

## INTERFACES TO 6H-SiC SUBSTRATES – TECHNOLOGY AND SIMULATION

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**Abstract.** This paper gives a short overview of inhomogeneities at the semiconductor metal interface. The model for the contact area is described, and the simulation results are presented and discussed. It is concluded that the contacts to the SiC substrate will include some errors. These inhomogeneities cause changes in the current distribution at the interface, which in turn, could lead to the creation of hot spots. With the help of electrothermal simulations, it is possible to determine the location and current peak value of the hot spot and therefore to avoid damaging the device.

**Key words:** silicon carbide, Schottky interface, current suppressing effect, contact modelling, physics oriented SPICE simulation.

### 1. INTRODUCTION

#### Aspect one – technology

Silicon carbide is known to be a superior semiconductor for the development of high frequency, high power, high temperature, and radiation hard devices [<sup>1,2</sup>]. In the case of SiC technology, the fabrication of p-n junction using diffusion technology is not feasible because of the low diffusion rates of dopants [<sup>3</sup>]. Therefore, most of the SiC structures have been based on multiple epitaxial layers in conjunction, and the trench process is used to form the devices and the contacts to the buried epitaxial layers.

Different metals (mostly gold, platinum and titanium) could be used to form a contact barrier to 6H-SiC. In [<sup>2</sup>], a new etching technique for 6H-SiC, which utilizes amorphization by high dose ion-implantation, and wet chemical etching has been introduced. The etching technique yields smooth etched surfaces with vertical sidewalls.

The high performance of SiC-based devices has been limited because of the lack of a high temperature contact technology [4]. Thus, high temperature contacts are a critical phase of the technology, impeding further device and system development. Since diffusion welding technology offers extra high lateral homogeneity and relatively deep interface penetrate, it probably avoids these difficulties for different metals mentioned further. Metal-diamond-like nanocomposite (Me-DLN) is, however, potentially an interesting high temperature contact material. The W-DLN technology and electrical characteristics of W-DLN Schottky contacts have been reported in [5]. Unfortunately, the structure of the interface area has an extremely high level of inhomogeneities (nanocomposite structure of the interface). The electrical properties of the interface are controlled by the electrical properties of the tungsten SiC interface. Therefore, the selection of the metal incorporated into the Me-DLN SiC contact should strongly influence the electrical properties of the contact. In spite of the nearly ideal results reported for the Schottky contacts, the question of existing inhomogeneities at the interface remains. This assumption is supported by the results in [6]. It is proposed that the defects at the SiC metal interface result in lowering of the barrier height in the localized regions, and thus, significantly affect the I-U characteristics of the Schottky contacts.

These inhomogeneities (caused, e.g., by grain size effects, diffusional creeps, other boundary effects) lead to the local characteristics at the interface. It means that the interaction of several metals or other materials at the semiconductor interface will lead to the formation of different local barriers at the different subregions with different contact properties, and the current flows through different subregions which have different resistance. Sometimes the so-called multi-level and alloy-type Schottky contacts are manufactured to diminish the contact transition resistance, which also could lead to another type of inhomogeneities. This, in turn, leads to potential barrier variations at the interface along the contact area. The variation of the Schottky barrier height and thickness may occur partially or simultaneously when there is a simultaneous interaction of some type of metals (or those of metals and semiconductor elements) on semiconductor substrate in both microscopic and macroscopic aspects. Therefore, the height of the metal-semiconductor (MS) contact barrier will be a combination of several local barrier heights (Fig. 1).

### Aspect two – modelling

Many explanations and models have been developed to describe the inhomogeneities at the Schottky contacts (e.g., [7-9]). The first model for these structures was proposed in [7]. This model was extended to parallel connected (lateral) diodes with lateral dimensions comparable to the Debye length of the given semiconductor, where the diodes are no longer independent and the potential, and therefore the electron transport of each individual patch may be no longer treated independently [8].

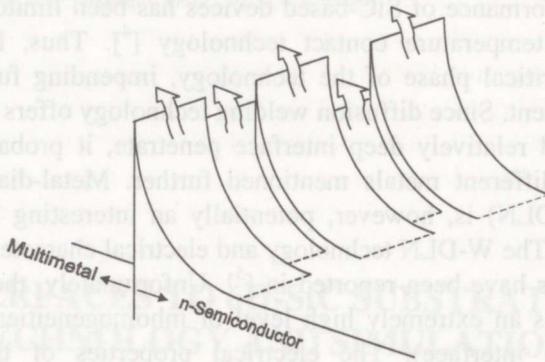


Fig. 1. The Schottky interface at different barrier heights.

The most applicable model for the so-called effective barrier height was reported by Mojzes and his co-workers [10] for the Si and GaAs Schottky contacts. Later, similar results were reached by Rang [11] for SiC. Unfortunately, these results that neglected the influence of simultaneous presence and distribution of different metal atoms (or different atomic groups along the inhomogeneous interface), using the so-called effective barrier height, could lead to some error in the evaluation of the electrical properties of the MS contacts. The current distribution at the contacts caused by inhomogeneities (e.g., creation of hot spots, etc.) is described in [12].

Thus, the aim of this work is to try to design a relatively simple 2D model for describing a thermoelectrical behaviour of the Schottky interfaces and to apply this model to 6H-SiC power Schottky structure with inhomogeneities at the contact.

## 2. DESCRIPTION OF THE MODEL

The current transport in MS contacts is mainly due to majority carriers. There exist four processes:

- transport of electrons from the semiconductor over potential barrier into the metal;
- recombination in the space-charge region;
- hole injection from the metal to the semiconductor;
- quantum-mechanical tunnelling of electrons through the barrier.

The first three mechanisms are described by diffusion-drift theory, and the current is known as thermionic emission current. The latter forms the tunnelling current. However, in this paper, we do not include the tunnelling part into the whole current. The tunnelling current will dominate ( $J^T > J^{ED}$ ) at higher doping levels and lower temperatures, and therefore in the first approximation it could be neglected. The influence of tunnelling current will be discussed elsewhere [13].

First, the equivalent circuit for 2D model of the MS contact area is designed. The interface area is modelled with the help of ideal diodes, the resistors describe the substrate volume, and the anisotropy of the 6H-SiC is taken into account, using different types of vertical and lateral resistors. To keep the homogeneous current density from the bulk of Schottky structure, the so-called current density generators are introduced. For the most commonly used triangular basic cell configuration, it is enough to describe cylindrical volume around the contact area of the Schottky structure (Fig. 2a). The basic cell of the model is described as a toroid (Fig. 2b). Figure 3a shows the discretization net, and Fig. 3b shows the SPICE 2D equivalent circuit model. The net is denser in these regions, where the barrier height of the MS contact is changing.

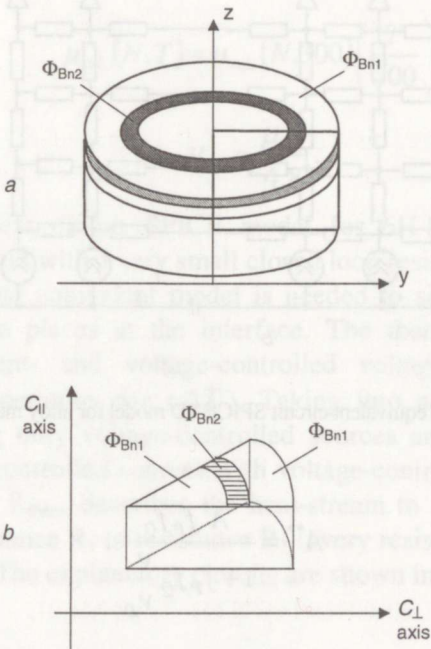


Fig. 2. 2D model area (a) and basic cell (b) description.

Using the thermionic-emission theory, the diode current density will be expressed as

$$J = J_s \left( \exp \frac{U}{n\varphi_T} - 1 \right), \quad (1)$$

where

$$J_s = A^{**} T^2 \left( \exp - \frac{q\Phi_{Bn}}{\varphi_T} \right), \quad (2)$$

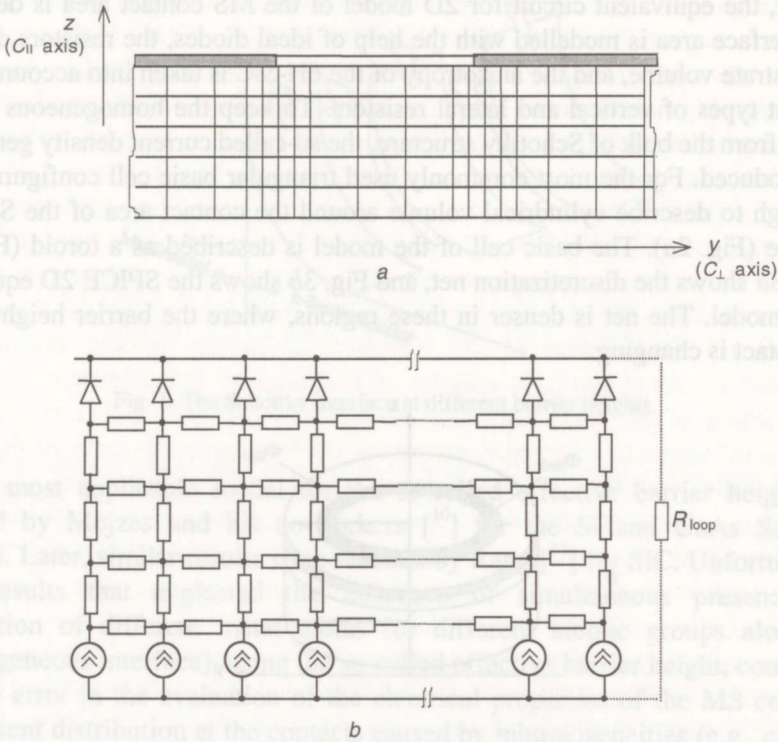


Fig. 3. Discretization net (a), equivalent circuit SPICE 2D model for alloy metal Schottky interface (b).

$$A^{**} = \frac{A^* f_P f_Q}{1 + f_P f_Q \frac{V_R}{V_D}} \quad (3)$$

Let us assume  $f_P = f_Q = 1$ , where  $f_P$  is the probability of electron emission over the potential maximum, and  $f_Q$  is the ratio of the total current flow, considering the quantum-mechanical tunnelling and reflection, to the current flow neglecting these effects. Effective Richardson constant is  $A^{**} = A^* / (1 + v_R / v_D)$ , and  $A^* = A(m^* / m_0)$ , where  $A = 120 \text{ AK}^2 / \text{cm}^2$ ,  $(m^* / m_0)_\perp = 0.25$  and  $(m^* / m_0)_\parallel = 1.7$ . Thus, for 6H-SiC,  $A^*_\perp = 30 \text{ AK}^2 / \text{cm}^2$  and  $A^*_\parallel = 204 \text{ AK}^2 / \text{cm}^2$ . The effective recombination (thermal) velocity will be determined as  $v_R = (A^* T^2) / (q N_C)$ , and the effective diffusion velocity  $v_D = \mu E_M \{1 - [(3\pi / 64)(\mu E_M / C_S)]\}$ , where the effective density of states in the

conduction band  $N_C = 3.368 \cdot 10^{19} (T/300)^{3/2}$ , and the speed of sound in semiconductor is  $C_S = 1.224 \cdot 10^6$  cm/s.

The MS contact itself is described with the help of ideal diodes; the parameters of each of them are calculated using thermionic-diffusion theory, neglecting the tunnelling mechanism through the barrier as mentioned earlier.

For charge carrier mobilities, the so-called two-level description (local model) is used

$$\mu_{n\perp}(N, 300) = \frac{415}{1 + \left( \frac{N_D + N_A}{1.11 \cdot 10^{18}} \right)^{0.59}}, \tag{4}$$

$$\mu_{n\perp}(N, T) = \mu_{n\perp}(N, 300) \left( \frac{T}{300} \right)^{-2.07}, \tag{5}$$

$$\mu_{n\parallel} = \frac{\mu_{n\perp}}{4.8}. \tag{6}$$

The 2D equivalent circuit SPICE model for 6H-SiC substrate Schottky interfaces is completed with a very small closed loop resistor  $R_{loop}$ .

The electrothermal equivalent model is needed to simulate the self-heating behaviour of certain places at the interface. The thermal behaviour will be handled over current- and voltage-controlled voltage sources, which are proportional to temperature rise ( $\Delta T$ ). Taking into account that by analog-behaviour-modelling only voltage-controlled sources are allowed, we have to replace the current-controlled sources with voltage-controlled sources over  $F_{copy}$  and  $R_{ref}$ . Resistance  $R_{therm}$  describes the heat-stream to surface (heat-reservoir) and  $R_{R1R2}$  from resistance  $R_1$  to resistance  $R_2$  (every resistance creates additional two nodes  $a$  and  $c$ ). The explanatory circuits are shown in Figs. 4 and 5.

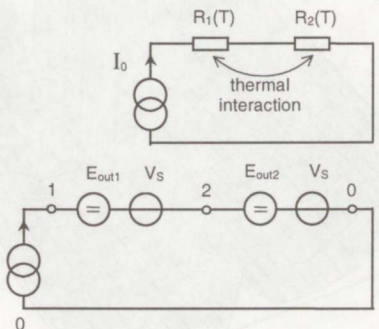


Fig. 4. Elements taking into account the thermal behaviour.

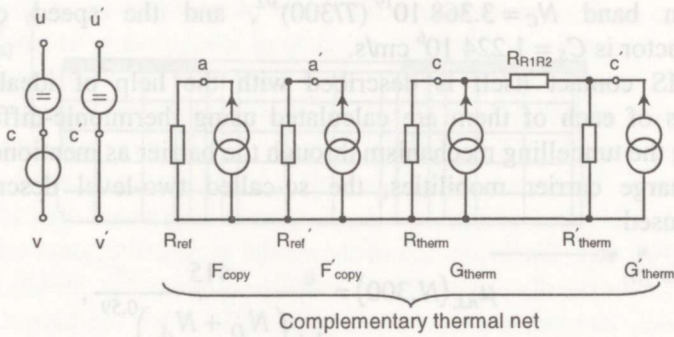


Fig. 5. Complementary thermal net.

### 3. RESULTS AND DISCUSSION

The current distribution at the Schottky interface, depending on the average current density, is shown in Fig. 6. Obviously, a strong current “push-out” effect in the vicinity of the boundary, where the overjump from the higher barrier height to the lower one takes place, could be observed. The current pressing from the region of higher barrier height into the region with lower barrier height can explain this. This so-called extra current has two peaks in the contact region with lower barrier height, which means that the current “push-out” effect exists near the boundaries, where the barrier height change takes place. Because of the symmetry of the effect described further, it is enough to look only for one symmetric part of this picture (Fig. 7). In our opinion, this rather unexpected behaviour of the current could be explained by the anisotropy of the 6H-SiC

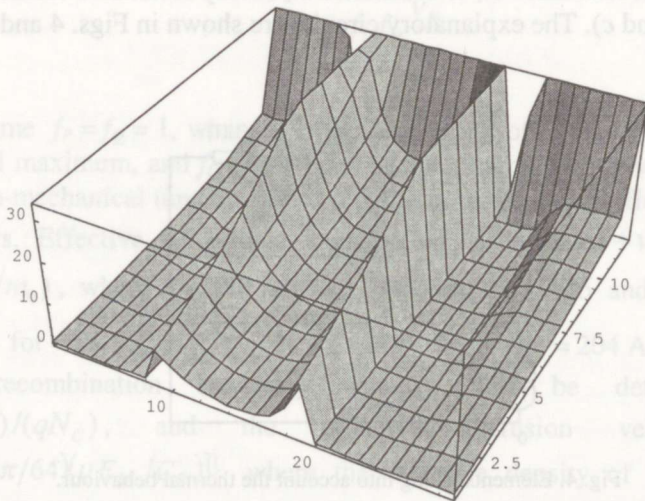


Fig. 6. Current “suppressing” effect at the contact with inhomogeneities.

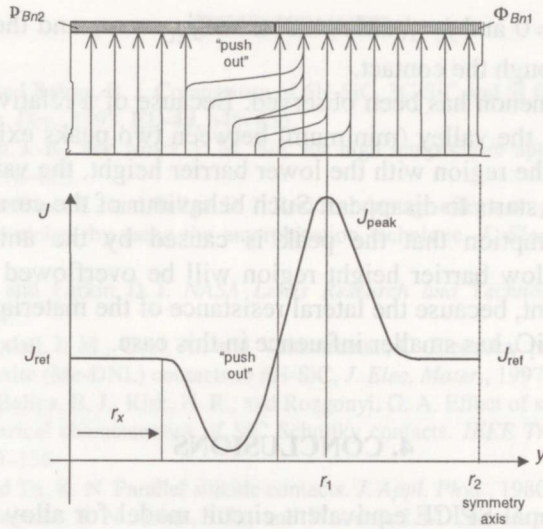


Fig. 7. The characteristic picture of the current distribution along the Schottky alloy (Au-Pt-Au system on C - face to SiC) contact to 6H-SiC substrate. The current “push-out” effect is clearly seen in this region, where the higher barrier height is replaced by the lower barrier height.

substrate. The difference in current densities could reach the factor of two. Thus, we could also say that the resistance in the direction  $\perp$  exceeds the resistance in the direction  $\parallel$  in the same magnitude. Therefore, the current flows more easily in the direction  $\parallel$  than in the direction  $\perp$  of the substrate material, and the current “push-out” effect in the vicinity of the boundary, where the change of the barrier height takes place, could be easily followed.

The current “push-out” effect, which leads to the creation of the so-called hot spot, could be analysed as follows: changing the circle area causes a change in the current passing through this circle (Fig. 7). An extra current occurs

$$dI = j2\pi r dr, \quad (7)$$

which could be expressed as

$$I_{p0} = j\pi r_x^2 \left( \frac{r_1^2}{r_x^2} - 1 \right). \quad (8)$$

Full contact current density is

$$j_C = j(1 + j_{EC}), \quad (9)$$

where

$$j_{EC} = r_x^2 \left( \frac{r_1^2}{r_x^2} - 1 \right) / r_1^2 \left( \frac{r_2^2}{r_1^2} - 1 \right). \quad (10)$$



If  $r_x = r_1$ , then  $j_{EC} = 0$  and  $j = j_C$ . If  $r_x = 0$ , then  $j_{EC} = \infty$ , and the whole current will be pressed through the contact.

Another phenomenon has been observed. Because of a relatively large lower barrier height area, the valley (minimum) between two peaks exists. Decreasing the dimensions of the region with the lower barrier height, the valley (minimum) between two peaks starts to disappear. Such behaviour of the current distribution supports our assumption that the peak is caused by the anisotropy of the substrate. Smaller low barrier height region will be overflowed quickly by the "out-pushed" current, because the lateral resistance of the material, caused by the anisotropy of 6H-SiC, has smaller influence in this case.

#### 4. CONCLUSIONS

A two-dimensional SPICE equivalent circuit model for alloy metal Schottky interfaces to 6H-SiC substrate has been described. The anisotropy of the substrate material has been taken into account. It is shown that by modelling the alloy metal contacts, strong current "push-out" effect exists, which is probably caused by the anisotropy of the material. This "push-out" effect occurs near the boundaries, where one metal transfers in compound to another.

It was clearly shown that by modelling alloy metal Schottky contacts using the equalized, so-called effective barrier height, it would describe the current density distribution along the whole contact with some error. Using the effective barrier height gives us the equal current density distribution along the contact, and the creation of hot spots (rings) will not be taken into account.

Recently, in [14] it was shown that the barrier height depends very strongly on the temperature above 300 K (for Au contacts to *n*-type 6H-SiC substrates, the barrier lowering about 30% was reported by the temperature rise from 300 K up to 450 K). Thus, it means that for *n*-type substrates (system Au-Pt-Au), the current suppressing effect should decrease with the temperature rising due to the additional barrier lowering effect in the Au region (assuming that for Pt, the barrier height temperature dependence is weak). The latter effect should be involved into further simulations and discussions.

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## 6H-SiC ALUSTE KONTAKTID: TEHNOLOOGIA JA SIMULEERIMINE

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On esitatud lühiülevaade metalli ja pooljuhi üleminekuale esinevatest mittehomoogensustest ning kirjeldatud üleminekuale matemaatilist mudelit. On toodud simuleerimise tulemused ning neid hinnatud. Tehnoloogiast tingituna sisaldab metalli SiC üleminekuale vigu – mittehomoogensusi, mis põhjustavad voolutiheduse jaotuse ebaühtlust üle kontakti pinna. Viimane nähtus omakorda aga võib olla kuumade punktide tekke alus. Simulatsiooni abil on määratud kuumade punktide asukoht ning voolu tippväärtused selles. Tulemuste põhjal on võimalik ennustada Schottky struktuuri purunemist.