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## **Determination of the Schottky barrier height in diodes based on Au–TiB<sub>2</sub>–*n*-SiC 6H from the current-voltage and capacitance-voltage characteristics**

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**Abstract.** We present the results of investigation of the barrier height and ideality factor in Schottky barrier diodes based on Au–TiB<sub>2</sub>–*n*-SiC 6H relying on measuring the current-voltage and capacitance-voltage characteristics. Improving the accuracy of the methods that take into account the effect of the series resistance in calculating the ideality factor and barrier height has been shown with the Cheung method and direct approximation one. It has been ascertained that an inconsistency between real current-voltage characteristics and its model – the temperature dependence of the barrier height, the ideality factor dependence on the voltage – introduces the basic error into the calculated parameters in the diode under study.

**Keywords:** Schottky barrier, wide-gap semiconductor, ideality factor, current-voltage and capacitance-voltage characteristics.

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### **1. Introduction**

Schottky barrier height (ShBH) and ideality factor are the most important parameters of the Schottky contact. A number of methods for their determination, including determination from the current-voltage characteristic, is well known [1-20]. Attempts to generalize and systematize the existing methods were made in a number of papers [1-4], but estimation of accuracy, carried out in the most of works, does not take into account the peculiarities of contacts to wide-gap semiconductors.

Considering the accuracy of determining ShBH, as applied to the contacts based on wide-gap semiconductors, it is necessary to take into account three factors: the accuracy of measurements of initial values (current, voltage, capacitance), accuracy of the approximation method and accuracy of correlation between the proposed mechanism of charge transport and that implemented in reality.

In this work, a batch of Schottky barrier diodes (ShBD) based on Au–TiB<sub>2</sub>–*n*-SiC 6H were investigated using different methods, a comparison of these results was made, and the reasons of their differences were discussed.

### **2. Samples under study**

Schottky barrier diodes based on Au–TiB<sub>2</sub>–*n*-SiC 6H were created on bulk semiconductor with the concentration of dislocations  $<10^2 \text{ cm}^{-2}$  [19]. The concentration of non-compensated impurities in semiconductors, which was obtained from the capacitance-voltage (*C–V*) characteristics, amounted  $(2...3) \cdot 10^{18} \text{ cm}^{-3}$ . The layers TiB<sub>x</sub> with the thickness ~50 nm and those of Au with the thickness 100 nm were successively deposited using the magnetron sputtering onto the surface of *n*-6H-SiC (0001), subjected to photon

cleaning. Back ohmic contacts were formed using the magnetron sputtering Ni(100 nm), TiB<sub>x</sub>(100 nm) and Au(100 nm) with followed RTA at  $T_a = 1000^\circ\text{C}$  for 60 s.

### 3. Calculation of barrier parameters from current-voltage characteristics

The method described by Rhoderick [5] is the most simple in implementation among the methods considered. In accord with this method, the current through the Schottky diode is described by the relation:

$$I = I_0 \exp(qV/nkT) [1 - \exp(-qV/kT)]. \quad (1)$$

Plotting the current-voltage characteristics in the coordinates  $\ln(I) / [1 - \exp(-qV/kT)] \propto V$  and approximating the line part with straight line  $y = a + bx$ , the coefficients  $b = \ln(I_0)$  and  $a = q/nkT$ , were obtained, and knowing these coefficients it is easy to find  $\phi_b$  and  $n$ . With automating the method, it is convenient to determine the ideality factor, when plotting the dependence:

$$\frac{dV}{d \ln(I)} \frac{q}{kT} = n(V). \quad (2)$$

If in the curve  $n(V)$  there present is the portion weakly dependent of the voltage, then from this range of voltages the values of ideality factor and ShBH were determined using the Rhoderick method. It is worth noting that for wide-gap semiconductors, often even in a highlighted portion in the curve, it is impossible to assert that the ideality factor does not change with voltage. This dependence will make an error into accuracy of determining the ideality factor and, therefore, the barrier height, which is substantially greater than the error introduced by the measurement inaccuracy. Typical local maximum  $n$  for low voltages and increase of the ideality factor with the voltage at high voltages were observed by several authors [3, 7, 21, 22].

The advantage of the Rhoderick method is the ability to describe forward and backward branches of the current-voltage characteristics with one dependence, as well as the account of measurements at  $V < 3kT/q$ . The disadvantages of the method include the lack of account for the influence of the series resistance.

In practice, for small values of ShBH or large series resistance, it is impossible to separate the portion unaffected by the series resistance, there is no portion of the  $I$ - $V$  curve that is described by Eq. (1). One way to solve this problem was proposed by Norde. He has developed a method to determine the barrier height at the voltages  $V > 3kT/q$  and with account of the large series resistance.

The Norde method [7] was developed for the ideality factor close to unity for the cases when the effect of series resistance on the current-voltage characteristics introduces a significant error in determination of the

barrier height by using the simpler methods. For correct description of the current-voltage characteristics at  $V > 3kT/q$ , the formula (1) must be modified to the form  $I = A^{**} T^2 S \exp(q(V - IR_s - \phi_b)/kT)$ , where  $R_s$  is the series resistance.

It is easy to see that, plotting the function  $F(V) \equiv V/2 - kT/q [\ln(I/T^2) - \ln(A^{**}S)]$ , we obtain  $F(V) = IR_s + \phi_b - V/2$ : the slope of the function  $-1/2$ , with the prevalence of the voltage drop on the series resistance the slope will be  $1/2$ . If there is a portion with a slope of  $-1/2$ , the barrier height is determined as the cut-off portion of linear approximation of this portion on the ordinate axis. If the effect of series resistance is large in the whole voltage range, there used is the search of minimum of function  $F$ , which is achieved at some values  $V_{\min}$  and  $I_{\min}$ , then the values of the series resistance and barrier height can be obtained as  $R_s = kT/qI_{\min}$  and  $\phi_b = F(V_{\min}) + V_{\min}/2 - kT/q$ , respectively.

Along with its advantages, the method has some drawbacks: in many cases, the ideality factor is not equal to unity, which introduces errors into results of calculations. The latter are performed from a single point of the current-voltage characteristics, which may also negatively affect the accuracy of calculations. Below we will consider a number of studies, in which attempts were made to neutralize these disadvantages.

The Lien method [8] is based on the construction of several Norde-like functions of the form, where  $\gamma$  is an arbitrary parameter,  $\gamma > n$ . From these curves, the current value  $I_{\min}$  can be obtained, when  $G(I_{\min})$  is minimal. For  $V > 3kT/q$ , taking the series resistance into account, the formula (1) can be rewritten as follows:

$$I = I_s \exp(q(V - IR_s)/kT). \quad (3)$$

We can see that from determining  $G$  and formula (3), the dependence of  $I_{\min}(\gamma)$  is linear and is described by the expression  $I_{\min}(\gamma) = (\gamma - n)kT/qR_s$ . The series resistance is determined using the slope of the dependence, the ideality factor – from the cut-off portion. The barrier height can be found extrapolating the  $G_{\min}(\gamma)$  dependence to the value  $\gamma = n$ . Proposed in the papers by Cibils and Buitrago [9] is a similar modification of the Norde method, however, instead of the  $\gamma$  parameter, some parametric voltage performing the same function was introduced.

Proposed in the method by Cheung *et al.* [10] is transformation of the formula (3):

$$V = \frac{nkT}{q} \ln(I) + \exp(\ln(I)) R_s - \frac{nkT}{q} \ln(A^{**} T^2 S) + n\phi_b,$$

whence  $\frac{dV}{d \ln(I)} = \frac{nkT}{q} + IR_s$ . That is, plotting the

dependence  $\frac{dV}{d \ln(I)} \propto I$  and approximating it with the straight line, we obtain the coefficients  $a = nkT/q$  and  $b = R_s$ . To determine the barrier height, we shall plot the

dependence  $H(I) \equiv V - nkT/q [\ln(I/T^2) - \ln(A^*S)]$ . As seen from Eq. (3),  $H(I) = IR_s + n\phi_b$ , i.e., approximating the dependence with the straight line, we obtain the coefficients  $R_s$  and  $n\phi_b$ . The advantage of the Cheung method lies in determination of the series resistance along with the barrier height and ideality factor, which not only gives an additional information about the contact, but it is also convenient from the viewpoint of automating the calculation process. The disadvantages include the applicability of the method only at the voltages  $V > 3kT/q$ .

Werner [11] examined three different methods for determining the parameters of Schottky diode from the current-voltage characteristics. One of them coincides with the Cheung method. However, as it was shown, the other from the methods considered by Werner, which we will name the Werner method, gave the most accurate values  $\phi_b$ ,  $n$  and  $R_s$ . The Werner method uses the differential conductance of the real diode  $L = dI/dV$  at a forward bias. For  $V - IR_s > 3kT/q$ , with taking into account the equation (3), it can be written:

$$\frac{L}{I} = \frac{q}{nkT} (1 - LR_s), \quad (4)$$

whence it follows that plotting the dependence  $L/I = f(L)$  and approximating it with a straight line, one can calculate  $R_s$  from the slope coefficient, and one can get the value of the ideality factor from the cut-off portion.

Carried out in the work by Aubry and Meyer [3] was a comparative analysis of the methods by Lien and Werner, and it was shown that the methods have mathematically similar procedures, accordingly, their accuracy and limitations are close.

Another way to solve the identified problem is to use the methods of direct approximation (DA) to the entire length of the current-voltage characteristics with the simplified expression (3) [12] or more complete one that takes into account the shunt resistance [13-16]. The disadvantage of the method is the relative complexity of the calculation, however, we have developed a program [17], allowing easily-to-make calculations with the majority of the above methods, including the batch calculation parameters, which is important for statistical measurements.

In all the cases described above, the product of the effective Richardson constant by the effective area is assumed to be known. However, this product can be determined experimentally in a case when the temperature measurements of the current-voltage characteristics were performed. For this purpose, it is necessary to use the method of activation energy (AE) [9] or the Sato method [18].

However, ShBH obtained using these two methods is determined on the assumption that its dependence on temperature is missing. In the presence of a linear

temperature dependence of ShBH, the resulting value is often denoted by  $\phi_{b0}$ , to indicate that this value obtained by extrapolating to zero temperature. But this is true only for the linear temperature dependence of ShBH, in the case when it is nonlinear we shall obtain different  $\phi_{b0}$  values for different temperature ranges. In this case, it should be sure to specify the range of temperatures, in which the measurements were performed, as well as to take into account the error in determining the value  $\ln(A^{**}S)$  equal to  $q\beta/k$ , where  $\beta$  is the temperature coefficient of ShBH.

The method of activation energy [5] determines  $\ln(I_0)$  with one of the above methods (by Rhoderick, Cheung and DA) for each temperature separately. Plotting the dependence  $\ln(I_0/T^2) \propto q/kT$  and approximating it with the straight line, we obtain the coefficients  $a = \ln(A^{**}S)$  and  $b = \phi_{b0}$ .

The Sato method [18] lies in the fact that for determining the barrier height, taken is not  $\ln(I_0)$  but the specific point on the  $I-V$  characteristic, which is obtained from minimum  $F1_{\min}$  of the function  $F1 = (qV/2kT) - \ln(I/T^2)$  at certain current  $I_{\min}$ . In this case, the following equality must be fulfilled

$$\begin{aligned} F2 &\equiv 2F1_{\min} + (2-n)\ln(I_{\min}/T^2) = \\ &= 2 - n \left[ \ln(SA^{**}) + 1 \right] + (qn\phi_{b0}/kT), \end{aligned} \quad (5)$$

whence the barrier height  $\phi_{b0}$  and  $\ln(A^{**}S)$  are determined as coefficients of the linear approximation  $a = 2 - n \left[ \ln(SA^{**}) + 1 \right]$  and  $b = n\phi_{b0}$  for the known ideality factor.

Along with the method of the current-voltage characteristics for determining the barrier height, the method of the capacitance-voltage characteristics is often used. According to [2, 5], the dependence of capacitance on the applied voltage in the reverse-biased Schottky barrier is described by the equation:

$$\frac{1}{C^2} = \frac{2(\phi_b - V - kT/q)}{q\epsilon_s N_d}, \quad (6)$$

where  $C = (C_E - C_0)S$  is the reduced capacitance;  $C_0$  – capacitance of a case, contacts;  $C_E$  – experimentally determined capacitance;  $N_d$  – concentration of uncompensated donors;  $\epsilon_s$  – permittivity of semiconductor.

If the concentration  $N_d$  is constant over the whole area of depleted layer, when plotting the dependence  $1/C^2$  on  $V$ , we get a straight line. Approximating this line, we shall obtain the coefficients:

$$a = -\frac{2}{q\epsilon_s N_d} \quad \text{and} \quad b = \frac{2(\phi_b - kT/q)}{q\epsilon_s N_d}.$$

From these, it is simply to calculate the concentration of uncompensated carriers and ShBH:

$$N_d = -\frac{2}{q\epsilon_s a} \text{ and } \varphi_b = \frac{b\epsilon_s N_d}{2} + kT.$$

The method can be implemented only under condition of uniform doping semiconductor, owing to which one can also determine the parameter  $C_0$ , achieving the linearity of dependence  $1/C^2$  on  $V$  (minimum of errors in linear approximation).

#### 4. Results and discussion

The parameters of the Schottky barrier calculated by various methods at the temperatures 340 and 480 K are listed in Tables 1 and 2, respectively. For the calculations by using the AE method, applied here are the results of the saturation current determined by the Rhoderick method. The resulting value of ShBH is strongly underestimated (see Table 1). The reason for this is the temperature dependence of  $\varphi_b$ . It is seen that the value of the barrier height obtained from AE and Sato methods is close to the value obtained using linear extrapolation to zero of the temperature dependence of ShBH, calculated by the Roderick method (figure).

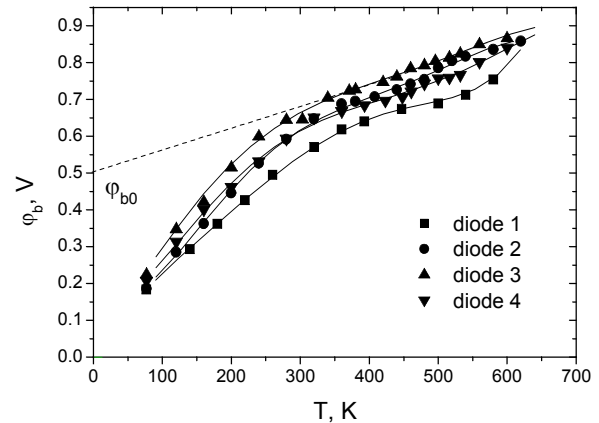
**Table 1. The parameters of the Schottky barrier calculated using different methods. The calculation is performed for the temperature close to 340 K.**

Method of calculation	$n$	$\varphi_b$ , V	$\ln(A^{**}S)$	$R_s$ , Ohm
Rhoderick	$1.51 \pm 0.05$	$0.704 \pm 0.003$	$-4.646^*$	
Cheung	$1.50 \pm 0.01$	$0.704 \pm 0.003$	$-4.646^*$	$934 \pm 30$
DA	$1.493 \pm 0.005$	$0.704 \pm 0.002$	$-4.646^*$	$951 \pm 40$
AE		0.50	-4.0	
Sato		0.52	-4.1	
$C-V$		0.98		

Note. The asterisk \* denotes the value taken for calculation.

**Table 2. The parameters of the Schottky barrier calculated using different methods. The calculation is performed for the temperature close to 480 K.**

Method of calculation	$n$	$\varphi_b$ , V	$R_s$ , Ohm
Rhoderick	$1.6 \pm 0.12$	$0.789 \pm 0.005$	
Cheung	$1.5 \pm 0.15$	$0.79 \pm 0.01$	$400 \pm 25$
DA	$1.45 \pm 0.05$	$0.786 \pm 0.003$	$370 \pm 25$



Temperature dependence of the barrier height calculated using the Rhoderick method.

The reason for increasing the error of calculation of the barrier height in all three methods is the reduction of the length of the logarithmic plot of current-voltage characteristics and increasing in the complexity of determining its boundaries. In the case of the Cheung method, the error is maximum, since in this case the account of the portion of current-voltage characteristics  $V \sim kT/q$  plays a significant role in the total measurement accuracy.

#### 5. Conclusions

Considering the series resistance and portion of current-voltage characteristics at  $V \sim kT/q$  can contribute a substantial correction to the value of the determined series resistance, and therefore, the methods of Lien, Werner as well as direct approximation are preferable to determine the height of the potential barrier at the small extent of the exponential portion of the current-voltage characteristics, as for example, it is observed for the current-voltage characteristics of the investigated diode at  $T \geq 480$  K. The values of the barrier height, obtained by the method of activation energy and Sato, are only valid in the absence of the temperature dependence of ShBH.

It has ascertained that an inconsistency between the real current-voltage characteristics and its model – the temperature dependence of the barrier height, ideality factor dependence on the voltage – introduces the basic error into the calculated parameters in the diode under study. In relation with the foregoing, it can be concluded that for the wide-gap semiconductors, at this stage of their study, the greatest accuracy is inherent to methods allowing to detect and identify a discrepancy between the model and measured data, namely, methods by Lien, Werner and Cheung. The necessity to study the temperature dependence of the ideality factor for correct determination of the mechanism responsible for the charge transfer and Schottky barrier height has been shown.

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