Schottky Barrier Height Inhomogeneity of Ti/n-GaAs Contact Studied by the $I-V-T$ Technique *

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(Received 2 August 2001)

The current–voltage characteristics of Ti/n-GaAs Schottky diodes measured over a temperature range of 78–299 K have been interpreted on the basis of thermionic emission across an inhomogeneous Schottky contact. The experiment shows that the apparent barrier height (ϕ_{ap}) increases from 0.437 eV at 78 K to 0.698 eV at room temperature. The plot of ϕ_{ap} versus $1/T$ does not exhibit a simple linear relationship over the whole temperature range, indicating that the barrier height distribution is more complicated than the frequently observed single Gaussian distribution. A new multi-Gaussian distribution model is developed. Our experimental results can be explained by a double Gaussian distribution of the barrier heights. The weight, the mean barrier height, and the standard deviation of the two Gaussian functions are 0.00001 and 0.99999, 0.721 and 0.696, 0.069 and 0.012 eV, respectively.

PACS: 73.30.+y, 73.40.Ns, 85.30.De

The classical model of a metal–semiconductor contact (or Schottky diode) assumes the junction to be abrupt with a fixed barrier height. However, such a description fails to account for the observed temperature dependence of diode parameters determined from the corresponding current–voltage ($I-V$) characteristics on the basis of thermionic emission (TE) theory. The discrepancies could be attributed to the barrier inhomogeneities present in the Schottky diodes.[1−12] To describe the barrier inhomogeneities, two different approaches are adopted. One is Tung's "pinch-off" model,[3,13] which takes into account the interaction between neighbouring patches with different Schottky barrier height (SBH). The pinch-off effect is appreciable only when the barrier inhomogeneity is large and the low-barrier patch is very small. The other approach is the parallel conduction model, which is based on non-interaction of patches with different barrier heights.[14] The spatial barrier inhomogeneities have been described with some distribution functions, e.g. Gaussian[1,2,6,12,15,16], log–normal[17] and constant.[18]

The Gaussian distribution function is widely used because of its simplicity, clear physical meaning and validity for small barrier inhomogeneity and moderate size of low-barrier patches. The Gaussian distribution model has been successfully used to explain non-ideal behaviour of real Schottky contact, for example, the linear decrease of apparent barrier height with the inverse of absolute temperature.[1,2] One must admit that the actual distribution is very complicated. Sometimes, a simple distribution function may not be accurate enough to depict the experiment. In this Letter we develop a multi-Gaussian distribution model and apply it to describe the barrier inhomogeneities of a Ti/n-GaAs Schottky contact.

The substrate used for the metal contact in this study is an n-GaAs/n$^+$-GaAs(100) substrate. The 1.5 μm thick epitaxial n-GaAs layer was grown by molecular beam epitaxy. The electron concentration and mobility of n-GaAs layer are $2.0 \times 10^{16}\,\mathrm{cm^{-3}}$ and $3000\,\mathrm{cm^2/V{\cdot}s}$, respectively. After ultrasonic cleaning in isopropyl alcohol, acetone, and absolute alcohol, the substrate was loaded into a metal deposition system. After the chamber was evacuated to a base pressure of 7×10^{-7} Torr, 10 nm Ti and 20 nm Al films were deposited sequentially through holes (0.8 mm diameter) in a metal mask by Ar ion beam sputtering. The metal deposition was done at a pressure of 5×10^{-5} Torr with Ar ion energy of 1 keV and ion beam current of 60 mA. The $I-V-T$ measurement was carried out in a temperature controller. The measurement temperature ranged from 78 to 299 K. A Keithley 2400 source meter controlled by a computer was used to measure the $I-V$ characteristics of the Ti/n-GaAs Schottky diode.

The current across an ideal Schottky barrier at a forward bias V_a, based on the TE theory, is given by the relation when $V_a > 3kT/q$[19]

$$I(V_a) = A_d A^{**} T^2 \exp\left(-\frac{\phi_{b0}}{kT}\right) \exp\left[\frac{q\,(V_a - IR_s)}{nkT}\right], \tag{1}$$

where A_d is the diode area, A^{**} is the effective Richardson constant of n-GaAs ($4.4\,\mathrm{Acm^{-2}K^{-2}}$),[19] T is the temperature in Kelvin, k is the Boltzmann

*Supported by the Open Project from the State Key Laboratory of Functional Materials for Informatics and the Shuguang Project from Shanghai Municipal Education Commission and Shanghai Education Development Foundation.

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constant, q is the electronic charge, ϕ_{b0} is the barrier height in eV at zero-bias, n is the ideality factor, and R_s is the series resistance of the diode. For most non-ideal Schottky diodes, the current–voltage can still be well described by Eq. (1), except that ϕ_{b0} and n should be replaced by ϕ_{ap} and n_{ap}, i.e.

$$I(V_a) = A_d A^{**} T^2 \exp\left(-\frac{\phi_{ap}}{kT}\right) \exp\left[\frac{q(V_a - IR_s)}{n_{ap}kT}\right]. \tag{2}$$

Table 1. Extracted apparent barrier height ϕ_{ap}, apparent ideality factor n_{ap} and diode series resistance R_s of Ti/n-GaAs Schottky diode at different temperatures.

T (K)	ϕ_{ap} (eV)	n_{ap}	R_s (Ω)	T (K)	ϕ_{ap} (eV)	n_{ap}	R_s (Ω)
78	0.437	1.89	49	140	0.662	1.16	68
80	0.443	1.87	49	146	0.676	1.13	70
83	0.472	1.75	50	154	0.682	1.11	73
87	0.492	1.68	50	161	0.685	1.11	75
90	0.503	1.62	52	170	0.690	1.09	78
97	0.534	1.51	55	179	0.690	1.09	80
100	0.547	1.47	56	190	0.691	1.08	86
103	0.553	1.46	56	206	0.692	1.07	93
111	0.569	1.41	58	216	0.692	1.07	97
119	0.599	1.33	61	233	0.693	1.06	102
129	0.623	1.26	64	252	0.693	1.06	107
134	0.643	1.21	66	299	0.698	1.05	118

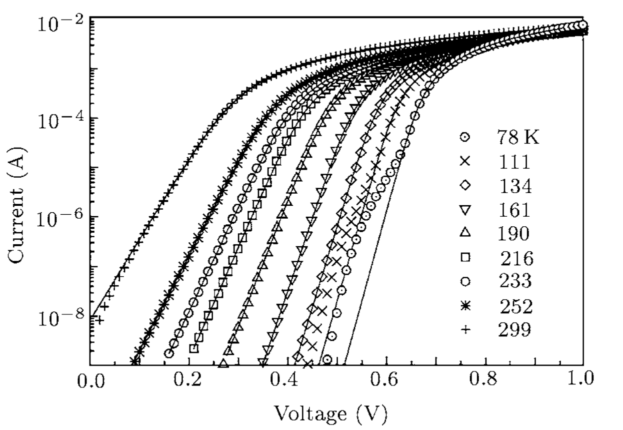

Fig. 1. Current−voltage characteristics of the Ti/n-GaAs Schottky diode at some typical temperatures.

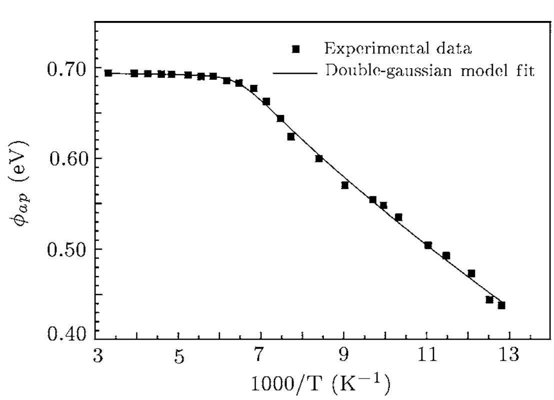

Fig. 2. Variation of the apparent barrier height ϕ_{ap} as a function of $1000/T$. The solid line is the fitted curve using Eq. (9) where the fitting parameters ρ_1, $\bar{\phi}_1$, σ_1, $\bar{\phi}_2$, and σ_2 are 1×10^{-5}, 0.721 eV, 0.069 eV, 0.696 eV, 0.012 eV, respectively.

Figure 1 shows the temperature-dependent I–V characteristics of the Ti/n-GaAs Schottky diode in our experiments. The solid lines are the fitted curves according to Eq. (2) taking ϕ_{ap}, n_{ap}, and R_s as the fitting parameters. The knee portions observed in the $I-V$ curves at very low temperatures (below 134 K) have been neglected in the present fit. Their origin will be discussed later. All the parameters extracted from the experimental data of ϕ_{ap}, n_{ap}, R_s at different temperatures are listed in Table 1.

Figure 2 shows the plot of ϕ_{ap} versus $1/T$. If the barrier height distribution can be described with a Gaussian function, the relationship between ϕ_{ap} and $1/T$ should follow a straight line whose slope is proportional to the square of the standard deviation and whose intercept at ϕ_{ap} axis corresponds to the mean value of the barrier height. However, the experimental relation of ϕ_{ap} versus $1/T$ shown in Fig. 2 is not simply a straight line in the whole temperature range, indicating a more complicated distribution of barrier height existing in the diode. Generally, it should be more reasonable to use an arbitrary SBH distribution to describe an inhomogeneous Schottky contact than any pre-assumed distribution. Only when the theoretically predicted results reach good agreement with experimental results, can the assumed distribution be accepted. In principle, one can assume an infinite number of Gaussian distributions with different mean values and standard deviations, present simultaneously across the metal–semiconductor interface with different probabilities. Here we use an arbitrary distribution function $\rho(\phi)$ to describe the inhomogeneities, and we can obtain the $I-V$ equation based on the parallel conduction model[14]

$$I(V_a) = A_d A^{**} T^2 \left[\exp\left(\frac{qV_a}{n_{ap}kT}\right) - 1\right] \cdot \int_0^{\infty} \rho(\phi) \exp\left(-\frac{\phi}{kT}\right) \mathrm{d}\phi, \tag{3}$$

where

$$\rho(\phi) = \sum_i \frac{\rho_i}{\sigma_i\sqrt{2\pi}} \exp\left[-\frac{\left(\phi - \bar{\phi}_i\right)^2}{2\sigma_i^2}\right]$$

is expanded by the Gaussian distribution function with ρ_i representing the weight, σ_i representing the standard deviation and $\bar{\phi}_i$ representing the mean value of each Gaussian function. The normalization of $\rho(\phi)$ requires $\sum_i \rho_i = 1$. Comparing Eq. (3) with Eq. (2), we can obtain

$$\begin{aligned}\phi_{ap} = &-kT \ln\left[\rho_1 \exp\left(-\frac{\bar{\phi}_1}{kT} + \frac{\sigma_1^2}{2k^2T^2}\right)\right. \\ &+ \rho_2 \exp\left(-\frac{\bar{\phi}_2}{kT} + \frac{\sigma_2^2}{2k^2T^2}\right) + \cdots \\ &\left.+ \rho_n \exp\left(-\frac{\bar{\phi}_n}{kT} + \frac{\sigma_n^2}{2k^2T^2}\right)\right].\end{aligned} \tag{4}$$

For the single Gaussian distribution, Eq. (4) is reduced to the well-known relation

$$\phi_{ap} = \bar{\phi}_1 - \frac{\sigma_1^2}{2kT}. \tag{5}$$

In principle, an infinite number of Gaussian distributions is needed for the multi-Gaussian distribution model but, in practice, one may use a limited number of Gaussian distributions as long as the experimental results are well interpreted. Since the apparent barrier height ϕ_{ap}versus $1/T$ does not show a simple linear relationship in our experiments, we have to use more than one Gaussian distribution. Here we try a double-Gaussian distribution. In other words, the barrier height distribution can be written as follows

$$\begin{aligned}\rho(\phi) &= \rho_A(\phi) + \rho_B(\phi) \\ &= \frac{\rho_1}{\sigma_1\sqrt{2\pi}} \exp\left[-\frac{\left(\phi - \bar{\phi}_1\right)^2}{2\sigma_1^2}\right] \\ &\quad + \frac{\rho_2}{\sigma_2\sqrt{2\pi}} \exp\left[-\frac{\left(\phi - \bar{\phi}_2\right)^2}{2\sigma_2^2}\right],\end{aligned} \tag{6}$$

where

$$\rho_A(\phi) = \frac{\rho_1}{\sigma_1\sqrt{2\pi}} \exp\left[-\frac{\left(\phi - \bar{\phi}_1\right)^2}{2\sigma_1^2}\right] \tag{7}$$

and

$$\rho_B(\phi) = \frac{\rho_2}{\sigma_2\sqrt{2\pi}} \exp\left[-\frac{\left(\phi - \bar{\phi}_2\right)^2}{2\sigma_2^2}\right] \tag{8}$$

are the two different Gaussian distribution functions, and $\rho_1 + \rho_2 = 1$ is satisfied for normalization. Then we can have the relationship of ϕ_{ap} versus T for an inhomogeneous Schottky diode with double-Gaussian distribution of barrier heights

$$\begin{aligned}\phi_{ap} = &-kT \ln\left[\rho_1 \exp\left(-\frac{\bar{\phi}_1}{kT} + \frac{\sigma_1^2}{2k^2T^2}\right)\right. \\ &\left. + \rho_2 \exp\left(-\frac{\bar{\phi}_2}{kT} + \frac{\sigma_2^2}{2k^2T^2}\right)\right].\end{aligned} \tag{9}$$

We use Eq. (9) by taking $\bar{\phi}_1$, σ_1, $\bar{\phi}_2$, σ_2, and ρ_1 as the fitting parameters ($\rho_2 = 1 - \rho_1$) to fit the experimental data, and the results are shown as the solid line in Fig. 2. The good agreement of the experimental data (solid square) with the fitting curve indicates that the SBH inhomogeneity of our Ti/n-GaAs contact can be well described by a double-Gaussian distribution. The fitting parameters ρ_1, $\bar{\phi}_1$, σ_1, $\bar{\phi}_2$ and σ_2, are 1×10^{-5}, 0.721 eV, 0.069 eV, 0.696 eV, 0.012 eV, respectively. Using these parameters, we can plot this double-Gaussian distribution curve as shown in Fig. 3.

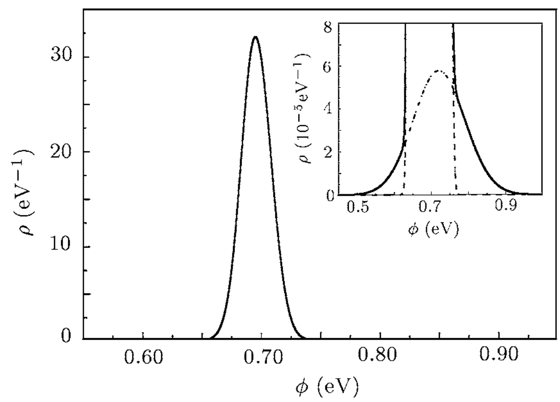

Fig. 3. Distribution curve of the double-Gaussian distribution function with the parameters extracted from the fitting results; *ρ(φ)* is the double-Gaussian distribution function. The inset depicts the detailed distribution information with the solid line representing *ρ(φ)*, the dash-dot-dotted line representing $\rho_A(\phi)$, and the dashed line representing $\rho_B(\phi)$.

From Fig. 3, we can see that the distribution curve is mostly contributed from the second Gaussian distribution $\rho_B(\phi)$. The first Gaussian distribution $\rho_A(\phi)$ contributes very little. However, this little part plays a very important role when the diode works at low temperatures. The difference between the mean values of these two Gaussian distributions is only 0.025 eV. Therefore it is not easy to produce "pinch-off" for such a distribution.[3] The standard deviation of the distribution is about 12 meV, so the homogeneity of this Ti/n-GaAs Schottky diode seems not to be too bad. From the fitting results, we can also know that the occupation area of these two Gaussian distributions are 5 μm^2 for $\rho_A(\phi)$ and 0.005 cm^2 for $\rho_B(\phi)$. It should be pointed out that this double-Gaussian distribution function described above is effective in the whole experimental temperature range. This is different from the multi-Gaussian distribution model previously proposed by Chand and Kumar.[6] In their model (a *single* Gaussian model), Eq. (5) can be used to fit the experimental ϕ_{ap} versus $1/T$ relation of linear fitting in several temperature ranges with several different sets of ϕ and σ. Obviously, it is easier to fit experimental data by this method, however, the assumption of the model, i.e. "dynamic" behaviour of Gaussian distribution still remains questionable.[6] The dynamic behaviour may be explained by the temperature dependence of the semiconductor energy gap (therefore barrier height) and the temperature dependence of band-bending (therefore pinch-off effect).[2,16] If this is true, the mean barrier height and the standard deviation should monotonically decrease with the increase of temperature. Chand and Kumar[6] found there are three temperature ranges with different mean barrier heights and standard deviations. However according to their fitting results, the mean barrier height and standard deviation do not vary monotonically with temperature.

As we mentioned before, the diode exhibits excess leakage, i.e. knee portion at low bias in $I-V$ characteristics at temperatures below 134 K. Such knees can be attributed to the presence of very-low SBH patch(es) covering a small region (within the diode area of high SBH) which will give rise to a large current at a low bias and a saturated current even at a moderate bias because of very large series resistance. Here we may have an estimation of occurrence probability of those very low SBH patches which can only be appreciable below 134 K. We use Eq. (2) to fit the excess current region (knee portion) of the $I-V$ curve at, for example, 78 K. The extracted series resistance R_s is about 5000 Ω. If the series resistance is assumed to result from the spreading resistance of N low-barrier patches with a uniform radius r, then R_s can be written as

$$R_s = \frac{1}{N} \times \frac{\rho}{2\pi r}, \tag{10}$$

and the total area of these patches is

$$A_0 = N\pi r^2 = \frac{1}{N} \times \frac{\rho^2}{4\pi R_s^2}, \tag{11}$$

where ρ is the resistivity of n-GaAs at 78 K, $\sim 0.02\,\Omega\cdot$cm in our case. By taking N to be one, the upper limit of occurrence probability of this distribution A_0/A_d can be estimated to be 2.5×10^{-10}, five orders of magnitude lower than the relatively small Gaussian distribution determined by our double-Gaussian distribution model. This is reasonable because only a small area with a low barrier height will exhibit such temperature-dependent behaviour.

It should be pointed out that in the present model we have not included the temperature- or bias-dependent effects of mean barrier height and standard deviation. Therefore the ideality factor variation is beyond the scope of our discussion. However the inclusion of temperature- or bias-dependent effects into our multi-Gaussian distribution model is straightforward.

In conclusion, the experimental current–voltage characteristics of the Ti/n-GaAs Schottky contact have been successfully interpreted on the basis of a new double-Gaussian distribution model which assumes the simultaneous existence of two Gaussian distributions of barrier height at the metal–semiconductor interface. The model explains the nonlinear behaviour of ϕ_{ap} versus $1/T$, without any assumption of "dynamic" behaviour of barrier height mean value and standard deviation. Our results suggest that the SBH distribution of a real inhomogeneous Schottky contact may not be described by a simple function.

References

[1] Song Y P, Van Meirhaeghe R L, Laflere W H and Cardon F 1986 *Solid-State Electron.* **29** 633

[2] Werner J H and Guttler H H 1991 *J. Appl. Phys.* **69** 1522

[3] Tung R T 1992 *Phys. Rev.* B **45** 13 509

[4] Palm H, Arbes M and Schulz M 1993 *Phys. Rev. Lett.* **71** 2224

[5] Weitering H H, Sullivan J P, Carolissen R J, PerezSandoz R, Graham W R and Tung R T 1996 *J. Appl. Phys.* **79** 7820

[6] Chand S and Kumar J 1997 *Appl. Phys.* A **65** 497

[7] Detavernier C, Van Meirhaeghe R L, Donaton R, Maex K and Cardon F 1998 *J. Appl. Phys.* **84** 3226

[8] Osvald J 1999 *J. Appl. Phys.* **85** 1935

[9] Tung R T 2000 *J. Appl. Phys.* **88** 7366

[10] Osvald J 2000 *J. Appl. Phys.* **88** 7368

[11] Tung R T 2000 *Phys. Rev. Lett.* **84** 6078

[12] Zhu S Y, Van Meirhaeghe R L, Detavernier C, Cardon F, Ru G P, Qu X P and Li B Z 2000 *Solid-State Electron.* **44** 663

[13] Sullivan J P, Tung R T, Pinto M R and Graham W R 1991 *J. Appl. Phys.* **70** 7403

[14] Ohdomari I and Tu K N 1980 *J. Appl. Phys.* **51** 3735

[15] Chin V W L, Green M A and Storey J W V 1990 *Solid-State Electron.* **33** 299

[16] Zhu S Y, Detavernier C, Van Meirhaeghe R L, Cardon F, Ru G P, Qu X P and Li B Z 2000 *Solid-State Electron.* **44** 1807

[17] Horvath Zs J 1992 *Mater. Res. Soc. Symp. Proc.* **260** 367

[18] Osvald J 1992 *Solid-State Electron.* **35** 1629

[19] Rhoderick E H and Williams R H 1988 *Metal–Semiconductor Contacts*, 2nd edn (Oxford: Clarendon) chap 1 p 39