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Modelling of inhomogeneities of SiC Schottky interfaces

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Abstract

In this general paper, a short description of the generation of inhomogeneities at SiC Schottky interfaces due to technology and crystal growth is given. The problem of the local and the effective barrier heights is described. Finally, simulation results of the current crowding phenomenon and specific contact resistivity are presented.

1 Introduction

Metallic films are required to provide interconnection between semiconductor devices and the outside world, which, in the majority of cases, forms with the semiconductor substrate a certain type of junction. Depending mostly on barrier height between the metal and semiconductor, two extreme types of contacts from the point of view of current flow will be created: nearly linear (Ohmic contact), and strongly non-linear (Schottky contact). For the Schottky contacts the most important characteristics are the low leakage currents, good adherence with low stress, surface smoothness (for large area contacts), no reaction with other metals and low electromigration.

In electronics, Al is the most used metallic film of choice for the formation of Schottky interfaces, but unfortunately Al suffers from a low melting point limitation. Taking into account, for example, the high working temperature of SiC devices, Al should not to be a prospective material for the manufacture of Schottky interfaces in such devices. Al also exhibits undesirable electro-migration behaviour. Therefore, other metals, such as W, Mo, Ti or their alloys could be used. However, it is interesting to state that the alloys of these metals with Al or even with Au may be used (see e.g. [1]). Cu metallization has recently

been seen as a promising metallization material (see e.g. [2]) and often intermetallics (mostly Cu-Al alloys) are also used for metallization purposes. Unfortunately, in such systems the development of quasi-crystalline layers is often observed, as is shown, for example, in [3]. Here the danger exists that those intermetallics generally, but especially Cu-Al alloys, transfer themselves to the quasi-crystal state and thereby strongly influence the quality and reliability of the interface.

The quality (defect free) of the contact area is a very important phenomenon. Today the bonding technology seems to give the highest defect-free interfaces for Schottky contacts. The bonding method is physically different from the traditional metallization technologies. The bonding technique is based on the idea that the atoms of metals and semiconductors (or some other materials, e.g. ceramics) can penetrate into each other (not very deeply) and form much better quality contacts with less inhomogeneities at the surface. The procedure takes place at the room- to medium-temperature level (not exceeding 600°C) and under pressure (not exceeding 50 MPa). The most well known bonding technologies are diffusion welding (bonding) and laser-induced welding (bonding). The first is used mostly in power electronics and the latter in microsystems (see also e.g. [4-6]).

In this paper we first give an overview of Schottky interface inhomogeneities created by technology and crystal growth and we discuss the modelling and simulation possibilities for such interfaces. The new data for current crowding dynamic behaviour and specific contact resistance for SiC Schottky structures will be presented.

2 Technology-caused inhomogeneities at the Schottky interfaces

There are basically two different major technologies for manufacturing Schottky interfaces to SiC surfaces – deposition and bonding (diffusion) methods.

Using deposition, the technology-created inhomogeneities are *cracks* in the deposits as the result of poor adhesion, the presence of particulates or unevenness, and/or the relief of the stress in the film, *grain size variations* in the deposits, *step coverage*, which results because of the directionality of the deposition from the evaporating or sputtering sources of low mobility of the deposited atoms, molecules, or ions, and the enhanced topography (deeper steps), *metallurgical and chemical interaction* caused inhomogeneities, and *electromigration* causes considerable material transport in metals because of the enhanced and directional mobility of atoms.

The deposition methods allow manufacturing of SiC substrates with either Ohmic or Schottky contacts from very different metals (Al, Au, W, Ti, Pt, and Re) or their alloys. After all, with the help of deposition methods, the ohmic contacts to *Si-face* of SiC are more traditional than to *C-face* of SiC. This can be explained in a relatively simple way – the adhesion between *Si-face* and metal (normally Al, Ti, Ni, and Pt) is more similar to this one, what takes place by forming of Me-Si contacts. Another reason is that subsequent annealing decreases significantly the number of dissociations in the case of the Me-Si-face

of SiC than in case of the Me-C-face of SiC. The possible influence of inhomogeneities on the electrical characteristics for deposited SiC Schottky structures is described in [7].

Bonding is the youngest technology compared to the previously discussed one for manufacturing of high quality Schottky and Ohmic contacts, especially on large areas. This technology creates much less inhomogeneities at the interface, because *cracks* in the traditional meaning of the understanding for bonded interfaces are not probable, due to the extra high adhesion rate in bonded junctions. *Grain size variations* are also less interesting phenomena for bonded interfaces due to the plastic deformation of metal film, but *electromigration* can also cause considerable material transport in metals in this case, because it is based, as in the previous case, on a current-induced atomic diffusion caused by a momentum transfer from the electron wind to the atoms in a conductor, which is dimension dependent. Taking into account the possible extra high temperatures at contacts during the work of SiC devices, thermally induced extra currents (current crowding at the interface) could introduce the selective electromigration of the contact material, for example in Schottky contacts under high forward current densities. This last phenomenon has been very poorly investigated, but considering the very good thermal conductivity of SiC the selective migration will be strongly decreased. This, in turn, could lead to the situation that the selective electromigration processes in contacts with inhomogeneities at high current densities might have no significant meaning. However, further investigations are needed in this specific area. In Ref. [8] it is stated that an additional amorphous interfacial phase will be formed between Al and SiC whether the sample is bonded in vacuum or in air. Today it is not clear, if such an introduced phase should be considered as an inhomogeneity or not.

The bonding method also allows the manufacture of SiC substrate Schottky and Ohmic contacts from very different metals (Al, Au, Pd, Pt, and Mo) or their alloys. After all, with the help of the bonding method, Al Schottky contacts to SiC might have problems in their later operating life due to relatively low melting point of Al. Due to the extremely good atomic level binding, in the case of the *C-face* this results in the development of a relatively high potential barrier at the interface. In general, it is assumed that the strong carbide-formers (also known as reactive metals) such as Ti, Ta, Mo can form Ohmic contacts whereas the non-carbide formers (known also as non-reactive metals) such as Al and Au generally give rectifying behaviour. However, the situation is more complex, because for both the surface treatment and orientation can directly affect the behaviour of the interface.

A very special case for every metallization method is the crystal growth defects. It should be mentioned that the epitaxial layer thickness grown on the *C-face* of 4H-SiC had a rather irregular topology on the periphery of wafer surface compared with the layer in the centre region of the wafer. In addition, over the whole surface big rough asperities (50 μm height) of disoriented 4H-SiC crystals and comparatively deep craters have been observed. As an illustration, Fig. 1 shows the comparison of surface profiles in the periphery and in the central region of epitaxial layer areas measured by us.

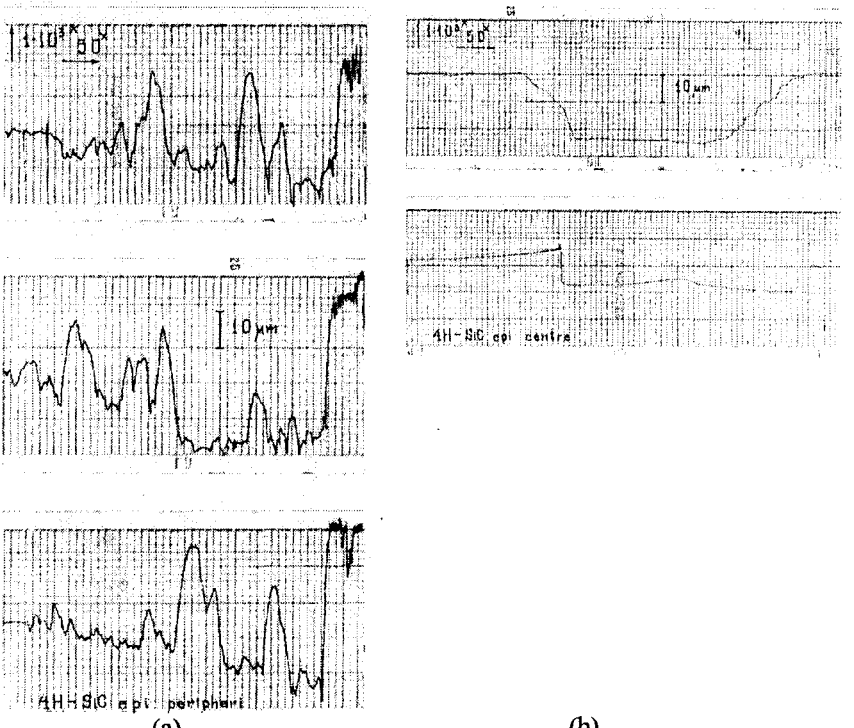


Figure 1: Roughness of the epitaxial layer surface: (a) periphery and (b) centre region.

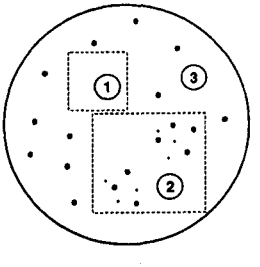


Figure 2: Distribution of micropipes (dots on the picture) at 4H-SiC episurface. ① area nearly free of micropipes; ② area, where micropipes clusters are located; and ③ area where the non-regular distribution of micropipes is present.

Another problem, connected to the previous one, is the high density of micropipes at the surface of the SiC epilayer. Fig. 2 shows a typical picture of our investigations of the distribution of micropipes on the surface of a 4H-SiC

epilayer. Such irregularities of the epitaxial layer may limit the fabrication of large-area metal–semiconductor contacts; consequently, only those parts of the wafers cut from the central regions can be used in the manufacture of properly functioning devices and for determination of their electrical characteristics.

3 Modelling and simulation of contact properties

Being familiar with the nature of creation of inhomogeneities at the SiC surface, we have to mention the modelling of such interfaces. We believe that the defects at the SiC metal interface result in lowering of the barrier height in localized regions, and thus significantly affect the *U-I* characteristics of the Schottky contacts. These inhomogeneities 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 interface properties, and the current flows through different subregions which have different resistance. This, in turn, leads again to potential barrier variations at the interface along the contact area. Therefore, the height of the metal–semiconductor (MS) contact barrier will be a combination of several local barrier heights (see Fig. 3).

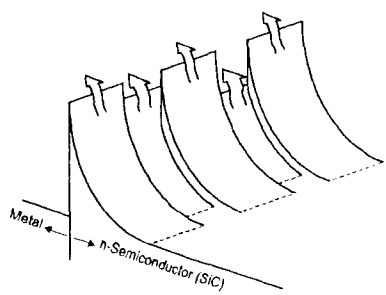


Figure 3: Schematic picture of SiC Schottky interface at different barrier heights.

The general model of Schottky interface with inhomogeneities will be formed by N different barrier heights on the same semiconductor substrate. The model of such a structure looks like so that each diode formed by the same inhomogeneity has almost identical characteristics, which is described with a local potential barrier. Therefore, the electrical properties of the contact could be characterized by the macroscopic parameters. Many models have been developed to describe the inhomogeneities at the MS Schottky junctions (see e.g. [9-12]).

We describe the set of primary diodes, and it will be assumed that they will not influence each other at the interface. Therefore the electrical properties of contact will be characterized by the macroscopic parameters such as the effective barrier height, the ideality factor, the *U-I* and *C-V* characteristics. This

assumption could cause some difficulties by modelling of micropipe-induced inhomogeneities.

Let the total area of the contact be S. With S_i will be described the part of interfacial area occupied by all primary diodes of the i-th inhomogeneity. (N_{ij} is the subarea of the j-th primary diode formed by i-th inhomogeneity; S_{ij} is the subarea of the j-th primary diode formed by the i-th inhomogeneity).

Then

$$S_i = \sum_{j=1}^{M_i} N_{ij} S_{ij}, \quad i = 1, 2, \ldots, N, \tag{1}$$

where N is the number of metals (inhomogeneities) at preparing the contact. M_i is the number of elementary diodes of i-th inhomogeneity.

In practice we have

$$S = \sum_{i=1}^{N} S_i \ , \tag{2}$$

and we could define the ratio R_i

$$R_i = \frac{S_i}{S}, \quad i = 1, 2, \ldots, N \ . \tag{3}$$

Generally, almost every electrical parameter of the MS contact depends on this ratio.

The total current across the interfacial area will be described by:

$$I = I_{ED} + I_T \ , \tag{4}$$

where I_{ED} is the total current over the barrier expressed with emission–diffusion theory and I_T is the total tunnelling current through the barrier.

Using current density terms, eqn (4) will take a form as follows:

$$I = J \cdot S = \sum_{i=1}^{N} \left(J_i^{ED} + J_i^T \right) S_i \ . \tag{5}$$

This equation means that the total current through the total interfacial area of the contact is equal to the sum of currents through the areas S_i and the electrical parameters of the contact can be described by the individual parameters of the elementary contacts.

Often $J^T << J^{ED}$ (because of determining the barrier height by $U \approx 0$ V), and therefore it is assumed that there does not exist any tunnelling through the barrier at all, and therefore the expression (5) could be written as follows:

$$I = J \cdot S = \sum_{i=1}^{N} J_i \cdot S_i \ , \tag{6}$$

where J_i is the thermionic emission–diffusion current density of the i-th inhomogeneity (diode). Further, we assume that there is no lateral fluctuation of the potential at the contact and therefore we may write $U_i \equiv U$.

The barrier height ϕ_{Bi} will be

$$\phi_{Bi} = \varphi_T \ln \frac{A_i^* T^2}{J_{Si}} \quad , \tag{7}$$

and the ideality factor η_i is given as

$$\eta_i = \frac{1}{\varphi_T} \frac{dU}{d\ln(J_i)}, \quad i = 1, 2, \ldots, N \quad . \tag{8}$$

The current transport in metal–semiconductor contacts is mainly due to majority carriers. Four basic transport processes under forward bias (the inverse processes occur under reverse bias) are shown on Fig. 4 (see e.g. [13]). In addition, the edge leakage current due to a high electric field at the contact periphery, or interface current due to traps at the metal–semiconductor interface may occur, but are directly not included in this particular model.

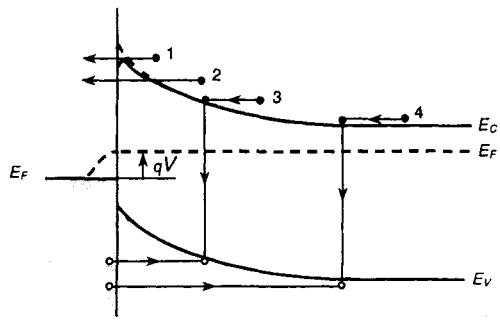


Figure 4: Four basic transport processes under forward bias.

1. Transport of electrons from the semiconductor over potential barrier into the metal (dominant mechanism in moderately doped semiconductors operated at moderate temperatures);
2. Quantum-mechanical tunnelling of electrons through the barrier (important for heavily doped semiconductors and for most Ohmic contacts);
3. Recombination in the space-charge region;
4. Hole injection from metal to the semiconductor (equivalent to recombination in the neutral region).

3.1 Thermionic emission–diffusion transport

Pure thermionic emission is based on Bethe's theory [14], where two superimposed current fluxes (one from metal to semiconductor, the other from semiconductor to metal) are treated separately. The pure diffusion theory is based on Schottky's assumption [15], where the processes in the depletion region near the interface define the current. A synthesis of thermionic and diffusion approaches to current flow is described in terms of the effective recombination velocity v_R at the potential energy maximum:

$$J_i^{ED} = q(n_m - n_0)v_R \,, \tag{9}$$

where n_m is the electron concentration at energy maximum and n_0 is a quasi-equilibrium electron density at the same point. The last term defines the density that would occur if it were possible to reach equilibrium without altering the magnitude or position of the potential energy maximum. Assuming that $\phi(W) = -V$, where W is the width of depletion layer, the n_m and n_0 could be defined taking into account the effective density of states in the conduction band N_C, and the imref function $\phi(x_m)$ at x_m.

After some mathematical operations the effective diffusion velocity can be defined as:

$$v_D = \left[x_m (q/\mu kT) \exp\left\{ -(q/kT)(\phi_{Bn} + \psi) \right\} dx \right], \tag{10}$$

which describes the transport of electrons from the edge of the depletion layer at W to the potential energy maximum. If the electron distribution is Maxwellian for $x \geq x_m$, and if no electrons return from metal other than those associated with the current density qn_0v_R, the semiconductor acts as a thermionic emitter. Then v_R is the thermal velocity given by

$$v_R = A^* T^2 / qN_C \,, \tag{11}$$

where A^* is the effective Richardson coefficient, and $A^* = A(m^*/m_0)$, where A = 120 A/K^2/cm^2. For 6H-SiC $(m^*/m_0)_\perp = 0.25$ and $(m^*/m_0)_\parallel = 1.7$ [16], thus for 6H-SiC $A^*_\perp$ = 30 A/K^2/cm^2 and $A^*_\parallel$ = 204 A/K^2/cm^2. But, then in [17] for 6H-SiC the value of 194.4 A/K^2/cm^2 for the effective Richardson coefficient $A^*_\parallel$ is reported. For the 4H-SiC in [18] the effective Richardson constant A^* is calculated as 146 A/K^2/cm^2 by using the effective mass of (m^*/m_0) = 0.2 from [19].

The effective Richardson coefficient depends additionally on the diffusion velocity of charge carriers. Therefore, often an improved effective Richardson coefficient A^{**} is used to describe the processes at the interface. The improved effective Richardson coefficient is calculated as $A^{**} = A^*/(1 + v_R/v_D)$.

The values for v_R at room temperature are shown in [20] for 6H-SiC. Unfortunately, using data available for 6H-SiC, the value of v_R at room temperature calculated from formula (11) would be different from measured values. For example, for $v_{R\perp}$ we get 5.0×10^5 cm/s and for $v_{R\parallel}$ the value of 3.4×10^6 cm/s was obtained. The difference between measured and calculated values of thermal velocities in 6H-SiC seems to be caused by an inadequate definition of the effective density of states in the conduction band for different crystal polarities of 6H- SiC.

For anisotropic materials, as SiC, the anisotropy must be taken into account and for v_D it could be made using crystal polarity dependent mobilities of charge carriers.

3.2 Tunnelling transport

The electron and hole diffusion equations depend on the underlying Boltzmann equation so that, initially, a way of putting tunnelling into the Boltzmann

equation must be found. The normal Boltzmann equation is, in effect, the mathematical expression of an intuitive and basically classical picture of particle diffusion. Tunnelling, on the other hand, is essentially quantum mechanical in nature and does not agree well with the localized electronic picture underlying the Boltzmann equation. To overcome this problem, the WKB (Wentzel-Kramers-Brillouin) method must be used. To obtain a modified continuity equation, including tunnelling, the so-called "supply function" must be defined and the tunnelling probability determined. The supply function for electrons has the following form (see e.g. [21]):

$$S_x^{x'} = \frac{A_n T}{k}\left(\ln\left[1+\exp\left\{\varphi_F(x')-\varphi_C(x')\right\}/\varphi_T\right]-\ln\left[1+\exp\left\{\varphi_F(x)-\varphi_C(x)\right\}/\varphi_T\right]\right), \quad (12)$$

where k is the Boltzmann constant, T is the absolute temperature, φ_F and φ_C are the Fermi and conduction band edges, respectively, $\varphi_F = kT/q$.

Tunnelling probability can be expressed as:

$$P_x^{x'} = \exp\left(-|W|\right) \quad (13)$$

with

$$W = \frac{\sqrt[2]{(2m^*)}}{\mathrm{h}} \int_x^{x'} \left[\varphi_C(x'') - \varphi_C(x)\right]^{1/2} dx'',$$

where m^* is the electron effective mass, h is Planck's constant $(\hbar = h/\pi)$, $x \in [0,d]$, $x' \in [0,x]$, $x'' \in [x,d]$, and d is the depletion layer thickness determined by the doping concentration and applied voltage. To determine the value of x' corresponding to a given value x, we need to know the dependence of φ_C on x. This will be determined by the variation of doping concentration with x through the solution of Poisson's equation.

Therefore, Boltzmann statistics is valid for our model, and the Einstein–Nernst relationship is found to hold for describing the diffusion constants. The permittivity is anisotropic and the values for 6H-SiC are $\varepsilon_{\parallel} = 10.03$ and $\varepsilon_{\perp} = 9.66$ and for 4H-SiC $\varepsilon = 9.66$ in both directions.

For a metal-n-SiC structure the transport equation for tunnel current takes the following form:

$$J_i^T - q\int_d^x E(x) S_x^0 P_x^0 dx \ . \quad (14)$$

A two-level description (local model) of charge carrier mobilities and the barrier lowering due to mirror forces (Schottky effect) has to be included.

On the basis of the model described the PSPICE environment of the slightly simplified simulator package SCHOTSIC has been developed at the Department of Electronics TTU.

Simulations at different ambient temperatures (300–900 K) show the strong dependence of current suppressing effect on temperature. The self-heating effect is higher at lower temperatures. Higher semiconductor intrinsic resistance in the case of lower temperatures explains this fact. Although the self-heating effect is low at high temperatures, the effect becomes important at low temperatures

because of thermal expansion. The dynamic behaviour of the current crowding is shown in Fig. 5 for 4H-SiC Schottky structures without and with a heat sink, when the structure has been influenced with a current pulse. Unfortunately, the PSPICE environment does not allow one to build up the thermal feedback loop directly into simulation and therefore the results presented here must be taken as characteristic ones. So, the next generation models should should be more exact. For example, the physical model, which is based on the numerical solution of Van Roosbroeck [22] equations, could be used.

Finally, we briefly discuss the specific contact resistance of the interface environment. The specific contact resistance is the reciprocal of the derivative of current density with respect to the applied voltage. At zero bias the specific resistance will be defined as:

$$R_C = \left(\partial J/\partial V\right)^{-1}_{V=0} . \tag{15}$$

The model described in eqn (15) has one large disadvantage: it does not take into account the influence of the substrate or epitaxial layer. Therefore, a more general model should be used. Using ideas suggested in [23] the resistivity of the Me-SiC interface could be calculated. In the following formulas all letters have their traditional meaning, except for b, which is the ratio μ_n/μ_p.

Specific resistivity R_C for n^+ substrate

$$R_{cn} = \frac{bD_p L_p \rho_p}{D_p sh\dfrac{w_n}{L_p} + v_{rec} ch\dfrac{w_n}{L_p}} . \tag{16}$$

In simulations we use $\mu_n = 120$ cm^2/Vs, $\mu_p = 20$ cm^2/Vs and $\tau_p = 89$ ns.

Specific resistivity R_C for p^+ emitter.

$$R_{cn} = \frac{bD_n L_n \rho_p}{D_n sh\dfrac{w_p}{L_n} + v_{rec} ch\dfrac{w_p}{L_n}} . \tag{17}$$

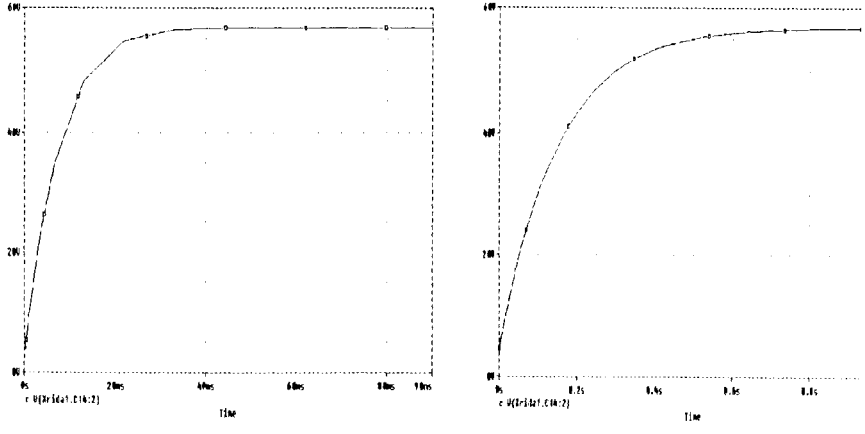
In simulations we use $\mu_n = 20$ cm^2/Vs, $\mu_p = 2$ cm^2/Vs and $\tau_n = 2.2$ ns.

Fig. 6 shows clearly that by the determination of the contact resistivity the thickness of substrate or epitaxial layer becomes very important in analysing thin layers under the metallic layer. From the other hand, it is also clearly seen that the increase of recombination velocity strongly decreases the value of R_{cp} or R_{cn}.

4 Conclusions

Two important aspects of metal–semiconductor interfaces have been discussed: manufacturing technologies, and modelling and simulation of interface areas. Special attention has been focused on interfaces to SiC Schottky interfaces.

Manufacturing technologies introduce different types of inhomogeneity as we have seen, which influence directly the electrical characteristics of the devices and have to be taken into account by modelling and simulation activities.



(a) (b)

Figure 5: Up-heating of the 4H-SiC Schottky structure (a) without heat sink, (b) with heat sink (the heat capacity was taken 1.0 Ws/K and density 3.12 g/cm^3.

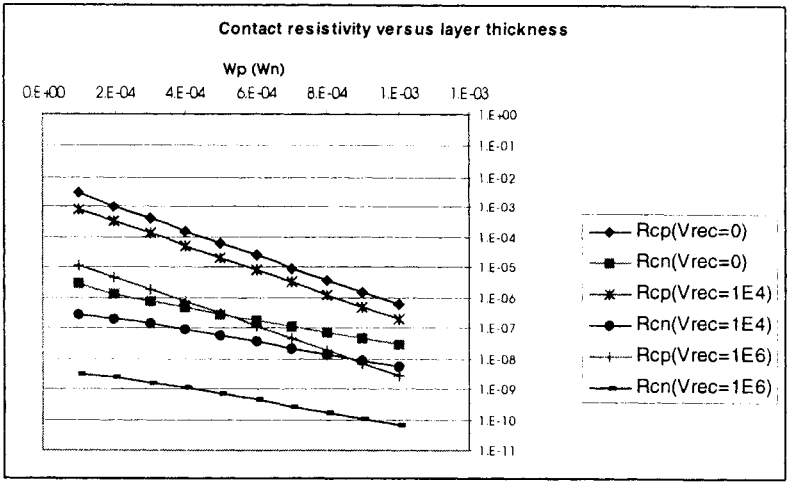


Figure 6: Contact specific resistivity [in Ωcm^2] dependence on substrate thickness and on recombination velocity at the contact interface for n^+ and p^+ layers.

To analyse the inhomogeneities at the Me-SiC Schottky interfaces, the PSPICE-based global model (from the SCHOTSIC package) has been developed. Unfortunately, for heat dynamic analysis the higher level models have to be used.

The heat propagation has been analysed and the conclusion has been reached that due to relatively high heat conductance the heat shock is not very sharp. The specific contact resistance calculations show that the epilayer resistivity plays an important role by the definition of this resistivity and must always be included in calculations.

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