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The effect of Schottky metal thickness on barrier height inhomogeneity in identically prepared Au/n-GaAs Schottky diodes

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Abstract
We have studied identically prepared Au(5 nm)/n-GaAs (35 dots) and Au(65 nm)/n-GaAs (38 dots) Schottky barrier diodes (SBDs) on the same n-type GaAs single crystal. A GaAs wafer has been prepared by the usual chemical etching, and evaporation of the metal has been carried out in a conventional vacuum system. The effective Schottky barrier heights (SBHs) and ideality factors obtained from the current–voltage (I–V) characteristics have differed from diode to diode. The SBH for the Au(5 nm)/n-GaAs diodes have ranged from 0.839 to 0.943 eV and the ideality factor n from 1.011 to 1.150. The SBH for the Au(65 nm)/n-GaAs diodes have ranged from 0.828 to 0.848 eV and the ideality factor n from 1.026 to 1.069. Our aim is to find the laterally homogeneous SBH values of the SBDs depending on Schottky metal thickness. The lateral homogeneous SBH values of 0.940 eV for the Au(5 nm)/n-GaAs and 0.866 eV for the Au(65 nm)/n-GaAs diodes have been calculated from a linear relationship between barrier height (BH) and the ideality factor, which can be explained by lateral inhomogeneities of the SBH, respectively.

1. Introduction

Metal-semiconductor (MS) contacts are used extensively in electronics, optoelectronics and microwave devices such as MESFETs, solar cells and microwave mixers. In these devices, the perfection of the Schottky interface plays an important role on the devices' characteristics. The interfaces between metals and semiconductors are very complex regions and their physical properties depend on surface preparation conditions [1, 2]. Although the Schottky interfaces have been researched over years, the barrier height (BH) inhomogeneity has attracted increasing attention in the last decades [3–10]. It has been reported in some works that the BH inhomogeneity is caused by grain boundaries, defects, multiple phases etc. in the MS interface. Song *et al* [3] have introduced an analytical potential fluctuation model (a barrier height Gaussian distribution model). Tung's model [9] assumed that there are small regions having lower BH compared to the junction's main BH at the junction. The existence of small local regions with different BHs was experimentally evidenced by using ballistic electron emission spectroscopy (BEES) [11, 12]. Some work has been done to describe the inhomogeneity of the Schottky barrier diodes (SBDs) [6, 13–17]. Furthermore, if the SBD shows an inhomogeneity, the correlation between BH and ideality factor may be approximated by a linear relationship. That is, the BH becomes smaller while the ideality factor increases, which can be explained by lateral inhomogeneities of the BH [18–21].

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Recently, Im *et al* [20] have done a direct comparison of naturally occurring nanometer-scale variations in the BH of a particular diode to the non-ideal macroscopic behaviour of the current–voltage (I–V) characteristics of that diode; they [20] have indicated that the nm-scale patches can be measured and quantified by the nm-resolution technique of BEEM, and that this would help determine whether the Tung model is mostly responsible for observed nonidealities in particular kinds of fabricated Schottky-diode structures. Leroy *et al* [21] have prepared small Au(30 nm)/n-GaAs Schottky barrier diodes (SBDs) using e-beam lithography and obtained the effective BHs and ideality factors from I–V measurements using a conducting probe atomic force microscope. They [22] have found a homogeneous BH value of 0.835 eV for the Au(30 nm)/n-GaAs SBDs from the linear relationship between effective BH and ideality factor values using the method of Schmitsdorf *et al* [18].

In this paper, we aimed to investigate whether the identically prepared Au(5 nm)/n-GaAs (35 dots) and Au(65 nm)/n-GaAs (38 dots) SBDs on the same n-type GaAs single crystal show the inhomogeneous behaviour or not. In addition, our aim was to observe the effect of the Schottky metal thickness on the SBH inhomogeneity, that is, to find the laterally homogeneous SBH values of the SBDs depending on Schottky metal thickness.

2. Experimental methods

A Si-doped n-type GaAs (from Wafer Technology, UK) wafer of 100 orientation, 3–5 × 10^{16} cm^{-3} donor concentration and two faces polished was used in this work. The wafer was cut into two pieces of 5 × 5 mm^2. Before, the n-GaAs samples were degreased in boiling trichloroethylene, acetone and methanol subsequently. To remove surface-damage layer and undesirable impurities, the n-GaAs were dipped in $3H_2SO_4 + H_2O_2 + H_2O$ solution at 80 °C for 15 s and in H_2O + HCl solution to remove the native oxide, and then followed by a rinse in de-ionized water of 18 MΩ, respectively. The samples were dried with high-purity nitrogen and inserted into the deposition chamber immediately after the etching process. Ohmic contacts were made by evaporation of In in vacuum of 10^{-5} mbar at room temperature, followed by rapid thermal processing at 300 °C during 10 min in an inert nitrogen atmosphere. They were immediately inserted into the evaporation chamber, separately, for forming Schottky contacts by evaporating (by using a tungsten boat) a 5 and a 65 nm Au layers. The evaporation rate was 0.1 nm s^{-1} and the substrate temperature was 110 °C. The dark current–voltage measurements were carried out by using a Keitley 487 picoammeter/voltage source at the room temperature.

3. Results and discussion

It is assumed that the forward bias current of the Schottky barrier diodes (SBDs) is due to thermionic emission current and it can be expressed as [1]

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

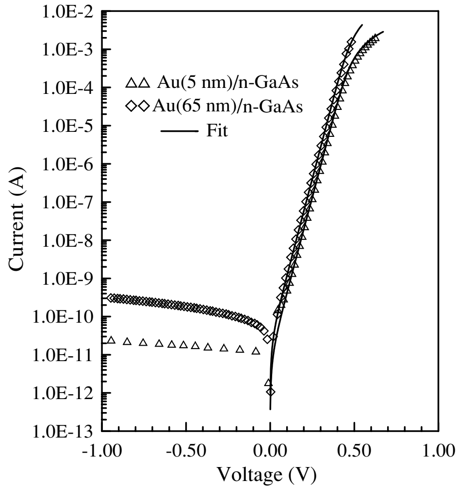

Figure 1. Forward and reverse bias current versus voltage characteristics of one of the Au(5 nm)/n-GaAs (35 dots) and Au(65 nm)/n-GaAs (38 dots) Schottky barrier diodes at room temperature. The full lines are the fits of equation (5) to the experimental data.

where

$$I_0 = AA^*T^2 \exp\left(-\frac{q\Phi_b}{kT}\right) \qquad (2)$$

is the saturation current density, $\Phi_{b,0}$ is the effective barrier height at zero bias which is determined from the extrapolated I_0 in the usual analyses of the experimental data on Schottky contacts, A^* is the effective Richardson constant equal to 8.16 A cm^{-2} K^{-2} for n-type GaAs, A is the diode area and n is an ideality factor and a measure of conformity of the diode to pure thermionic emission, determined from the slope of the straightline region of the forward bias ln I–V characteristics. The effective ideality factor and barrier height are given by

$$n = \frac{q}{kT}\frac{\mathrm{d}V}{\mathrm{d}(\ln I)} \qquad (3)$$

and

$$q\Phi_b = kT \ln\left(\frac{A^*AT^2}{I_0}\right) \qquad (4)$$

from equation (1), respectively. Figure 1 shows the room temperature forward and reverse bias I–V characteristics of one of the identically prepared Au(5 nm)/n-GaAs (35 dots) and Au(65 nm)/n-GaAs (38 dots) SBDs. The values of the effective ideality factor and barrier height Φ_b were calculated from the forward I–V characteristics according to equations (3) and (4), respectively. The BH for the Au(65 nm)/n-GaAs SBDs ranged from 0.828 to 0.848 eV and ideality factor n from 1.026 to 1.069. Φ_b value for the Au(5 nm)/n-GaAs SBDs ranged from 0.839 to 0.943 eV, and ideality factor n value from 1.011 to 1.150.

Figures 2 and 3 give a good picture of the scattering of the effective barrier height, experimentally measured for the two devices. The statistical analysis yielded a mean value of 0.894 ± 0.027 eV for the SBH of the Au(5 nm)/n-GaAs (35 dots) SBDs, and a mean value of 0.829 ± 0.010 eV for the Au(65 nm)/n-GaAs (38 dots) SBDs. Forment *et al* [12] reported a mean value of 0.880 eV for the SBH of the Au(5 nm)/n-GaAs SBDs using BEEM method which allows

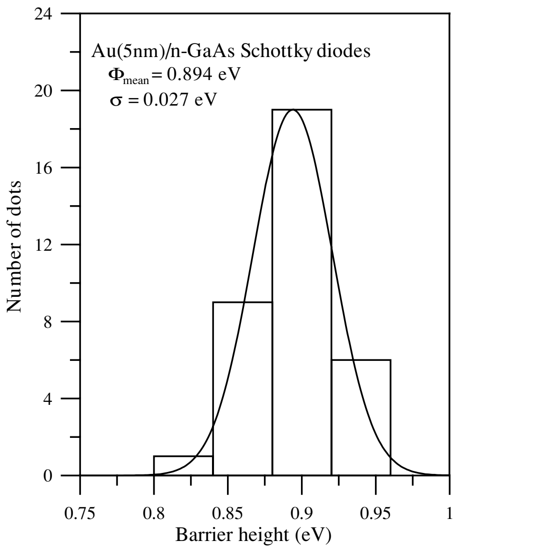

Figure 2. The Gaussian distribution of barrier heights from the forward bias I–V characteristics of the Au(5 nm)/n-GaAs diodes at room temperature.

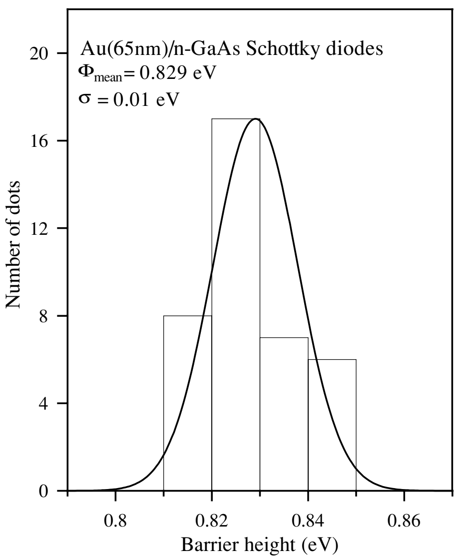

Figure 3. The Gaussian distribution of barrier heights from the forward bias I–V characteristics of the Au(65 nm)/n-GaAs diodes at room temperature.

us to determine the distribution of the SBH over the Schottky contact area on a nm-scale. This value, they [12] found for Au(5 nm)/n-GaAs SBDs with Gauss distribution, is in close agreement with our mean value of 0.894 ± 0.027 eV. As mentioned also by Schmitsdorf *et al* [18], we should emphasize that the histograms of figures 2 and 3 are shown here for completeness only because such statistical analysis disregards the pronounced correlation between the effective barrier heights and ideality factors. For discussions on the fundamental mechanism of barrier height (BH) formation, homogeneous BH rather than the effective BH should be considered only. Therefore, the standard deviations of the macroscopic barrier heights derived from the Gaussian distributions should be called the standard error. We will return to this point later.

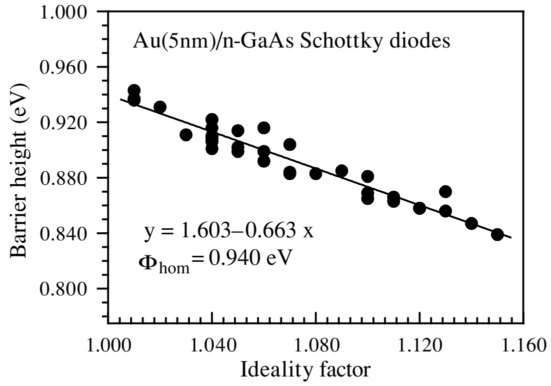

Figure 4. Experimental barrier height versus ideality factor plot of the Au(5 nm)/n-GaAs diodes at room temperature.

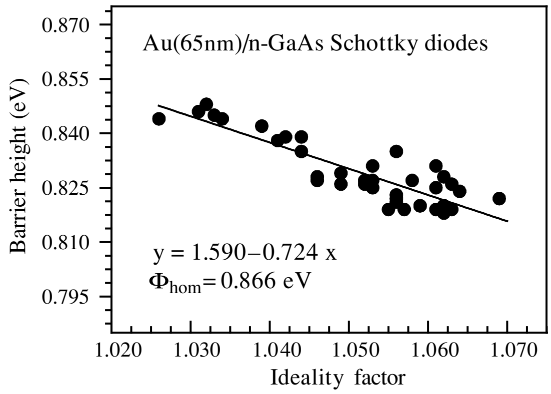

Figure 5. Experimental barrier height versus ideality factor plot of the Au(65 nm)/n-GaAs diodes at temperature room.

It is well known that in identically prepared ideal diodes (dots) on the same semiconductor substrate, the ideality factor value of the dots should be equal to each other or the BH values. It has been mentioned in [9, 14, 16–21] that, among identically prepared diodes, higher ideality factors have been found to accompany lower BHs due to inhomogeneity of the BH, and that the correlation between the experimental BHs and ideality factors has been approximated by a linear relationship. The ideality factor that is determined by the image-force effect only should be close to 1.01 or 1.02 [16–18]. Our data clearly show that the diodes have ideality factors that are considerably larger than the value determined by the image-force effect only. Therefore, these diodes are patchy [9, 14, 16–21]. As can be seen from figures 4 and 5, there is a linear relationship between experimental effective barrier heights and ideality factors of Schottky contacts that can be explained by lateral inhomogeneities of the barrier heights in Schottky diodes [12–24]. The straight lines in figures 4 and 5 are least squares to the experimental data. Mönch *et al* [17–19] have suggested that the extrapolation of the experimental BHs versus ideality factors plot to $n = 1$ will give the laterally homogeneous BH values. From figures 4 and 5, the laterally homogeneous BH values of approximately 0.940 and 0.866 eV were obtained for the Au(5 nm)/n-GaAs and Au(65 nm)/n-GaAs SBDs, respectively. As can be seen, the laterally homogeneous BH value decreases with increasing Schottky metal thickness.

As pointed out already by some authors [14, 16–21], the inhomogeneities may play an important role and have to be considered in the evaluation of experimental I–V characteristics. The application of standard procedures (equation (1)) gives the effective BH and ideality factors only. To explain commonly observed deviations from the standard thermionic emission theory (TET) (all the 'anomalies' of the BH and ideality factor), as mentioned above, Tung [14] has treated a system of discrete regions or 'patches' as low barrier imbedded in a higher uniform barrier. The patches are taken to be small relative to the size of the depletion region such that the interaction of the patch with the surrounding depletion region causes a pinch-off or saddle point in the potential barrier away from the interface. For small, discrete and low-density circular patches, Tung [14] gives the following form of the total current:

$$I = AA^*T^2 \exp\left(-\beta\Phi_{bo}^{\mathrm{hom}}\right)[\exp(\beta(V - IR_s)) - 1](1 + P), \tag{5}$$

which also consists of $V \leqslant 3$ kT q^{-1} values. The other terms except for $(1 + P)$ on the right-hand side of equation (5) are the thermionic emission current of a homogeneous Schottky contact of area A, the series resistance R_s and barrier height Φ_{bo}^{hom}. The additional current term P is the patch function and depends on the area density ρ and strength factors γ of the patches. The strength parameter γ of a given patch is related to its radius R_p and decrease in barrier at the interface Δ_p (the local lowering of the BH at the saddle point in front of a circular patch of radius R_p) and is given by

$$\gamma = 3\left(\frac{R_p^2\Delta_p}{4}\right)^{1/3}. \tag{6}$$

Furthermore, if the strength parameter γ has a Gaussian distribution for $\gamma \geqslant 0$, the patch function P can be expressed by

$$P = \frac{8\pi\rho\sigma^2\eta^{1/3}}{9(V_{bo} - V + IR_s)^{1/3}} \exp\left(\frac{\beta^2\sigma^2(V_{bo} - V + IR_s)^{2/3}}{2\eta^{2/3}}\right), \tag{7}$$

where σ is the standard deviation of γ around zero and $\eta = \varepsilon_s\varepsilon_o/qN_d$, ε_s and N_d are the dielectric constant and the dopant density of the bulk semiconductor. V_{bo} is the interface band bending of the uniform barrier outside the patch, and ρ is the patch density. Thus, equation (5) completely describes the current through nonuniform Schottky contacts that exhibit circular patches with a Gaussian distribution of the patch parameter γ and do not include the image-force lowering of the BH.

The full line in figure 1 displays a fit of equation (5) to the experimental forward I–V data. The fitting parameters were $\Phi_{bo}^{\mathrm{hom}} = 0.971$ eV, $R_s = 56\ \Omega$, $\sigma = 3.51 \times 10^{-5}$ cm$^{2/3}$ V$^{1/3}$ (the standard deviation of patch parameter γ) and $\rho = 1.12 \times 10^{10}$ cm^{-2} for the Au(5 nm)/n-GaAs SBDs. The fitting parameters were $\Phi_{bo}^{\mathrm{hom}} = 0.872$ eV, $R_s = 13\ \Omega$, $\sigma = 3.21 \times 10^{-5}$ cm$^{2/3}$ V$^{1/3}$ (the standard deviation of patch parameter γ) and $\rho = 1.17 \times 10^{10}$ cm^{-2} for the Au(65 nm)/n-GaAs SBDs. In addition, we used $N_d = 4 \times 10^{16}$ cm^{-3}, $A = 0.0177$ cm^2 and $T = 298$ K. The agreement between experimental data and fitted I–V curve in figure 1 is excellent, i.e. the experimental data are very well described by the thermionic emission theory of inhomogeneous Schottky contacts. From figures 4 and 5 which give the linear relationship between experimental effective barrier heights and ideality factors, the laterally homogeneous BH values of approximately 0.940 and 0.866 eV obtained for the Au(5 nm)/n-GaAs and Au(65 nm)/n-GaAs SBDs, respectively, are in close agreement with the values of 0.971 eV (Au(5 nm)/n-GaAs) and 0.872 eV (Au(65 nm)/n-GaAs) from the fit method to equation (5). Again, we should indicate that the barrier heights plotted in figures 2–5 result from the standard evaluation of the experimental I–V curves using equation (4) rather than fitting procedures employing equation (5). The standard deviations of patch parameters of $\sigma = 3.51 \times 10^{-5}$ cm$^{2/3}$ V$^{1/3}$ and $\sigma = 3.21 \times 10^{-5}$ cm$^{2/3}$ V$^{1/3}$ for the Au(5 nm)/n-GaAs and Au(65 nm)/n-GaAs SBDs, respectively, differ from the standard deviation of the macroscopic barrier heights derived from the Gaussian distributions, the values of 27 and 10 mV given in figures 2 and 3, respectively. The standard deviations of the macroscopic barrier heights derived from the Gaussian distributions should be called the standard error. We have obtained the standard deviation values of $\sigma_m = 6.37$ mV and $\sigma_m = 5.34$ mV for the Au(5 nm)/n-GaAs and Au(65 nm)/n-GaAs SBDs, respectively, following the calculation procedure in [20]. There is an underlying assumption that patchiness and statistical variations are one and the same. We have used the formula $\sigma_p = (V_{bo}/\eta)^{1/3}\sigma$, the fractional coverage $C_p = \pi\rho\sigma_p^2\ (16w^4/\eta)^{1/3}/(9V_{\mathrm{bo}})$ and $\sigma_m = C_p^{1/2}\sigma_p$, where w is the semiconductor depletion width and σ_m is the overall standard deviation of the model in [20].

As explained above, we have explained the linear relationship between experimental effective barrier heights and ideality factors of Schottky contacts in figures 4 and 5 by means of the lateral inhomogeneities of the barrier heights in Schottky diodes. We have two slopes in these figures, 0.663 for Au(5 nm)/n-GaAs and 0.724 for Au(65 nm)/n-GaAs SBDs. It can be instructive to see whether the slope correlates with the patch parameters. This is a relationship between the apparent ideality factor and the fluctuations in the barrier heights in Tung's model [9, 14]. As we all know, the ideality factors represent a direct measure of the interface uniformity [4–9, 16–19]. This finding and the assumptions that the patches have smaller barrier heights than homogeneous contact explains the experimentally observed reduction of the barrier heights with increasing ideality factors [18]. That is, one obtains larger ideality factors and smaller barrier heights when the inhomogeneity of the barrier increases. The larger slope $\partial\Phi/\partial n$ for the different effective barrier height versus ideality factor plots shows that the barrier inhomogeneity decreases or the standard deviation value of the patch parameter decreases [14, 18]. As can be seen from figures 4 and 5, a BH value of 0.84 eV for the Au(5 nm)/n-GaAs corresponds to an ideality factor value of 1.155 while this BH value for the Au(65 nm)/n-GaAs corresponds to an ideality factor value of 1.038.

Briefly, it has been seen that the relationship between the effective BHs and ideality factors of the Au/n-GaAs SBDs can be explained by lateral inhomogeneities of the BH. The laterally homogeneous BH values of approximately 0.940 and 0.866 eV were obtained for the Au(5 nm)/n-GaAs and Au(65 nm)/n-GaAs SBDs. The values of 0.971 eV (Au(5 nm)/n-GaAs) and 0.872 eV (Au(65 nm)/n-GaAs) have been calculated directly applying the theoretical I–V relationship derived for the thermionic emission at inhomogeneous contacts to the experimental I–V characteristics. Thus, it has been seen that the experimental and theoretical values are in agreement with each other according to the BH inhomogeneity model.

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