



# Analysis of barrier height inhomogeneity in Au/n-GaAs Schottky barrier diodes by Tung model

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## ABSTRACT

The apparent barrier heights and ideality factors of identically fabricated gold Schottky contacts on n-GaAs (14 dots) were determined from forward bias current–voltage characteristics at room temperature. A statistical study on the experimental barrier heights and ideality factors of the diodes was performed. The obtained results indicate that the barrier heights and ideality factor parameters of Schottky diodes are different from one diode to another, even if they are identically prepared. The experimental BH and ideality factor distributions obtained from current–voltage characteristics were fitted by a Gaussian function, and their mean values were found to be  $0.664 \pm 0.024$  and  $1.700 \pm 0.129$  eV, respectively. The lateral homogeneous BH value of 0.738 eV for the gold Schottky contacts on n-GaAs was obtained from  $\Phi_{b0}$  vs *n* plot by using  $n_{if} = 1.026$  and  $\Delta\Phi_{inf} = 42$  meV. It is concluded that the higher ideality factors accompany with the lower BHs or vice versa due to inhomogeneities. Also, a theoretical modelling of the formation mechanism of the Schottky barrier across the metal–semiconductor interfaces was successfully applied with the assumption of a statistical distribution of the patch characteristics. This model was assisted to lead to the explanation of many anomalies in the experimental results.

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## 1. Introduction

The electrical properties of metal–semiconductor (MS), metal–insulator–semiconductor (MIS) Schottky diodes have been investigated because of their importance in electronic device applications [1–3]. The performance and reliability of any Schottky contact are highly influenced by interface quality between the deposited metal and the semiconductor surface. In order to understand the conduction mechanism of the Schottky barrier diodes (SBDs), many attempts have been made. Generally, the SBD parameters have been determined over a wide range of temperatures and doping concentrations to understand the nature of the barrier and conduction mechanism. The analysis of the current–voltage (*I*–*V*) characteristics of Schottky barriers on the basis of thermionic emission diffusion (TED) theory reveals an abnormal decrease of the barrier height (BH) and increase of the ideality factor with decreasing temperature [4]. Also, the ideality factor has been found to increase with increasing carrier concentration, while barrier height obtained from *I*–*V* measurements decreases with increasing doping level. Explanation of the possible origin of such anomalies have been proposed by taking into account the interface state density distribution [5], quantum-mechanical tunneling [6,7],

image-force lowering and most recently the lateral distribution of BH inhomogeneities [8,9]. In addition, a Gaussian distribution of the BH over the contact area has been assumed to describe the inhomogeneities as another way too [10].

Gallium arsenide is one of the most popular semiconductors that has intrinsic electrical properties superior to silicon, such as a direct energy gap, higher electron mobility, a high breakdown voltage, chemical inertness, mechanical stability, and lower power dissipation. These advantages of gallium arsenide make it attractive for optoelectronic devices, discrete microwave devices and/or large-scale integrated electronic devices. Due to the technological importance of MS GaAs SBDs, a full understanding of the nature of the electrical characteristics of SBDs in the system is of great interest. Newman et al. [11] have been studied the electrical transport characteristics of nine metals on n-GaAs and n-InP as a function of doping level on (110) surfaces. Furthermore, Horváth et al. [12] have been presented experimental results obtained on n-type InP using various Schottky metal on untreated and/or HF, HF+Na<sub>2</sub>S and HCl treated surface. The experimental BHs and ideality factors obtained from the *I*–*V* characteristics differ from diode to diode even if they are identically prepared SDs. The application of standard procedures gives effective barrier heights and ideality factors only. Furthermore, there is a linear relationship between experimental effective BHs and ideality factors of Schottky contacts that can be explained by lateral inhomogeneities of the BHs in SBDs [4–7], that is, the BHs become the smaller

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as the ideality factors increase. An investigation indicates that the experimentally observed dependence of the effective barrier heights and the ideality factors of real metal–semiconductor contacts can be explained by lateral inhomogeneities of the barrier height. The barrier heights of laterally homogeneous contacts may be obtained by extrapolation of experimental  $\varphi_{ap}$  vs  $n$  relation corresponding to image-force-controlled ideality factor  $n_{if}$  [9]. The spatial variation of barrier heights in inhomogeneous Schottky diodes is described mainly by the Gaussian distribution function. Non-ideal behaviour of  $I$ – $V$  characteristics may be due to the spatially inhomogeneous barrier heights and potential fluctuations at the metal–semiconductor interface that consists of low and high barrier areas. The barrier inhomogeneities may be caused by inhomogeneities in the interfacial oxide layer composition, non-uniformity of the interfacial charges and interfacial oxide layer thickness, grain boundaries, multiple phases, facets, defects, a mixture of different phases and etc. Thus, the current across the MS contact may be greatly influenced by the presence of the BH inhomogeneity and this inhomogeneity leads to large ideality factors. However, the diode current is the sum of the contributions of small local patches of lower SBH inserted in a large region of uniform higher SBH and the presence of a wide distribution of low-SBH patches may occur barrier inhomogeneity [5–13]. Some authors have been able to account for much of the observed non-ideal behaviour by assuming certain distributions of microscopic BHs for the different diodes. Forment et al. [13] obtained an average value of 0.883 eV using BEEM to measure local BHs on a nanometer scale for Au/n-GaAs SBDs. Leroy et al. [14] measured an average BH of 0.819 eV of the whole contact for Au/n-GaAs SBDs using a conducting probe-AFM, instead of local nanometer-scale BHs. They have concluded that a lower average of an effective BH was obtained due to averaging over the whole contact.

In present study, we aim to experimentally investigate whether the Schottky BHs and ideality factors obtained from the  $I$ – $V$  characteristics differ from diode to diode, even if the samples are identically prepared or not. We analyze this procedure by considering theoretical results obtained by Tung for the current–voltage relationship of non-uniform Schottky contacts. For this purpose, the  $I$ – $V$  measurements of Au Schottky contacts on n-GaAs substrate were performed at room temperature and BHs and ideality factors were calculated using thermionic emission theory.

## 2. Experimental details

Schottky barrier diodes (SBDs) were fabricated on n-type GaAs (Si-doped) substrate with (100) orientation and a doping concentration of  $2.6 \times 10^{16} \text{ cm}^{-3}$ . The substrate was sequentially cleaned with trichloroethylene, acetone, methanol and then rinsed in deionised water. The native oxide on the surface was etched in sequence with acid solutions ( $\text{H}_2\text{SO}_4:\text{H}_2\text{O}_2:\text{H}_2\text{O} = 3:1:1$ ) for 60 s, and ( $\text{HCl}:\text{H}_2\text{O} = 1:1$ ) for another 60 s. After a rinse in deionised water and a blow-dry with nitrogen, a low resistance ohmic contact on the back side of the sample was formed by evaporating of In at a pressure of  $2 \times 10^{-5}$  Torr, followed by an annealing at 375 °C for 5 min in nitrogen atmosphere. Then, the above procedures were also used to clean the front surface of GaAs wafer. Finally, circular dots with a diameter of approximately 2 mm of Au were then evaporated through a molybdenum mask at a pressure of  $2 \times 10^{-5}$  Torr to form the Schottky barriers.  $I$ – $V$  measurements of the devices were made using a Keithley 4200 SCS semiconductor characterization system.

## 3. Results and discussion

The current through a Schottky barrier diode according to thermionic emission (TE) theory is given by the following relation [15,16]:

$$I = I_0 \exp\left(\frac{q(V - IR_s)}{nkT}\right) \quad (1)$$

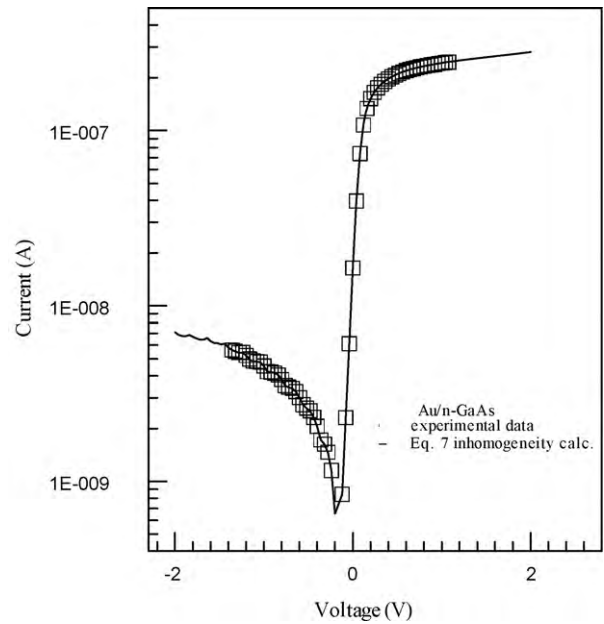


Fig. 1. Experimental forward and reverse bias current vs voltage characteristics of one of the n-GaAs SBDs at room temperature. The full line is a fit of Eq. (7) to the experimental data.

where,  $V$  is the applied voltage,  $n$  is the ideality factor and  $I_0$  is the reverse saturation current given by:

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

Where  $q$  is the electronic charge,  $A^*$  is the effective Richardson constant,  $k$  is the Boltzmann constant,  $T$  is the absolute temperature and  $\Phi_{b0}$  is the zero-bias barrier height. From Eq. (1), the ideality factor  $n$  can be written as:

$$n = \frac{q}{kT} \left( \frac{dV}{d \ln I} \right). \quad (3)$$

Fig. 1 shows the reverse and forward  $I$ – $V$  characteristics of one of the Au/n-GaAs SBDs at room temperature. The barrier height  $\Phi_{b0}$  for the Au/n-GaAs SBDs obtained from semi-logarithmic  $I$ – $V$  characteristics was varied from 0.623 to 0.722 eV and the ideality factor was varied from 1.530 to 1.846.

The  $I$ – $V$  characteristics deviate from the linearity due to the series resistance and interfacial layer. Thus, the series resistance is effective parameter in  $I$ – $V$  characteristics of the diode and it cannot be ignored. In order to check effect of series resistance on  $I$ – $V$  characteristics, we used Norde [4] method given by the following relation:

$$F(V) = \frac{V_0}{\gamma} - \frac{kT}{q} \left( \frac{I(V)}{A^* AT^2} \right) \quad (4)$$

where  $\gamma$  is the integer (dimensionless) greater than  $n$ .  $I(V)$  is the current obtained from the  $I$ – $V$  characteristics of the diode. The plot of  $F(V)$  vs voltage for the diode is shown in Fig. 2. The  $F(V)$  gives a minimum point and thus, the barrier height and series resistance values of the diode are calculated by the following relations:

$$\Phi_b = F(V_0) + \frac{V_0}{\gamma} - \frac{kT}{q} \quad R_s = \frac{kT(\delta - n)}{qI_0} \quad (5)$$

where  $F(V_0)$  is the minimum point of  $F(V)$ . Using Eq. (5), the barrier height and the  $R_s$  values for the diode were found to be 0.71 eV and 302.543 k $\Omega$ , respectively. The series resistance causes a non-linear region of forward bias  $I$ – $V$  curve of the diode. Figs. 3 and 4 show histograms of the  $\Phi_{b0}$  and  $n$  for 14 Au/n-GaAs SBDs. The experimental

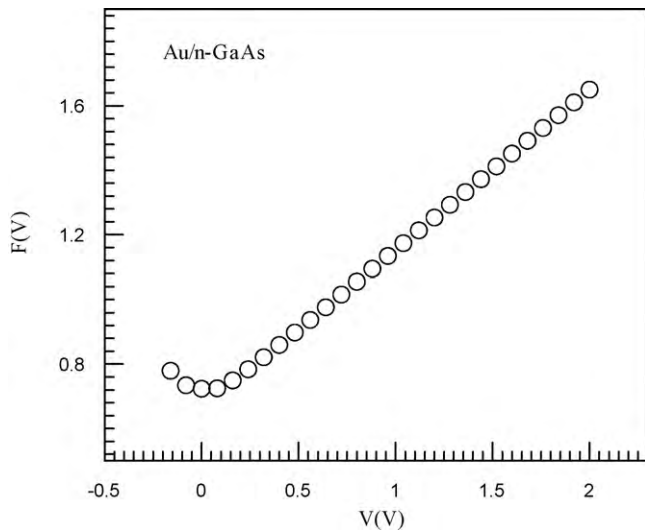


Fig. 2.  $F(V)$  vs  $V$  plot of the Au/n-GaAs Schottky diode.

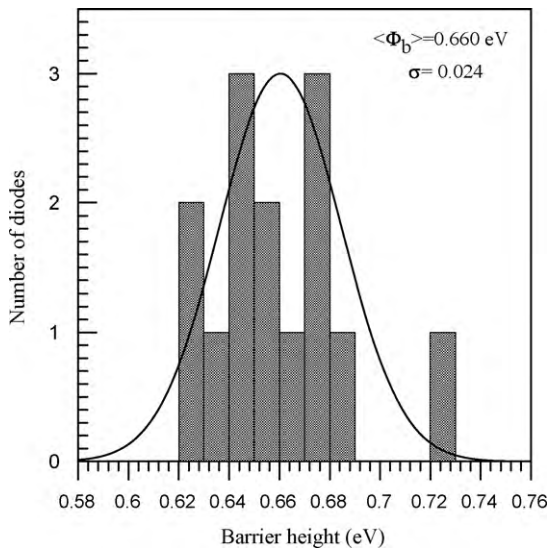


Fig. 3. Gaussian distribution of SBHs from the forward bias current–voltage characteristics of n-GaAs SBDs at room temperature.

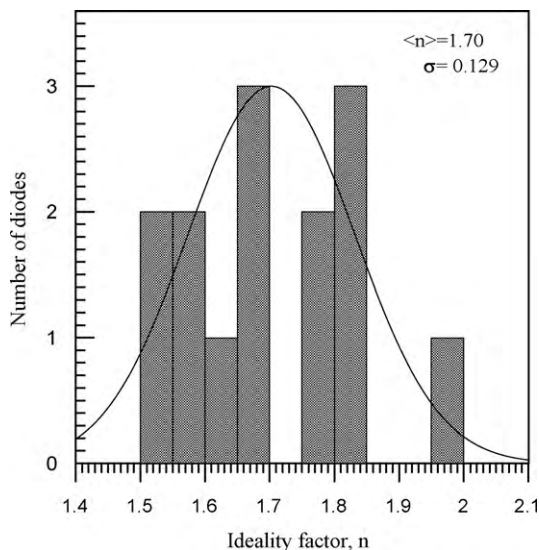


Fig. 4. Gaussian distribution of ideality factors from the forward bias current–voltage characteristics of n-GaAs SBDs at room temperature.

distribution of the  $\Phi_{b0}$  and  $n$  was fitted by the Gaussian function. Statistical analysis yields the mean  $\Phi_{b0}$  and  $n$  as  $0.664 \pm 0.024$  and  $1.700 \pm 0.129$  eV, respectively. Forment et al. [13] and Leroy et al. [14] reported the average SBHs value of  $0.883 \pm 0.018$  and  $0.819 \pm 0.01$  eV for Au/n-GaAs, respectively. Dogan et al. [15] have obtained the homogeneous SBH value of 0.862 eV for Ni/n-GaAs. The obtained barrier height of the studied diode is lower than that of those diodes. The standard deviations we find here are greater than the both obtained in Refs [13,14]. The obtained results indicate that the experimental BHs and ideality factors obtained from the  $I$ – $V$  characteristics can differ from diode to diode even if they were identically prepared on the same sample. Fig. 4 shows the plot of the  $\Phi_{b0}$  vs  $n$  of identically prepared Au/n-GaAs SBDs at room temperature. It was seen that ideality factors were decreased, while the BHs were increased or vice versa due to inhomogeneities. As seen in Fig. 4, there is a linear relationship between  $\Phi_{b0}$  and  $n$  parameters of Au/n-GaAs Schottky contacts. This finding may be attributed to lateral inhomogeneities of the BHs in Schottky diodes [5,17–25]. In addition, it has been mentioned by Tung and co-workers [5,17] and Mönch and co-workers [18–21] that the higher ideality factors among identically prepared diodes were often found to accompany lower observed BHs. Due to lateral inhomogeneities of the BH, both parameters differ from one diode to another. However, their variations are correlated in that  $\Phi_{b0}$  becomes smaller with increasing  $n$ . Extrapolations of such  $\Phi_{b0}$  vs  $n$  plots to the corresponding image-force-controlled ideality factors  $n_{if}$  give the BHs of laterally homogeneous contacts. They are then compared with the theoretical predictions for ideal Schottky contacts. The observation of large ideality factors when the diode is in a state of maximum confusion is in good agreement with the interpretation of ideality factors based on SBH inhomogeneity. There are certainly other sources for SBH inhomogeneity which may be imagined. For example, there may be a mixture of different metallic phases with different SBHs at a MS interface due to incomplete interfacial reaction. Additionally, there may be doping inhomogeneity at the MS interface and dopant clustering. The contamination at a MS interface is often present at the MS interfaces of diodes prepared by the routine processing methods used in the semiconductor electronics industries. These contaminants may act directly to introduce inhomogeneity or they may simply promote inhomogeneity, through the generation of defects, additional interfacial chemical phases and etc. Even if the absence of chemical contaminants, SBH inhomogeneity may be present. Thus, interface roughness may contribute to the presence of SBH inhomogeneity due to effectively increasing or decreasing the low-SBH patches. Finally, there are numerous structural defects, grain boundaries, dislocations, stacking faults, at MS interfaces, and these may contribute to SBH inhomogeneity [17]. The straight line in Fig. 5 is the least-square fitting to the experimental data. The extrapolation of the  $\Phi_{b0} = -0.112n + 0.853$  plot for  $n_{if} = 1.026$  results in the laterally homogeneous BH of about 0.780 eV for the Au/n-GaAs SBDs, adding the image-force lowering value. This value is in close agreement with the values obtained as in [14,26]. The  $n_{if} = 1.026$  and  $\Delta\Phi_{imf} = 42$  meV image-force lowering values were determined by Eqs. (5) and (6) in Ref. [27] at room temperature. This homogeneous BH, which is the real meaningful characteristic value for MS system, is essential to develop theories of physical mechanisms determining these BHs about Schottky contacts [28]. Schmitsdrof et al. [9] have justified this procedure by numerical simulations of  $I$ – $V$  curves which are used for Tung's theory of laterally inhomogeneous contacts with Gaussian distributions of the parameter characterizing such patchy metal–semiconductor interfaces. These results suggest that the formation mechanism of the SB is locally non-uniform at common [5,9]. Furthermore, the reason of low BHs and high  $n$  values in inhomogeneity model based on small local regions or patches with lower BH than the junction's main BH assumed to exist at

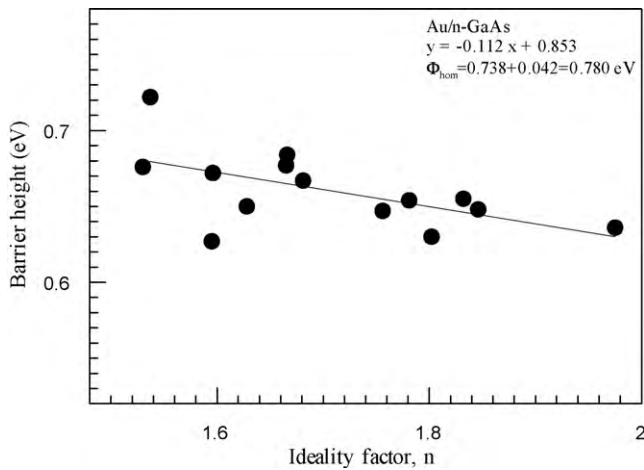


Fig. 5. Experimental barrier height vs ideality factor plot of n-GaAs SBDs at room temperature.

the junction may be explained by the patch density. According to the investigations by Schmitsdrof et al. [9], the larger patch density and/or standard deviation of the patch-parameter is, the larger the respective ideality factor is. So, it has been speculated that the reason of the experimentally observed reduction of the BHs with increasing ideality factors is inhomogeneity of the contact comprising patches with smaller BHs. Therefore, the ideality factor is a direct measure of the interface uniformity. Tung [29] has treated the SBH inhomogeneity to account for local variations in transport properties. In this model, when the regions of low SBH are comparable to or smaller than the semiconductor depletion width  $w$ , the conduction path in front of this patch becomes frequently “potentially pinched-off” by the surrounding high barrier region. The condition for pinch off is given by [5]:

$$\frac{\Delta}{V_{bb}} > \frac{2R_p}{w} \quad (6)$$

where  $\Delta$ ,  $V_{bb}$ ,  $R_p$  are the barrier height reduction at the interface of the patch compared to the homogeneous value, the interface band bending of the uniform barrier outside the patches, the radius of a circular patch, respectively. The total current through the inhomogeneous MS contact which exhibits circular patches with Gaussian distribution of the patch-parameter  $\gamma = 3(Rp^2\Delta/4)^{1/3}$  is given by the following relation [5]:

$$I = AA * T^2 \exp\left(\frac{-\Phi_{b0}^{hom}}{kT}\right) [\exp(q(V - IR_s)/kT) - 1](1 + J) \quad (7)$$

The total junction current is consisted of two terms. One of which is the characteristic of the current through the whole area with a uniform SBH. The other is current through the patches. The patch function  $J$  can be expressed as:

$$J = \frac{AA_{eff}\rho}{(IR_s - V)^{1/3}} \exp\left[\frac{q^2\sigma^2(V_{b0} - V + IR_s)^{2/3}}{2k^2T^2\eta^{2/3}}\right] \quad (8)$$

where  $\sigma$  is standard deviation of  $\gamma \geq 0$ ,  $A_{eff} = (8\pi\sigma^2/9)(\eta/V_{b0})^{1/3}$ ,  $\eta = \epsilon_s\epsilon_0/qN_d$  and  $V_{b0}$  is the interface band bending of the uniform barrier. Thus, Eq. (7) completely describes the current through inhomogeneous Schottky contacts that exhibit circular patches with a Gaussian distribution of the patch-parameter. The diode current determined by Eq. (7) is shown in Fig. 1, the agreement between experimental data and fitted  $I$ - $V$  curves in Fig. 1 is excellent. This means that the experimental data are very well described by the pinch-off theory of Tung. The fitting parameters for  $I$ - $V$  plot calculated with Eq. (7) of a Au/n-GaAs SBD are  $\Phi_{hom} = 0.722$  eV,  $R_s = 302.543$  k $\Omega$ ,  $\sigma = 8.7 \times 10^{-5}$  cm $^{2/3}$  V $^{1/3}$  (the standard deviation of

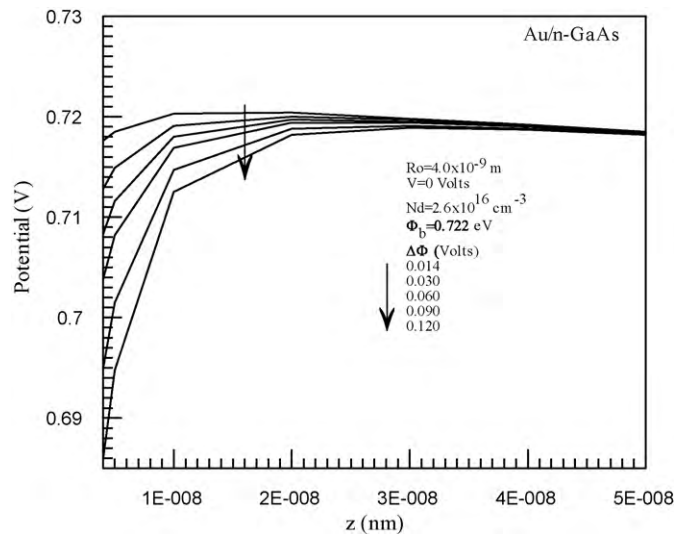


Fig. 6. The potential of the conduction-band minimum of the semiconductor for patch with SBH differences as a function of the distance  $z$  from the MS interface to the inside of the semiconductor.

patch parameter  $\gamma$ ) and  $\rho = 5.6 \times 10^{13}$  cm $^{-2}$ ,  $N_d = 2.6 \times 10^{16}$  cm $^{-3}$ ,  $A = 0.031$  cm $^2$ ,  $V_{b0} = 0.0168$  V and  $T = 300$  K. The combined effect of all the low-SBH patches is as if there were a big low-SBH region in the diode with an effective area of  $(\Phi_{eff})$  and effective SBH in an inhomogeneous SBD is given by the following relations [5]

$$\Phi_{eff} = \Phi_{b0}^{hom} - (\Delta\Phi), \quad \Delta\Phi = \frac{\sigma^2}{2kT} \left(\frac{V_{b0}}{\eta}\right)^{2/3} \quad (9)$$

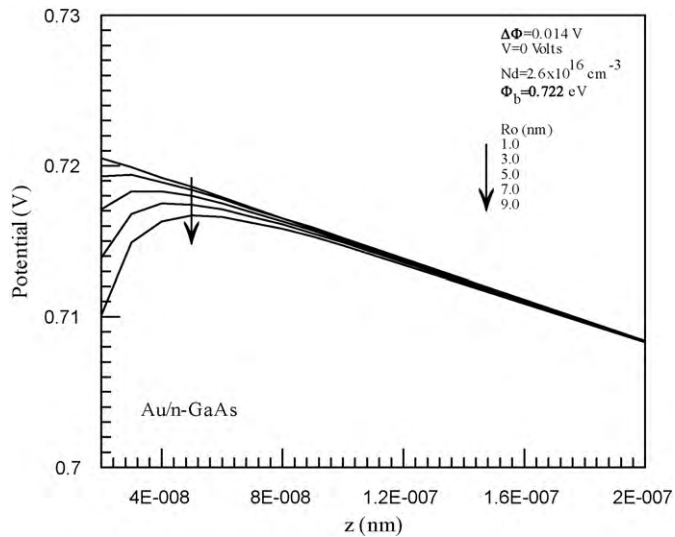
For a current described by Eq. (7), the ideality factor is given by [5]:

$$n \approx 1 + \Gamma \quad \Gamma \approx \frac{\sigma^2 V_{b0}^{-1/3}}{3kT\eta^{2/3}} \quad (10)$$

From above equation,  $\Delta\Phi$ , patch radius and  $\Gamma$  values were found to be 0.014 eV, 31.90 nm, 0.537, respectively. Furthermore, the value of  $n = 1.537$  ( $1 + 0.537 = 1.537$ ) from the fitting parameters is the same as the value of 1.537 obtained from the experimental  $I$ - $V$  characteristics for the Au/n-GaAs SBD. This patch radius is 24.74% of the depletion layer width in the homogeneous regions. Leroy et al. [14] have obtained a patch radius value for Au/n-GaAs SBDs, what is equivalent to 8% of the depletion layer width  $w$  in the homogeneous regions. Thus, it has been also achieved the characterization of the patches with lower BH. The potential distribution also varies from region to region if the SBH varies locally at Au/GaAs interface. Small areas with low SBH are easily “pinched-off” when surrounded by regions with SBH. The potential distribution of low SBH circular patches is given by [5]:

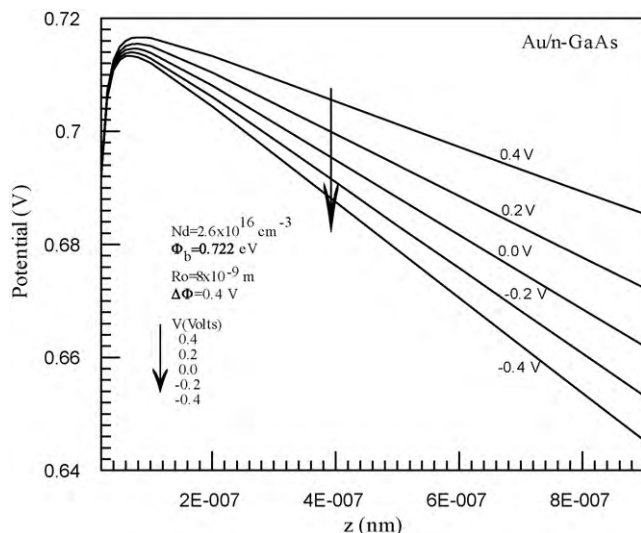
$$V(0, z) = V_{bb} \left(1 - \frac{z}{w}\right)^2 + V_n + V_a - \Delta\Phi \left[1 - \frac{z}{(z^2 + R_0^2)^{1/2}}\right] \quad (11)$$

where  $w$  is depletion width and  $z$  is depth from surface. In Fig. 6, the potential distributions along  $V = 0.0$  V of low SBH circular patches are plotted for patches with different  $\Delta\Phi$ s. For a large  $\Delta\Phi$ , the potential in front of the patch is obviously pinched-off. When  $\Delta\Phi$  is less than some critical value, there is no potential pinch-off. In present study, we estimate that the critical  $\Delta\Phi$  for potential pinch-off is about 0.083 V using Eq. (9). The experimental value of  $\Delta\Phi$  obtained for the Au/GaAs SBD is less than the critical value. Thus, there is no pinch-off effect, as shown in Fig. 6. The larger  $\Delta\Phi$  is, the greater is the degree of pinch-off. The potential distributions of low SBH circular patches are plotted for patches with different radius  $R_0$  in Fig. 7. The slope at the small value of  $z$  for



**Fig. 7.** The potential of the conduction-band minimum of the semiconductor as a function of the distance  $z$ , calculated with Eq. (7), illustrating the influence of the radius of a low-SBH patch on potential pinch-off.

the potential distribution is positive. For a small  $R_0$ , the potential in front of the patch is obviously pinched-off, that is, while the low-SBH patch radius decreases, the patches become more pinched-off and the potential at the saddle point increases. The low patch radius value of 31.90 nm is due to the level of substrate and standard deviation value of  $\sigma = 8.7 \times 10^{-5} \text{ cm}^{2/3} \text{ V}^{1/3}$ . It is concluded that current transport occurs via the low barrier patches. Furthermore, the dependence of the potential on the applied bias has a very important effect on conduction mechanism at inhomogeneous SBDs. The potential barrier between the metal and the semiconductor increases with forward bias and decreases with reverse bias [5,17]. In Fig. 7, the potential distributions of a circular patch of low SBH are shown for different voltage biases across the Au/GaAs contact. As seen in Fig. 8, the saddle point potential slowly rises with forward bias and slowly decreases with reverse bias. Since the effective barrier height of the low-SBH region is due to the magnitude of the potential at the saddle point, a variation in the potential at the saddle point with bias is an indicative of a variation in effective SBH with bias.



**Fig. 8.** The variation of the potential of the conduction-band minimum as a function of the distance  $z$  with the applied bias for a low-SBH circular patch.

#### 4. Conclusions

We have investigated experimentally the possibility of the BH change of the Au/GaAs SBDs which prepared on the same surface. The mean BH for Au/GaAs SBDs was found to be 0.664 eV and thus, we have supplied the possibility of barrier height enhancement with a difference of about 99 meV between the BHs of the Au/GaAs SBD, due to the barrier patch formed on the n-GaAs surface. The laterally homogeneous BH value of 0.738 eV for the identically fabricated Au/GaAs SBDs was obtained from the linear relationship between the experimental BHs and ideality factors. The statistical analysis yields the mean effective SBH of  $0.664 \pm 0.024$  eV and the mean ideality factor of  $1.700 \pm 0.129$  for these devices from the  $I$ - $V$  characteristics. The mean BH value of 0.664 eV from the statistical distribution of SBHs is smaller than the lateral homogeneous BH value of 0.738 eV obtained from the linear relationship between BHs and ideality factors for the Au/GaAs SBD. Finally, it is concluded that the homogeneous BHs rather than BHs of individual contacts or mean values should be used to discuss the other theories (i.e. Tung's theory) on the physical mechanisms that determine the barrier heights of metal–semiconductor contacts. Tung's theory has been successfully applied the experimental data for total thermionic emission current including a patch function describing the inhomogeneities.

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