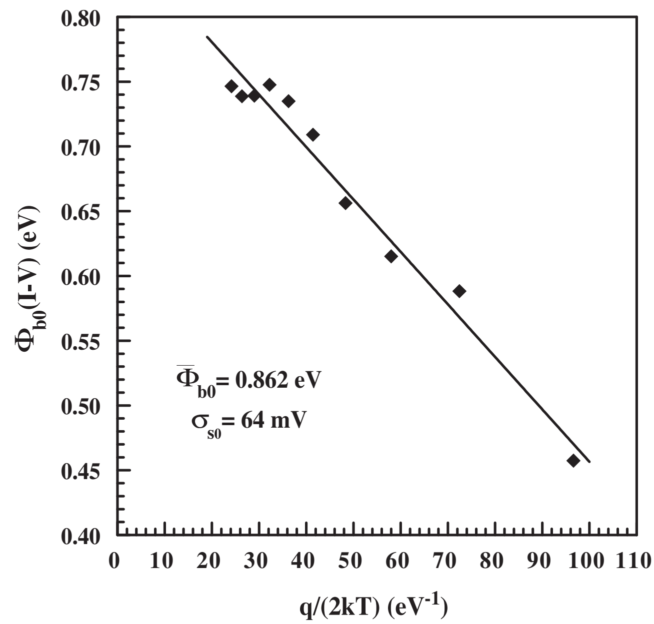

Fig. 3. Zero bias barrier height versus $q/2kT$ *plot* for Ni/n-GaAs/In Schottky diodes in the range 60–240 K.

This anomaly has been explained by the lateral distribution of the zero-bias BH [16,17]. The structural and morphological inhomogeneities at a metal-semiconductor (MS) interface can cause the barrier height (BH) to be spatially non-uniform [19]. The structural defects, grain boundaries in a metal, dislocations, stacking faults, doping inhomogeneity, and a mixture of different metallic phases are reasons of the inhomogeneities at the MS interface [8,17]. Recent studies have shown that zero-bias BH and ideality factor values obtained from I–V characteristics varies from diode to diode even if they are identically prepared [30–32]. Leroy et al. [31] have prepared 260 small Au/n-GaAs Schottky diodes. They have observed that zero-bias BH and ideality factor values exhibit a Gaussian distribution. They have used the Tung's [16] patchy model to explain their experimental results. Similar study has been made for Ni/n-GaAs [32]. Both studies have shown that there is a linear relationship between zero-bias BH values and ideality factor values that can be explained by lateral inhomogeneities.

Since the current transport across the MS interface is controlled by the thermionic emission over the Schottky barrier, the apparent barrier height depends on the temperature in the case of the existence of the Schottky barrier inhomogeneities at the MS interface. At low temperatures, it is intuitively clear that the current prefers to flow the region including low Schottky barriers. As the temperature increases, the current flows over regions including high Schottky barriers occurs as well as low Schottky barriers because the electrons have sufficient energy to flow over. As a result, the zero bias BH will increase with increasing temperature as in Fig. 2 [16,17,33,34].

It is commonly accepted that the BH has a Gaussian distribution with the zero bias mean BH ($\bar{\Phi}_{b0}$) and the Gaussian distribution of the BH is written by the following [10,17]:

$$\Phi_{b0} = \bar{\Phi}_{b0} - \frac{q\sigma_{s0}^2}{2kT}, \tag{6}$$

where σ_{s0} is the zero bias standard deviation of the BH distribution. From Fig. 2, it can be intuitively said that the distribution of the zero bias BH complies with the Gaussian distribution in the 60–240 K range. Therefore, the Gaussian distribution of the zero bias BH should be investigated in this range. Fig. 3 shows Φ_{b0} versus $q/2kT$ plots in the 60–240 K range. $\bar{\Phi}_{b0}$ and σ_{s0} were calculated as 0.862 eV and 64 mV, respectively, by using of linear fit to Φ_{b0} vs $q/2kT$ data. The value of σ_{s0} of our Ni/n-GaAs Schottky diodes is close with those reported for n-GaAs Schottky diodes in Refs. [5,12,14,17] and is not too large compared to the value of $\bar{\Phi}_{b0}$. Since the standart deviation is a measure of the barrier inhomogeneity [20], referring to 64 mV of σ_{s0}, it can be said that the interface quality of our Ni/n-GaAs Schottky diodes seems to be good.

The potential fluctuation model has been developed by Werner and Güttler [17] in order to explain the temperature dependence of the ideality factor. According to this model, the variation of the ideality factor with temperature is given by,

$$\frac{1}{n} - 1 = -\rho_2 + \frac{q\rho_3}{2kT} \tag{7}$$

where ρ_2 and ρ_3 are the voltage coefficients of the barrier height. In the case of temperature independent ρ_2 and ρ_3, a plot of n^{-1}-1 vs. $q/2kT$ should yield a straight line and those can be determined from the y-axis intercept and the slope of this plot. From Fig. 4, ρ_2 and ρ_3 were calculated as -6.94×10^{-4} and -5.73 mV in the temperature range of 60–240 K, respectively.

3.2. T_0 Effect

Most experimental results have showed that n may become temperature dependent [5,9,12–14,26–28]. The variation of n with temperature is called as "T_0 effect" or "T_0 anomaly" and can be expressed by the relation [35]

$$n = 1 + \frac{T_0}{T}, \tag{8}$$

where T_0 is a temperature independent constant. According to Eq. (8), nT vs. T plot will be a straight line and parallel to the unity slope line, if T_0 does not vary with the temperature. As can be seen in Fig. 5, the nT vs. T plot is linear, but it is not parallel to the unity slope line because of the temperature dependence of T_0 [14,28,36]. Similar behavior for Ni/n-GaAs diodes has been observed by several authors [14,28]. This case can be ascribed to presence of the high electric fields at the edge of the diode [36]. From Fig. 5, T_0 and the slope are determined as 51.23 and 0.85 K, respectively.

According to Werner and Güttler [17], Eq. (8) with the mysterious T_0 represents a coarse approximation to Eq. (7). In case of $\rho_2 \ll \rho_3/(2kT/q) \ll 1$, Eq. (8) may be written as:

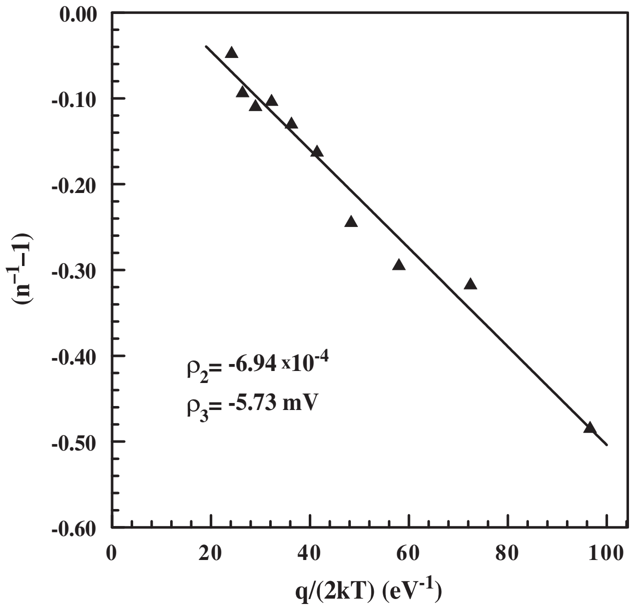

Fig. 4. $(n^{-1}–1)$ versus $q/2kT$ plot for Ni/n-GaAs/In Schottky diodes in the range 60–240 K.

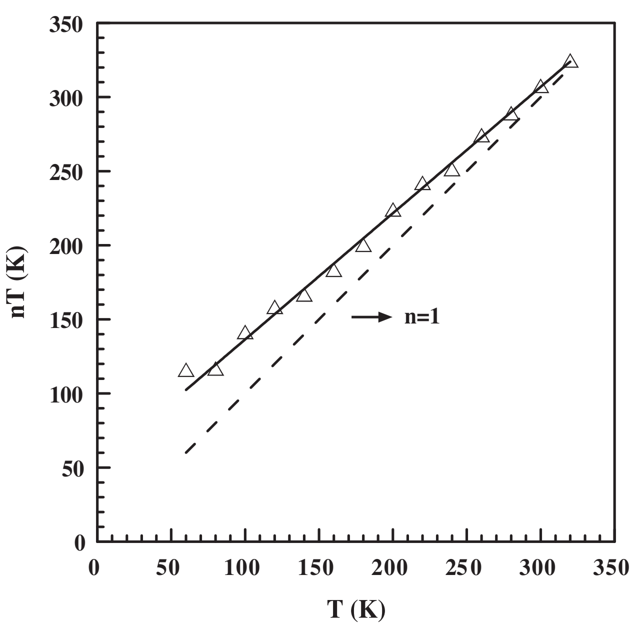

Fig. 5. Plot of nT versus T for Ni/n-GaAs/In Schottky diodes.

$$n \approx 1 - \frac{\rho_3}{2kT/q} \tag{9}$$

Equating Eqs. (8) and (9) thus yields,

$$T_0 \approx -\frac{\rho_3}{2k/q} \tag{10}$$

From Eq. (10), T_0 is calculated as 33.22. The new value of T_0 is different from the value of T_0 obtained from nT vs. T plot. The difference between T_0 values is reasonable when it is taken into that Eq. (10) is derived from an approximation. Furthermore, the temperature dependence of T_0 can be reason of this inconsistency.

3.3. Flat-band barrier height

A fundamental BH defined at zero electric field has been derived by Wagner et al. from relationship between the zero-bias BH and the ideality factor from an $I–V$ measurement. It is mostly called "flat-band barrier height" and is given as follows [37]:

$$\Phi_{bf} = n\Phi_{b0} - (n-1)\frac{kT}{q}\ln\frac{N_C}{N_D} \tag{11}$$

Here Φ_{bf} is the flat-band barrier height, N_C is the effective density of states in the GaAs conduction band, $N_D = 1.46 \times 10^{16}\ \text{cm}^{-3}$ is the donor concentration. A plot of Φ_{bf} vs. T is given for Ni/n-GaAs/In Schottky diodes in Fig. 6.

As can be seen from the figure, φ_{bf} depends on temperature linearly and decreases with increasing temperature in the temperature range measured. This dependence can be expressed as follows [5]:

$$\Phi_{bf} = \Phi_{bf}(T=0) + \alpha T, \tag{12}$$

Where $\varphi_{bf}(T = 0)$ is the flat-band barrier height extrapolated to the temperature axis and the α is its temperature coefficient. When we use simple linear regression to fit Φ_{bf} vs. T data, $\varphi_{bf}(T = 0)$ and α values are determined as 0.91 eV and -5.42×10^{-4} eV/K, respectively. The value of α is in good agreement with the temperature coefficient values of E_g reported in Refs. [38,39]. Therefore, it can be said that the variation in Φ_{bf} with the temperature is in entirely due to the temperature dependence of E_g. Similar result for Ni/n-GaAs Schottky diodes has been reported by Hackam [28].

3.4. Richardson and Modified Richardson plots

The value of I_0 and its reciprocal temperature were used to plot $\ln(I_0/T^2)$ versus $1/T$. This is the usual Richardson plot and yields straight line for ideal Schottky diode [35]. As can be seen from Fig. 7, the Richardson plot of Ni/n-GaAs/In Schottky diodes is not linear below 160 K due to strong temperature dependence of ϕ_{b0} and n [28,35,40]. The effective Richardson constant and BH at 0 K can be determined from linear part of $\ln(I_0/T^2)$ versus $1/T$ plot. BH at 0 K was calculated as 0.72 eV from the slope of the plot

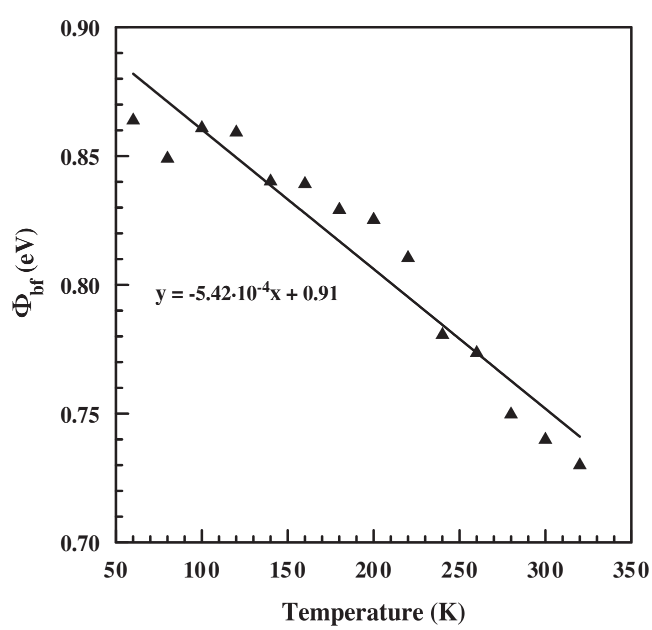

Fig. 6. The flat-band barrier height versus temperature plot obtained by means of Eq. (11).

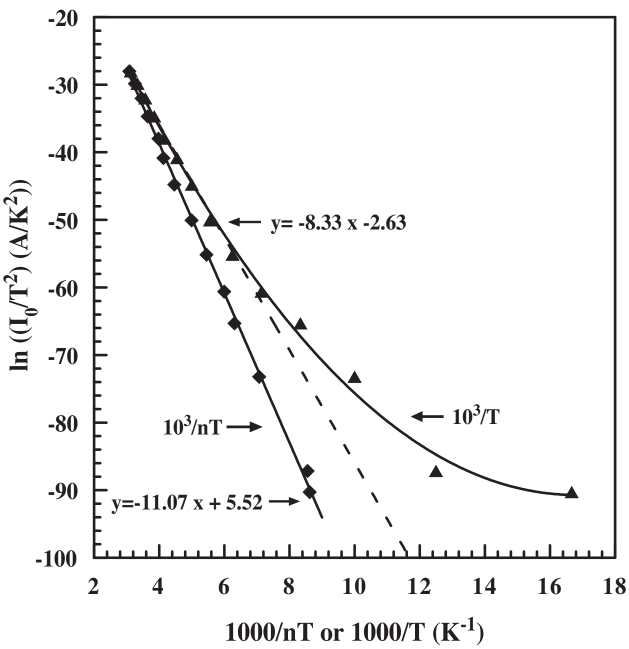

Fig. 7. Richardson and modified Richardson plots for Ni/n-GaAs/In Schottky diodes.

and A^* was found to be 4 A/cm^{2}K^2 from y-axis intercept of the plot. This value of A^* is in reasonable agreement with the theoretical value of 8.16 A/cm^{2}K^2 for n-GaAs.

The curved behavior of Richardson plot is eliminated by taking into temperature dependence of n [35]. Fig. 7 shows the modified Richardson plot. BH at 0 K and Richardson constant were determined as 0.954 eV and 1.39×10^4 A/cm^{2}K^2 from this figure, respectively. The values of BH at 0 K obtained from modified Richardson plot is in close agreement with the value of $\varphi_{bf}(T = 0)$. However, the value of Richardson constant is too large. Since the temperature dependence of barrier height is disregarded, this discrepancy occurs. This problem can be solved with help of the following equation [41]:

$$A^*_{\text{corrected}} = A^*_{\text{observed}} \exp\left[\frac{q}{k}\left(\frac{d\Phi_{bf}}{dT}\right)\right] = A^*_{\text{observed}} \exp\left[\frac{q}{k}\alpha\right] \tag{13}$$

The value of $A^*_{\text{corrected}}$ was calculated as 25.75 A/cm^{2}K^2 by using Eq. (13). This value of Richardson constant is closer to theoretical value of 8.16 A/cm^{2}K^2 for n-GaAs than 1.39×10^4 A/cm^{2}K^2.

4. Conclusions

The zero-bias barrier height and the ideality factor obtained from current–voltage (I–V) curves of Ni/n-GaAs/In Schottky diodes have exhibited temperature dependent behavior. At low temperatures, the temperature dependence of barrier height and ideality factors values of Ni/n-GaAs/In Schottky diodes has been interpreted by means of potential fluctuations model developed by Werner and Güttler. When σ_{s0} of 64 mV and n of 1.026 ± 0.014 at 300 K are taken into account, it can be said that the quality of Ni/n-GaAs interface is good. $\bar{\Phi}_{b0}$ was calculated as 0.862 eV. As the temperature increases, the ideality factor approaches unity. It can be said that the interface at Ni/n-GaAs is more homogeneous at higher temperature. This result proves that the inhomogeneity of SBH has a Gaussian distribution. From Eq. (6), it is clear that the zero-bias BH approaches mean SBH value when T is larger. Leroy et al. [31] emphasize that the homogenous barrier height analysis should be realized to understanding the physical mechanism of Schottky barrier formation between metals and semiconductors. In the view of this point, this study gives the information about interface of Ni/n-GaAs. $-\rho_2$ and ρ_3 were calculated as -6.94×10^{-4} and -5.73 mV in the temperature range of 60–240 K, respectively. The temperature dependence of the barrier height at high temperatures has been attributed to the variation of the semiconductor band gap with temperature. The $\varphi_{bf}(T = 0)$ and α values are determined as 0.91 eV and -5.42×10^{-4} eV/K, respectively. From nT versus T plot, T_0 is determined as 51.23 K. Furthermore, T_0 value was recalculated as 33.22 K with help of Werner and Güttler's [17] approximation. The Richardson constant values of 4 and 25.75 A/cm^{2}K^2 were determined from Richardson and modified Richardson plots, respectively. The BH at 0 K obtained from modified Richardson plot was determined as 0.954 eV. This value is in close agreement with the value of $\varphi_{bf}(T = 0)$. It is inferred from both our findings and experimental results in literature that the σ_{s0} and α are the important parameters of Schottky diodes. Therefore, it is strongly recommended that the values of σ_{s0} and α should be placed on commercial catalogue of Schottky diodes.

Acknowledgments

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