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Solid-State Electronics 49 (2005) 878–883
SOLID-STATE ELECTRONICS
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The barrier height inhomogeneity in identically prepared Au/n-GaAs Schottky barrier diodes

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Received 28 April 2004; received in revised form 13 December 2004; accepted 6 March 2005
Available online 14 April 2005

The review of this paper was arranged by Prof. S. Cristoloveanu

Abstract

We have prepared small Au/n-GaAs Schottky barrier diodes (SBDs) using e-beam lithography (EBL), and obtained their effective barrier heights (BHs) and ideality factors from current–voltage (*I*/*V*) characteristics, which were measured using a conducting probe atomic force microscope (CP-AFM). Although the diodes were all identically prepared, there was a diode-to-diode variation: the effective BHs ranged from 0.795 eV to 0.836 eV, and the ideality factor from 1.025 to 1.101. Lateral homogeneous BHs were computed from the observed linear correlation between BH and ideality factor using the method of Schmitsdorf et al. [Schmitsdorf RF, Kampen TU, Mönch W. J Vac Sci Technol B 1997;15(4):1221]. These homogeneous BHs were also obtained from the fit to the experimental *I*/*V* characteristics of the current through a "patchy" diode. From our model, the barrier height in the patches and their diameter could be determined. It are however the homogeneous BHs which should be used to make theories of the physical mechanisms responsible for the Schottky barrier height of the metal–semiconductor combination considered.

PACS: 73.30; 73.40.−c; 73.61.Ey

Keywords: Schottky barrier height inhomogeneities; Conducting probe-AFM; GaAs

1. Introduction

Metal–semiconductor (M–S) contacts are frequently used in integrated circuits, in light detectors and as solar cells. Barrier height (BH) and ideality factor are the fundamental parameters of Schottky barrier diodes (SBDs) [2]. Although they have been studied for over 50 years, it is only during the last decade that the inhomogeneity of the M–S interface has been considered [3,4]. In the early 1990s, Tung and co-workers showed that non-ideal behavior of the SBDs could be quantitatively explained by assuming a distribution of nanometer-scale interfacial patches of reduced SBH [2,5]. Several authors have found experimental evidence that nanometer-sized lateral variations in the SBH exist [6–11]. Moreover, Tung and co-workers reported theoretically [2,5,12] and Mönch and co-workers showed experimentally [1,13,14], that a correlation exists between effective BHs and ideality factors, which may be approximated by a linear relationship.

In this work we prepared small Au/n-GaAs Schottky diodes by EBL, and obtained current–voltage characteristics using a conducting probe-AFM. As was already done for Si substrates (e.g. [15,16]), and once (but only partially) for GaAs substrates [17], we confirm and give experimental evidence for the results reported by Tung

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0038-1101/$ - see front matter
doi:10.1016/j.sse.2005.03.005

and by Mönch. We tried to examine the influence of the patches, i.e. the inhomogeneities, by decreasing the diode size. Therefore we had to use a homebuilt conducting probe-AFM to make the *I*/*V* measurements. We will discuss various aspects of our procedure of contacting the diodes with this CP-AFM.

2. Experimental

2.1. General experimental details

The samples were prepared using n-doped GaAs(100) wafers (Si doped), obtained from Wafer Technology Ltd. The average carrier concentration is $N_D = 4 \times 10^{16}\ \mathrm{cm}^{-3}$. The resistivity varies from 0.076 to 0.078 Ω cm. Two samples of 5 × 5 mm were cut from the wafers. These were degreased in boiling trichloroethylene, acetone and methanol subsequently. Afterwards, they were chemically etched in a 3:1:1 (volume ratio) mixture of H_2SO_4 (95%):H_2O_2 (27%):H_2O at 80 °C, followed by a 5 s dip in 1:1 HCl (37%):H_2O at room temperature, to remove the native oxide; and finally they were rinsed in deionized (DI) water. Ohmic contacts were made by thermal evaporation of In in a vacuum of about 10^{-5} mbar, with the substrate held at room temperature, followed by annealing at 300 °C for 10 min in an inert atmosphere (N_2).

Contacts were patterned on a double PMMA-resist layer, by standard electron beam lithography (EBL) using a JSM T-330 (JEOL). Prior to the gold evaporation, the patterned samples were dipped for 5 s in HCl:H_2O and rinsed in DI water, to remove oxide remnants originating from the development of the resist film in an organic solution (MIBK:IPA, 1:2). The Schottky contacts were made by evaporating 30 nm of gold onto the sample at a rate of 0.15 nm/s in a vacuum better than 4×10^{-6} mbar, with a substrate temperature of 100 °C. Finally, a lift-off process was performed on the samples using acetone at room temperature. The contacts are all square shaped, and they had an area of 22,500 μm^2 (150 μm × 150 μm), 10,000 μm^2 (100 μm × 100 μm), 2500 μm^2 (50 μm × 50 μm), 400 μm^2 (20 μm × 20 μm), 100 μm^2 (10 μm × 10 μm), or their area was between 81 μm^2 (9 μm × 9 μm) and 36 μm^2 (6 μm × 6 μm) (these latter are referred to as the diodes with an area of <100 μm^2). There were more of the smaller contacts available to measure. Fig. 1 shows an example of these contacts.

2.2. The conducting probe-AFM procedure to measure the *I*/*V* characteristics

The *I*–*V* measurements were performed at room temperature, using a commercial AFM (Topometrix TMX 2010 Discovery) that was converted to a conducting probe-AFM to obtain *I*/*V* characteristics. The home-built *I*–*V* measuring unit contains a Keithley 616. All of the diodes were contacted with a Pt-coated tip (probe), without using the feedback mechanism of the AFM. The laser is switched off, to avoid a photocurrent that would originate from the scattering of the laserlight onto the sample. Then the tip is manually lowered onto the contact. As we do not use the feedback mechanism, we do not know what amount of force there is applied to the tip. From literature (e.g. [18]) it is known that the force needed for electrical measurements is of the order of μN, where for scanning purposes it is of the order of nN. We apply as much force as needed to observe a photocurrent (induced by the light of the internal microscope of the AFM). Once this is established, we switch off the light and apply a bias to check if we still have electrical contact. If the current fluctuates, we can increase the pressure of the tip on the contact, by increasing the bias on the *z*-piezo, thus pushing the sample towards the tip. If we cannot establish a good, stable current, we repeat the process or replace the tip (wear of the coating). It is easier to establish a stable contact with a rather stiff cantilever (with a spring constant of about 0.6–1.8 N/m) than with a more flexible cantilever (order of 50 mN/m). We have used Pt-coated tips, but also had tips with a Cr (20 nm)/Au (20 nm)-coating available. If we compare measurements done on the same contact, with different tip-coatings, there is no difference, as can be seen in Fig. 2. We prefer the usage of Pt-coated tips, due to the longer lifetime of the coating.

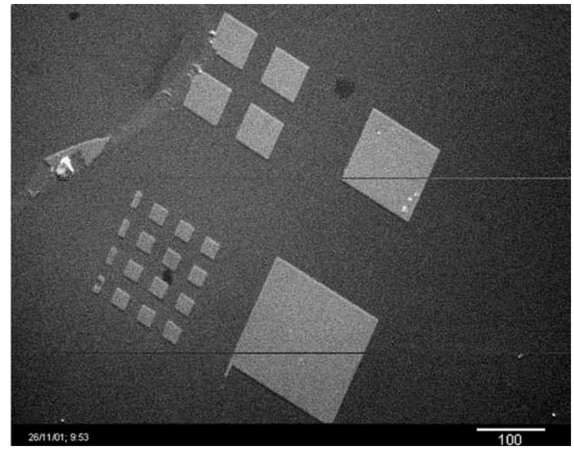

Fig. 1. SEM image of some typical Au/n-GaAs contacts that were measured. The marker indicates 100 μm.

Fig. 3 shows a forward and reverse *I*/*V* curve measured using the CP-AFM. We can clearly see the rectifying behavior of the contact. Due to the time consumption of measuring the reverse part, we have restricted our other measurements to the forward part of the *I*/*V* curve. To get an idea of the measuring-error, we have performed subsequent measurements on the same diode. After each measurement, the tip is lifted from the contact and then we re-establish electrical

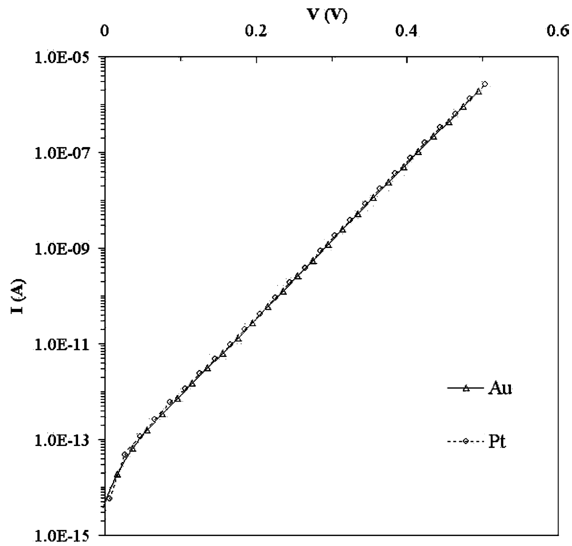

Fig. 2. Forward *I–V* characteristics of the same diode, measured with a different tip-coating. There is no difference noticeable. From these *I/V* characteristics we find ϕ_B^{eff} (Pt) = 0.831 eV, *n* (Pt) = 1.042 and ϕ_B^{eff} (Au) = 0.831 eV, *n* (Au) = 1.046.

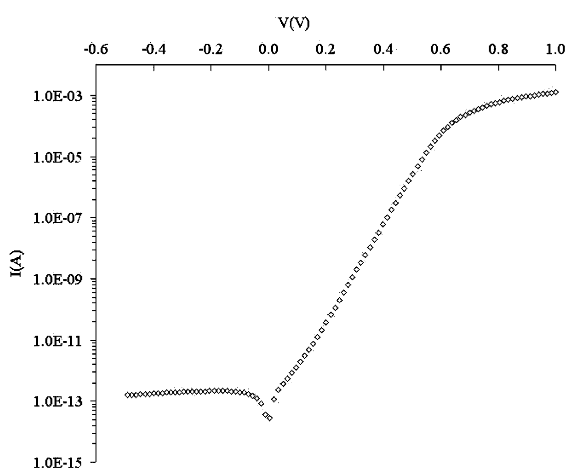

Fig. 3. Reverse and forward *I–V* characteristic of a Au/n-GaAs diode, measured using the CP-AFM.

contact (as described before). From these *I–V* characteristics we can calculate the effective barrier height and ideality factor (using Eq. (1)). The comparison of these parameters gives us an average measuring-error on the BH and ideality factor:

$$\mathrm{error}(\phi_{\mathrm{eff}}) = 0.002\ \mathrm{eV} \quad \text{and} \quad \mathrm{error}(n) = 0.005.$$

3. Theoretical background

3.1. Standard theory

The "standard theory" of thermionic emission describes the current–voltage relationship of the Schottky contacts as [19]

$$I_{\mathrm{te}}^{\mathrm{stand}} = I_0 \exp\left(\frac{qV}{nk_BT}\right)\left[1-\exp\left(-\frac{qV}{k_BT}\right)\right], \tag{1}$$

where

$$I_0 = AA_R^{**}T^2\exp\left(-\frac{\phi_B^{\mathrm{eff}}}{k_BT}\right),$$

is the saturation current, A is the diode area, A_R^{**} the effective Richardson constant, T the temperature, k_B the Boltzmann constant, q the electronic charge, ϕ_B^{eff} *the effective barrier height* at zero bias (which is defined by Eq. (1)) and n the ideality factor of the contact.

3.2. Pinch-off theory

Tung [2] analyzed the current transport in inhomogeneous Schottky contacts in detail. Traditionally, the electron transport at inhomogeneous SBs was treated by a parallel conduction model, as discussed by Ohdomari and Tu [20]. The parallel conduction model is, however, in significant error when the SBH varies spatially on a scale less than, or similar to the depletion region width. This error arises because the model fails to take into account the interaction between neighboring patches with different SBH. Tung takes into account this interaction (named "Pinch Off").

When he assumes an area density ρ_p of patches with a constant barrier height, and a Gaussian distribution

$$N(\gamma) = \frac{\rho_p}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{\gamma^2}{\sigma^2}\right), \tag{2}$$

of a patch parameter $\gamma = 3(R_p^2\Delta_p/4)^{1/3}$ [Δ_p being the deviation of the local barrier height from *the homogeneous value* Φ_{B0} (which is defined by Eq. (3)), R_p the radius of the circular patch, and σ the standard deviation], then the total current through such patchy diodes results as

$$\begin{aligned} I_{\mathrm{total}} = {} & AA_R^{**}T^2\exp\left(-\frac{\Phi_{B0}}{k_BT}\right)\left[\exp\left(\frac{q(V-R_sI_{\mathrm{total}})}{k_BT}\right)-1\right] \\ & \times\left[1+\frac{8\pi\rho_p\sigma^2\eta^{1/3}}{9(V_{b0}-V+R_sI_{\mathrm{total}})^{1/3}}\right. \\ & \left.\times\exp\left(\frac{q^2\sigma^2(V_{b0}-V+R_sI_{\mathrm{total}})^{2/3}}{2k_B^2T^2\eta^{2/3}}\right)\right], \end{aligned} \tag{3}$$

with $\eta = \epsilon_s\epsilon_0/qN_D$, R_s the series resistance of the semiconductor bulk and the measurement setup, and V_{b0} the band-bending of the uniform barrier at zero bias.

3.3. Lateral homogeneous barrier heights

Instead of fitting Eq. (3) to the experimental data, to obtain the homogeneous BH, Schmitsdorf et al. have shown (for Si substrates) [1,14] a much easier and quicker method to obtain the lateral homogeneous

BH. They plot the effective BH ϕ_B^{eff} versus the ideality factor, which they both obtain by fitting Eq. (1) to the experimental data. A straight line can be fitted to these $\phi_B^{eff}(n)$ data-points, using a simple least-squares fit. The extrapolation of this straight line to n_{if}, the ideality factor of the ideal diode with image-force included [19]

$$n_{if} = \left[1 - \frac{1}{4}\left(\frac{q^3 N_D}{8\pi^2(\epsilon_s\epsilon_0)^3}\right)^{1/4}\left(\Phi_{B0} - V - \xi - \frac{k_B T}{q}\right)^{-3/4}\right]^{-1}, \tag{4}$$

gives *the lateral homogeneous BH* ϕ_{lat}^{hom} of the M–S interface.

4. Results and discussion

Fig. 4 shows the forward *I–V* characteristics of two Au/n-GaAs diodes at RT. Each diode is from a different sample and both have an area of 400 μm^2 (20 μm × 20 μm). Although all 260 diodes from both samples were identically prepared, they exhibit different effective barrier heights ϕ_B^{eff} and ideality factors, which we calculated using Eq. (1) for a Richardson constant $A_R^{**} = 8.04 \times 10^4$ A m^{-2} K^{-2}. The diodes were by no means ideal; their ideality factors are larger than the ideality factor determined by the image-force effect (4) which is close to 1.01. As can be seen in Fig. 6, larger ideality factors are present here.

Figs. 5 and 6 give a good picture of the scattering of the effective barrier height ϕ_B^{eff} and the ideality factor, respectively, measured on 260 diodes. The averages for both parameters ($\bar{\phi}_B = 0.819$ eV and $\bar{n} = 1.057$) can be found in Table 1. The standard deviation of 10 meV we find here, is smaller than the one obtained in [21], which was 18 meV. Forment et al. [21] used BEEM to measure *local BHs* on a nanometer scale. In this paper we used a CP-AFM and measure *an average BH* of the whole contact (μm scale), instead of local nanometer-scale BHs. Due to this averaging over the contact, we find a smaller spread (10–18 meV [21]) and a lower average of effective BH $\bar{\phi}_B$ (0.819–0.883 eV [21]). The latter is because it are the lower barriers that carry the highest currents and hence dominate in the integration of the current over the total contact area, which is measured with the CP-AFM. The histograms are shown for completeness only, because they disregard the pronounced correlation between the effective barrier heights and the ideality factors [12–14], which will be discussed further in this paper.

Within the scatter of the effective BH and ideality factor, we could not find any correlation with the size of the

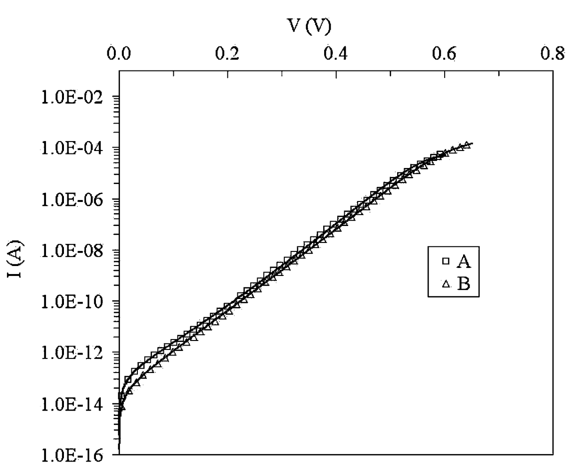

Fig. 4. Forward *I–V* characteristics of two Au/n-GaAs(100) diodes, at RT. Each one is from a different sample and they both have an area of 400 μm^2 (20 μm × 20 μm). ϕ_B^{eff} (A) = 0.815 eV, n (A) = 1.049; ϕ_B^{eff} (B) = 0.826 eV, n (B) = 1.055. The full lines are least-squares fits of the Tung relation, Eq. (3), for inhomogeneous Schottky contacts.

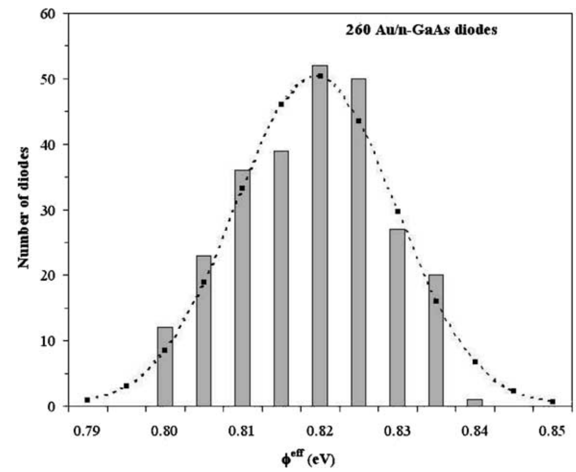

Fig. 5. Statistical distribution of effective BHs of the Au/n-GaAs diodes at RT. A Gaussian fit (dashed line) yields $\bar{\phi}_B = 0.819$ eV and a standard deviation of 10 meV.

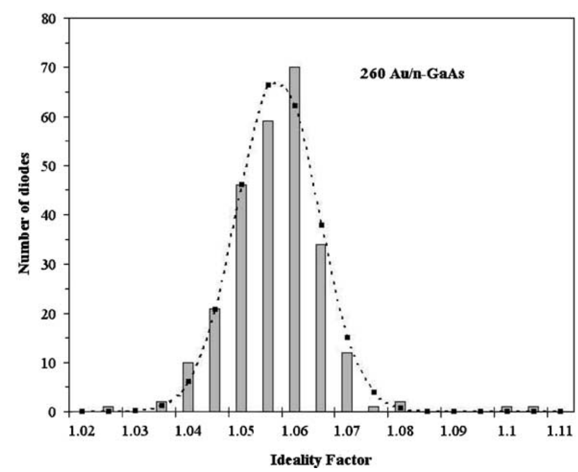

Fig. 6. Statistical distribution of the effective ideality factors of Au/n-GaAs diodes at RT. A Gaussian fit (dashed line) yields $\bar{n} = 1.057$ and a standard deviation of 0.008.

Table 1
Parameters calculated from the room temperature I–V characteristics of all the 260 Au/n-GaAs diodes

$\bar{\phi}_B$ (eV)	$\bar{n}$	ϕ_{lat}^{hom} (eV)	$\langle \Phi_{B0} \rangle$ (eV)	$\langle \sigma \rangle$ ($V^{1/3}$ $cm^{2/3}$)	$\langle \rho_p \rangle$ (cm^{-2})
0.819	1.057	0.835	0.848	6.226×10^{-5}	5.116×10^{10}

$\bar{\phi}_B$ and $\bar{n}$ are the Gaussian mean BH and ideality factor; ϕ_{lat}^{hom} is the lateral homogeneous BH from the linear correlation; $\langle \Phi_{B0} \rangle$, $\langle \sigma \rangle$ and $\langle \rho_p \rangle$ are the averages of the homogeneous BH, the standard deviation of the patch distribution, and of the area density, respectively, obtained from the fit of Eq. (3) to the data.

diodes, as shown in Fig. 7. Our original intention on using different sizes of diodes, was to measure Schottky diodes with decreasing sizes, going down to the scale of the depletion region. Due to technical problems, we did not succeed in this.

We obtained homogeneous barrier heights Φ_{B0} for all of the 260 diodes, by fitting Eq. (3) to the experimental I/V data (taking into account the physical relevance for each value of each parameter). The fitting parameters were the homogeneous BH Φ_{B0}, the standard deviation σ of the patch parameter γ, the patch density ρ_p and the series resistance R_s. As can be seen from Fig. 4, the fitted curve follows the experimental data closely. The average homogeneous BH $\langle \Phi_{B0} \rangle$ obtained in this way is 0.848 eV. The averages for all fitting parameters, $\langle \sigma \rangle$ and $\langle \rho_p \rangle$, are given in Table 1.

In their study of SBs on Si substrates, Schmitsdorf et al. [1,14] used sets of $\phi_B^{eff}(n)$ with ideality factors of $n < 1.4$ to make their linear fitting. To get an idea of the upper limit for the ideality factor (since we are using a different substrate), one should do a simulation as Schmitsdorf et al. have done. From all the fittings of Eq. (3) to every single experimental I/V curve, we calculated the average values $\langle \Phi_{B0} \rangle$ and $\langle \sigma \rangle$ for the 260 contacts (as can be found in Table 1). We used these averages $\langle \Phi_{B0} \rangle$ and $\langle \sigma \rangle$ in Eq. (3), and varied the patch density ρ_p stepwise from 0 to 1.0×10^{12} cm^{-2}. From each of these simulated I/V curves (each one is with a different ρ_p), we obtained an effective barrier height ϕ_{eff} and ideality factor n using Eq. (1). With these ϕ_{eff} and n obtained this way, we plotted the solid line shown in Fig. 8. This curve shows that for our system, there is a *linear correlation* between ϕ_{eff} and n (correlation coefficient of 0.9955) up to $n \leqslant 1.2$, so certainly for the region where our experimental data are located, i.e. for $n \leqslant 1.12$.

Because of this good linear correlation for all of our data, we can use the quicker method to fit to our data, as Schmitsdorf et al. [1,14] have done for Si. The dashed straight line in Fig. 9 shows the linear relationship (with a good correlation coefficient of 0.9987), and the extrapolation to $n_{if} = 1.01$ gives a lateral homogeneous barrier height ϕ_{lat}^{hom} of 0.835 eV.

Within the limits of the experimental error, the lateral homogeneous BH $\phi_{lat}^{hom} = 0.835 \pm 0.004$ eV matches the average of the homogeneous BHs $\langle \Phi_{B0} \rangle = 0.848 \pm 0.016$ eV (obtained from Eq. (3)). This agreement gives numerical evidence for the linear extrapolation method as proposed by Schmitsdorf et al. [1].

We take a closer look at the pinch-off theory for a more physical picture of the patches. We can write the local lowering of the barrier height at the saddle point in front of a circular patch of radius R_p as [2,22]

$$\delta\Phi_p^{sad} = \Phi_{B0} - \Phi_B^{sad} = 3\left(\frac{1}{2}\frac{\Delta_p}{qV_{b0}}\frac{R_p^2}{W^2}\right)^{1/3} qV_{b0}, \tag{5}$$

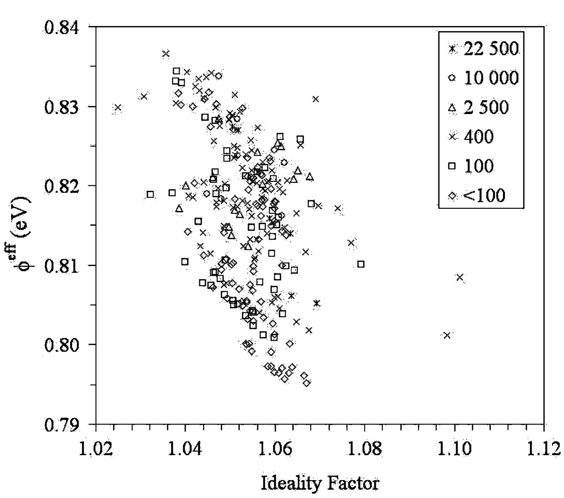

Fig. 7. The effective BH versus ideality factor plot for the 260 Au/n-GaAs diodes. Different symbols represent different sizes (in μm^2) of diodes. No correlation can be found between the size of the diode and the BH or ideality factor.

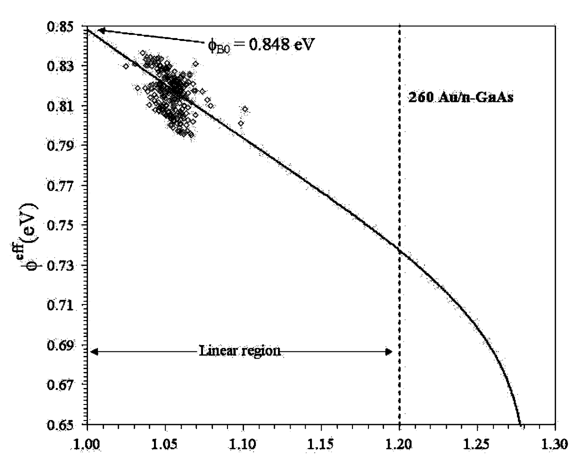

Fig. 8. The effective BH versus ideality factor plot for the 260 Au/n-GaAs diodes. The full line is a result of numerical simulations (details in text) and yields a correlation coefficient of 0.9955.

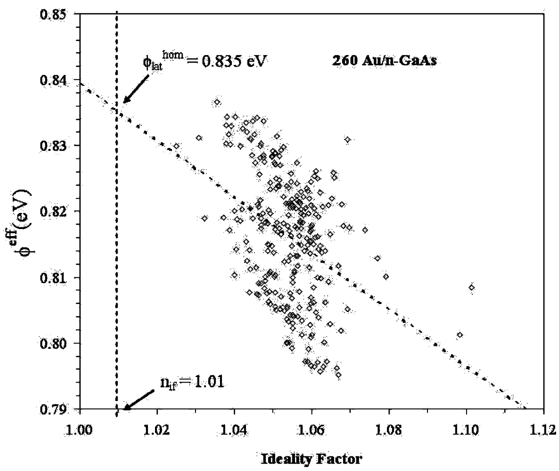

Fig. 9. The effective BH versus ideality factor plot for the 260 Au/n-GaAs diodes. The dashed line is the linear fit to the experimental effective BHs ϕ_B^{eff} (see Eq. (1)) and n, with a correlation coefficient of 0.9987.

where $W = [2\epsilon_s\epsilon_0(V_{b0} - \xi)/qN_D]^{1/2}$ is the depletion layer width. Also the standard deviation σ may be interpreted as an average patch-parameter

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

When we combine Eqs. (5) and (6) with the averages obtained here, we can make an estimation of the BH lowering by

$$\left\langle \delta\Phi_p^{sad} \right\rangle = \left\langle \Phi_{B0} - \Phi_B^{sad} \right\rangle = \sigma\left(\frac{2}{qV_{b0}W^2}\right)^{1/3} qV_{b0}. \tag{7}$$

This gives us $\left\langle \delta\Phi_p^{sad} \right\rangle = 0.1$ eV. Patches with this BH lowering would have a diameter of 12 nm (from Eq. (6)), what is equivalent to 8% of the depletion layer width W in the homogeneous regions.

5. Conclusion

We derived an average homogeneous barrier height of 0.848 eV for Au/n-GaAs Schottky diodes using Eq. (3) for a patchy diode. This agrees well with the lateral homogeneous barrier height of 0.835 eV, obtained using the linear correlation between the experimental effective barrier height and the ideality factor of the Schottky diodes, according to Schmitsdorf et al. [1]. Thus, it can be seen that the latter method is good for determining the homogeneous barrier height. Also, our homebuilt conducting probe-AFM proves to be reliable for the acquisition of I/V characteristics. We also succeeded to characterize the patches with lower BH (diameter 12 nm, BH lowering 0.1 eV). It is important to remark here, that it are the homogeneous BHs (instead of the effective BHs) which should be used to build theories of physical mechanisms determining these BHs, as it are these homogeneous BHs which are characteristic of the used metal–semiconductor combination (here Au and n-GaAs).

Acknowledgments

The authors would like to thank L. Van Meirhaeghe for technical support, and D. Deduytsche and C. Detavernier for helpful discussions.

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