

Modeling the Abnormal Behavior of the 6H-SiC Schottky Diode Using Lambert W Function

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Electrical study of Ni and Ti metals of Schottky contacts on *n*-6H-SiC epitaxial layers is performed, by current-voltage (*I-V*) characterization. Ni/6H-SiC shows inhomogeneous barrier height behavior. Thermionic emission model is coupled with the Lambert function to obtain an explicit form of the Schottky equation as well as to specify the number of branches necessary for modeling the abnormal behavior. The inhomogeneous barrier height for the investigated Ni/6H-SiC junction can be reproduced by a model that includes two Schottky branches, which give a low (*L*) and a high (*H*) Schottky barriers ($\phi_{bn}^L = 0.92$ eV, $\phi_{bn}^H = 1.56$ eV), as well as give a low and a high ideality factors ($n^L = 1.93$, $n^H = 1.23$).

Keywords: SiC, Schottky diodes, Lambert function, Inhomogeneous barrier height, Electrical measurement.

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1. INTRODUCTION

For more than sixty years, the semiconductor industry has been based on the use of silicon (Si). As the evolution of electronic components continues, we are currently at the limit of the physical properties of silicon in certain application areas [1, 2]. This limit has motivated the search for new materials with a wide bandgap that can offer superior performance to that of silicon.

Silicon carbide (SiC) with its wide bandgap, its critical electric field, and its high saturation electron drift velocity, gives the possibility of producing components in areas of operation that are inaccessible with Si. Its technological advancement makes SiC currently a high alternative candidate to silicon, more attractive than other wide bandgap semiconductors (diamond, AlN, GaN) [3].

Although there are all these traits, many steps are necessary to investigate highly efficient and miniaturized devices based on SiC, such as Schottky diodes. In particular, ohmic contacts with low contact resistance and Schottky contacts with controlled barrier height (ϕ_{bn}) between SiC and metal are critical points that can compromise the manufacturing quality of devices [4, 5].

The SiC semiconductor is also of considerable relevance for research such as Schottky diode inhomogeneity. Many researchers have already studied these effects [6]. The inhomogeneity is probably due to the quality of materials and interfaces with various defects such as carrots, growth pits and micropipes [7].

The barrier height inhomogeneity manifests itself in different forms in the static characteristic of a Schottky diode. The most frequent case is the double barrier. As its name suggests, the Schottky contact forms two barriers with different heights.

The most general form of inhomogeneity is when the barrier is made up of a multitude of barriers of different heights, locally delimited.

In this work, a generic model of the 6H-SiC Schottky diode has been proposed for the forward regime. It allows us to describe its abnormal behavior by using a systematic approach of several diodes in parallel. The particularity of this model is that it uses the properties of the Lambert function to obtain an explicit form of the Schottky equation as well as to specify the number of branches necessary for modeling abnormal behavior. Its simplicity of implementation makes it easy to integrate into SPICE simulator software.

2. EXPERIMENTAL DETAILS

The surface of SiC was prepared with chemical treatment and RCA cleaning for the control of metallic contamination and particles in the wafer reproduction process. After the RCA cleaning, the deposition of Ni and Ti metals on SiC surfaces was performed immediately. The epitaxial layers were *n*-type doped with doping concentrations of $5 \times 10^{15} \text{ cm}^{-3}$ and $8.8 \times 10^{15} \text{ cm}^{-3}$.

The ohmic contact is a nickel or titanium contact 2000 Å thick annealed for 10 min at 950 °C.

Schottky and ohmic contacts were covered in situ with a layer of platinum to prevent them from oxidizing, since platinum does not oxidize in air. The details of the deposition materials are shown in Table 1.

A "Semiconductor Parameter Analyzer" model HP4145B was utilized in order to obtain accurate readings of the electrical current. Each SMU is capable of being configured to generate an electrical potential ranging from 0 V to ± 100 V.

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Table 1 – Details on the deposited materials

| Sample | Concentration (cm ⁻³) | Epitaxial thickness (μm) | Dimension (cm) |
|-----------|-----------------------------------|--------------------------|----------------|
| Ni/6H-SiC | 5 × 10 ¹⁵ | 7 | 0.16 × 0.16 |
| Ti/6H-SiC | 8.8 × 10 ¹⁵ | 7 | 0.04 × 0.04 |

3. ELECTRICAL MEASUREMENTS AND MODELING

The *I-V* characteristics of Schottky diodes on *n*-type 6H-SiC wafer were obtained for values between - 40 and 5 V. Of these diodes, Ti/6H-SiC behavior is close to ideal, as shown in Fig. 1a. For the second diode, Ni/6H-SiC has "nonideal" forward characteristics, as seen the "knee" at log *I* vs *V* plot, as shown in Fig. 1b.

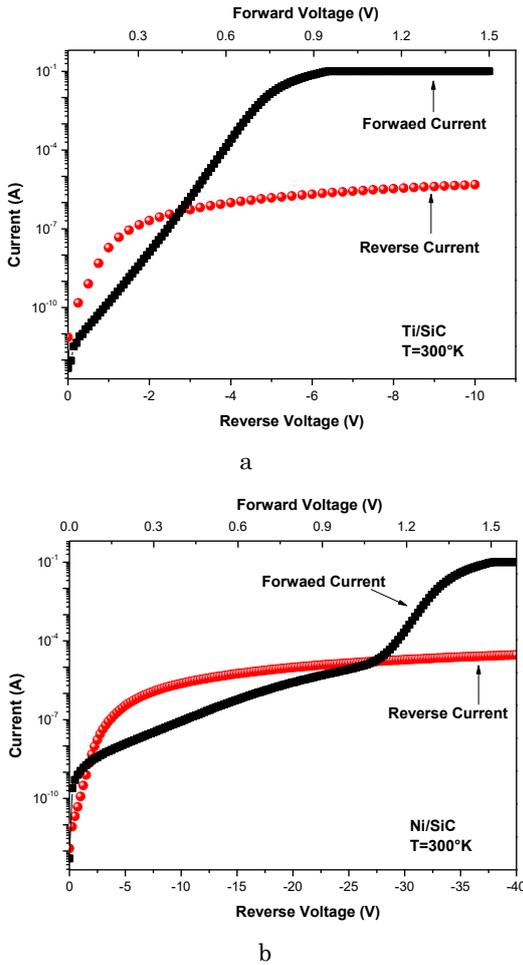


Fig. 1 – *I-V* characteristic showing the "single-barrier" for the Ti/6H-SiC contact (a) and the "double-barrier" for the Ni/6H-SiC contact (b)

The two characteristics show the presence of two types of diodes: a diode with normal behavior such as a Ti/SiC diode and the second type with abnormal and deformed characteristics of the Ni/SiC contact.

For electrical characteristics such as Schottky barrier height(s) and ideality factors, we use the equation of thermionic emission which describes the behavior in the direct mode of the Schottky diode.

After the proposal of the Schottky contact theory [8], several studies [9] propose a formulation of the thermi-

onic current in the following form:

$$I = I_S \left(\exp \left(\frac{q(V - IR_S)}{nkT} \right) \right) \tag{1}$$

The saturation current *I_S* is given by:

$$I_S = AA^*T^2 \exp \left(\frac{-q\phi_{bn}}{kT} \right), \tag{2}$$

where *q* is the electron charge, *k* is the Boltzmann constant, *T* is the absolute temperature, *A* is the effective diode area, *A** is the effective Richardson constant (for 6H-SiC it is 156 Acm⁻²k⁻² [7]), *R_S* is the series resistance, *φ_{bn}* is the barrier height, *n* is the ideality factor.

Note that the log *I* vs *V* plot of a near-ideal Schottky contact, as illustrated in Fig. 1a, has one linear area. The rollover zone of this plot occurs because *RS* restricts the amount of current that can be delivered through the diode. For *V* > 3*kT*/*q*, the mean value of the ideality factor *n* is given by the straight slope fitting of the linear area [10].

From the first region, we can define now *IS* as the value intersected on the current axis by the interpolated straight line. Then, using Eq. (2), we can deduce the barrier height *φ_{bn}* using the later saturation current.

Table 2 displays the Schottky diode parameters for Ti/6H-SiC.

Nonideal Ni/6H-SiC Schottky diode with a knee in the log *I-V* plot (see Fig. 1b) was modeled as having two parallel barrier heights.

The double barrier has been studied and modeled successfully in several reports [11]. This behavior would be visible when a small portion of the total surface of the contact (less than 1 %) forms a barrier lower than the ideal diode. In this case, the diode can be modeled as two Schottky diodes in parallel, whose parameters are different. According to this model, the current flowing through the diode is constituted by the sum of the currents flowing through the low barrier and through the high barrier. Using the thermionic current equation, we can find the parameters of each branch.

In order to determine the electrical parameters for each branch, we use the so-called "phenomenological" method, which allows us to precise the parameters of each diode.

The phenomenological model we present here allows us to avoid using the implicit nature of the thermionic equation and provides us with a set of parameters to adjust the model.

The proposed model uses the multi-branch approach. The particularity of this method is that it uses the properties of the Lambert function to obtain an explicit form of the Schottky equation as well as to specify the number of branches necessary for the modeling abnormal diodes. A schematic circuit model for a multi-branch case is shown in Fig. 2.

3.1 Formalization of the Multi-Branch Model

To explicitly define each branch of the model, we need to express the thermionic current suggested in Eq. (1) using the properties of the Lambert functions.

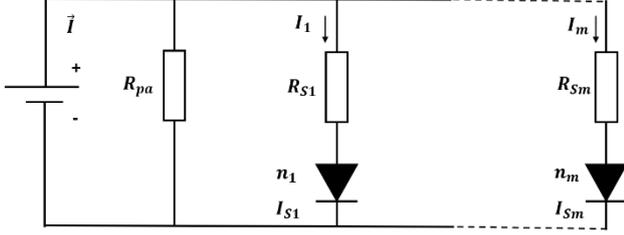


Fig. 2 – Multi-branch model of the Schottky diode defined by phenomenological parameters

First, the thermionic current terms are combined together:

$$I_S \exp\left(\frac{qV}{nkT}\right) = I_{TE} \exp\left(\frac{qR_s I_{TE}}{nkT}\right). \quad (3)$$

Then, by changing the variable, we get the W-Lambert function:

$$w = \frac{qR_s I_{TE}}{nkT}. \quad (4)$$

Eq. (3) then becomes:

$$w \exp(w) = \left(\frac{qR_s}{nkT}\right) I_S \exp\left(\frac{qV}{nkT}\right). \quad (5)$$

The W-Lambert function's property allows us to define w as follows:

$$w = W_0 \left[\left(\frac{qR_s}{nkT}\right) I_S \exp\left(\frac{qV}{nkT}\right) \right]. \quad (6)$$

After fulfilling the condition $W_0(x) = 0$ for $x = 0$, we deduce that the only main branch is obligatory for Eq. (1) [12].

By integrating w in Eq. (6), we can define the current of a branch by Eq. (7):

$$I_{TE} = \frac{nkT}{qR_s} W_0 \left[\left(\frac{qR_s}{nkT}\right) I_S \exp\left(\frac{qV}{nkT}\right) \right]. \quad (7)$$

In this way, we can express the current in analytical or numerical form, avoiding convergence problems that arise with the implicit form. Each branch of the model is defined by parameters independent of those of the other branches. The forward-biased current is given by Eq. (8), which is the sum of the currents in each branch:

$$I_{Total} = \sum_{i=1}^m I_{TE,i} = \sum_{i=1}^m \left(\frac{nkT}{qR_{s,i}}\right) W_0 \left[\left(\frac{qR_{s,i}}{nkT}\right) I_{S,i} \exp\left(\frac{qV}{nkT}\right) \right] + \frac{V}{R_{PA}}. \quad (8)$$

We choose two diodes for our case ($m = 2$). Fig. 2 can be reduced to the illustrated circuit model in Fig. 3, L and H designate the low and high Schottky barriers, respectively.

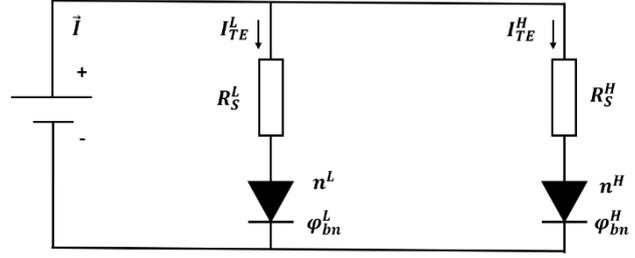


Fig. 3 – Double barrier thermionic model of Schottky diode

3.2 Extraction Method

To determine the physical Schottky diode parameters, the magical "FindFit" function was used. It is a nonlinear fitting technique commonly used in statistics; it converts parameters into numerical values, confirming the well-fitting of the model equation with the experimental data. This fitting tool determines the best fit globally in linear cases. In nonlinear applications, it just finds the best fit locally. For both cases, the least square fit is used by default. For nonlinear situations, some methods are internally integrated in the "FindFit" such as Levenberg-Marquardt, method of Brent Conjugate Gradient, principal axis Gradient, NMinimize, Newton and quasi-Newton [13].

The values obtained using the "FindFit" function are shown in Table 2.

As indicated in Table 2, the values of n , ϕ_{bn} , and I_s (A) for the diode modeled with one barrier ($\phi_{bn} = 0.82$ eV, $n = 1.18$) were significantly different from those modeled with two barriers (Region 1: $\phi_{bn} = 0.92$ eV, $n = 1.93$ and Region 2: $\phi_{bn} = 1.56$ eV, $n = 1.23$), the double-barrier diode has a high ideality factor and the barrier height presenting Schottky barrier inhomogeneity of the diode due to trap centers (defect centers) that generate tunnel currents (thermionic field emission TFE and field emission FE) [14-18]. Furthermore, it is clear that the double-barrier diode has greater reverse leakage currents than the near-ideal diode.

We consider that the computed values demonstrate a reasonable approximation of the "effective" low-barrier barrier height despite a slightly high ideality factor that might cause an underestimation of the low-barrier barrier height.

The term "effective barrier height" points out the possibility that low-barrier zones might have a combination of low barriers, with one of the barriers predominating in any particular diode, despite being described here as having a single or homogeneous barrier height.

For comparison, a preliminary study of inhomogeneous Schottky contacts [19] showed that regions with low Schottky barrier heights give bigger ideality factors. In more recent research [20] with SiC Schottky contacts, researchers used a model that was analogous to the previous one in order to match the experimental data. The researchers reported that the low-barrier ideality factors ranged anywhere between 1.45 and 3.9.

Table 2 – Electrical parameters calculated using the "FindFit" function

| Metal/property | | n | ϕ_{bn} (eV) | I_s (A) | Reverse leakage current at $V_R = 10$ V |
|----------------|-------------|------|------------------|-----------------------|---|
| Ti | | 1.18 | 0.82 | 2×10^{-12} | $\sim 4 \mu\text{A}$ |
| Ni | Branch 1(L) | 1.93 | 0.92 | 1.2×10^{-10} | $\sim 2 \mu\text{A}$ |
| | Branch 2(H) | 1.23 | 1.56 | 2×10^{-16} | |

4. CONCLUSIONS

The current-voltage measurements of Ni/6H-SiC and Ti/6H-SiC Schottky diodes showed surprising variations in the barrier height. The differences were described using single and double barrier models as well as quanti-

tative parameters as that of the ideality factor, Schottky barrier height, and reverse leakage current.

A generic model of the diode has been proposed for the forward regime. It allows us to describe the abnormal behavior of a 6H-SiC Schottky diode, considering the variation of the barrier height.

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Моделювання аномальної поведінки діода Шоттки на основі 6H-SiC за допомогою функції Ламберта

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Проведено електричне дослідження Ni і Ti металевих контактів Шоттки на епітаксійних шарах n-6H-SiC методом вольт-амперної характеристики. Ni/6H-SiC демонструє неоднорідну поведінку висоти бар'єру. Модель термоелектронної емісії поєднується з функцією Ламберта, щоб отримати явну форму рівняння Шоттки, а також визначити кількість гілок, необхідних для моделювання аномальної поведінки. Неоднорідну висоту бар'єру для досліджуваного переходу Ni/6H-SiC можна відтворити за допомогою моделі, що включає дві гілки Шоттки, які дають низький (L) і високий (H) бар'єри Шоттки ($\phi_{bn}^L = 0,92$ eV; $\phi_{bn}^H = 1,56$ eV), а також низький і високий коефіцієнти ідеальності ($n^L = 1,93$; $n^H = 1,23$).

Ключові слова: SiC, Діоди Шоттки, Функція Ламберта, Неоднорідна висота бар'єру, Електричні вимірювання.