Transactions on the Built Environment vol 12, © 1995 WIT Press, www.witpress.com, ISSN 1743-3509

Modelling of metal alloy contacts to semiconductor substrate

T. Rang
Institute of Electronics, Tallin Technical University,
Ehitajate tee 5, EE-0026 Tallin, Estonia

Abstract

Simple analytical model for metal - semiconductor non-ohmic (Schottky) contact using thermionic emission theory is described. This model is applied to alloy metal - n-SiC substrate contact. The ratio of areas, occupied by different metals at the surface interface will directly determine the effective barrier height of the Schottky contact. Already very weak presentage of the metal with lower barrier height in alloy, drastically decreases the effective barrier height at the interface. The anisotropy of the material has practically zero influence on barrier height. However, the current flow through the contact strongly depends on crystal direction and on the ratio of areas, occupied by different metals at the surface. Under certain circumstances this may occour the failure of the contact.

1 Introduction

Metallizations will not only be current carriers, but play an active role in determining semiconductor device properties, as in case of the gate electrode or Schottky barrier diode. To minimize interconnection resistance, to save valuable surface area or to avoid the migration of the contact material by higher current densities (e.g. for pure Al contacts to Si substrate the DC current density must not exceed 10^5 A/cm^2), multilevel (alloy) metallization schemes have been proposed. In practice it means that the metallization is used for influencing the potential barrier height [1].

The current transport in metal-semiconductor contacts is mainly due to majority carriers. There exists four processes:

- transport of electrons from the semiconductor over potential barrier into the metal;
- recombination of the charge carriers in the space-charge region;

- hole injection from the metal to the semiconductor;
- quantum-mechanical tunneling of electrons through the barrier.

Both, thermionic emission current (first three mechanisms) and tunneling current (last mechanism) depend directly on barrier height of contact. By the contacts, based on composition of the metallic film, it is suitable to introduce the effective barrier height, which in turn depends on inhomogenity of the area, occupied by each metal at the interface of contact. From the other hand the risk arises that the contact itself under real load conditions will be damaged due to strongly unequal current distribution over the contact area caused by different barrier heights at the interface. Fig.1 gives the simplified explanation for this situation. Using only two component metal compound by realisation of contact, the regions with barrier height ϕ_{B1} (e.g. black regions with area S_1) and ϕ_{B2} (e.g. white regions with area S_2) crop up. So, the relationship S_1/S_2 ($\phi_{B1}/\phi_{B2} \gtrless 1$) will play significant role in current distribution. Therefore, the determination of effective barrier height for compound metal-semiconductor contacts (the distribution of the different barrier heights over the whole contact) is one of the most important problem for the electrical description of the systems. The exact solution of this problem is not yet complete.

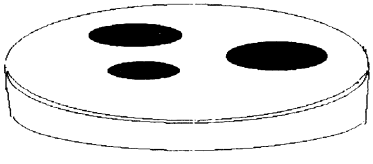

Figure 1: Schematic picture of the two-metal compound semiconductor substrate contact. The black rings have for example the barrier height ϕ_{B1} and the white area ϕ_{B2}.

Models described before (e.g. [2-7]) are incomplete, because of using essentially simplified theory of Scottky junction. The aim of this work is:

- to introduce new, more precise model for metal-semiconductor (MS) contacts (effective barrier height and nonideality factor);
- to apply this model to alloy-metal silicon carbide (anisotropic material) substrate contacts.

2 Description of the model

There are introduced two basically different techniques for preparing of the contacts to SiC surfaces - sputtering and joining technologies. For the contact fabrication different metals could be used, as for example Al, Ti, Pt, Au, and alloys of mentioned metals. So, the effective barrier height will depend on components of different metals, forming alloy. From another hand very often further formation of glassy phases takes place at the interface. Therefore, it is

very important to try to describe the behaviour of the barrier height under so called multimaterial situation.

The general multimetal contact to semiconductor will be formrd by N different metals on the same semiconductor substrate. So, each diode formed by the same metal, has almost identical electrical characteristics, which has a local potential barrier. We assume that the diodes do not influence on each other at the interface. Therefore, the electrical properties of contact will be characterized by the macroscopic parameters such as the effective barrier height and the effective ideality factor of the I-U characteristics of the junction.

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 metal. (N_{ij} - the subarea of the j-th primary diode formed by i-th metal; S_{ij} - the subarea of the j-th primary diode formed by the i-th metal).

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 involved by forming the contact. M_i is the number of elementary diodes (contacts) of i-th metal.

In practice we have

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

and we could define the ratio

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

The total current across the interfacial area will be described:

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

where I_{ED} is the total current over the barrier expressed with thermionic-emission theory and I_T is the total tunneling current through the barrier.

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

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

Eqn (5) means that the total current thrugh 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 own parameters of the elementary contacts (diodes).

Because of complexity of treatment of tunneling term and of the fact that relatively often $J^T << J^{ED}$ (because of determining the barrier height by $U \approx 0\text{V}$), at the moment we assume that there does not exist any tunneling through the barrier (see e.g. [8]). The expression for currents could be written as follows (see also [9]):

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

where J_i is the thermionic emission current density of the i-th subcontact (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 thermionic-diffusion term will be:

$$J_i = J_{Si}(\exp\frac{U}{n_i\,\varphi_T} - 1)\ , \tag{7}$$

where

$$J_{Si} = A_i^*\,T^2\exp\left(-\frac{\phi_{Bi}}{\varphi_T}\right),\quad i = 1,2,\ldots,N\ . \tag{8}$$

The barrier height ϕ_{Bi} will be

$$\phi_{Bi} = \varphi_T \ln\frac{A_i^*\,T^2}{J_{Si}}\ . \tag{9}$$

The barrier lowering effect is described as

$$\Delta\phi_{Bi} = 2E_{mi}\cdot x_{mi}\ , \tag{10}$$

where

$$E_{mi} = 2\frac{\Delta\varphi_{k0} - U - \varphi_T}{W_i}\ , \tag{11}$$

$$x_{mi} = \sqrt{\frac{q}{16\pi\,\varepsilon_S\,\varepsilon_0\,E_{mi}}}\ ,\quad i = 1,2,\ldots N. \tag{12}$$

and W_i is the depletion layer thickness, $\Delta\varphi_{k0}$ and φ_T are the built-in and thermal potential, respectivelly.

The idality factor n_i is given as

$$n_i = \frac{1}{\varphi_T}\frac{dU}{d\ln(J_i)}\ ,\quad i = 1,2,\ldots,N\ . \tag{13}$$

Eqns (1)-(13) form the general model of the contact. Assuming i = 2 (the alloy contact is consisting of two metals), the effective barrier height and the effective nonideality factor will get the following form:

$$\phi_B = \phi_{B2} - \varphi_T \ln\frac{R_2P_1 + R_1P_2\exp\left(\dfrac{\phi_{B2}-\phi_{B1}}{\varphi_T}\right)}{P}\ , \tag{14}$$

$$n = \frac{\left\{P_1\left[R_2P_1 + R_1P_2\exp\left(\dfrac{\phi_{B2}-\phi_{B1}}{\varphi_T}\right)\right]\right\}n_2 + \left[P_1n_1\exp\left(\dfrac{U}{n_1\varphi_T}\right) - P_2n_2\exp\left(\dfrac{U}{n_2\varphi_T}\right)\right]}{n_1n_2\left\{P_1\left[R_2P_1 + R_1P_2\exp\left(\dfrac{\phi_{B2}-\phi_{B1}}{\varphi_T}\right)\right]\right\}} \tag{15}$$

where

$$P = \exp\frac{U}{n\varphi_T} - 1;$$

$$P_1 = \exp\frac{U}{n_1\varphi_T} - 1; \qquad (16)$$

$$P_2 = \exp\frac{U}{n_2\varphi_T} - 1.$$

S_1 and S_2 are the subareas of the contact. So, $S_1 + S_2 = S$, $R_1 = S_1/S$ and $R_2 = 1 - R_1$.

3 Discussion

It can be seen that the barrier height and the ideality factor depend particullary on the interfacial areas, occupied by each type of metal at the interface. In general case the barrier height and the ideality factor depend also on applied voltage.

Let us see some examples for $i = 2$.

a) If we assume $n_1 = n_2 = 1$, then $n = 1$ and the effective barrier height will be

$$\phi_B = \phi_{B2} - \varphi_T \ln\left[R_2 + R_1 \exp\left(\frac{\phi_{B2} - \phi_{B1}}{\varphi_T}\right)\right]; \qquad (17)$$

b) In case $n_1 = n_2 \neq 1$, the ideality factor will be $n \equiv n_1 = n_2$ and the effective barrier height will be determined also by eqn (17);

c) In general case $n_1 \neq n_2 \neq 1$ and the effective ideality factor will be determined by eqn (14) and the effective barrier height by eqn (15).

It is clear that the value of effective barrier height is situated in the range of barrier heights of corresponding single metal - SiC contacts which form the MS contact. For the Au-Pt-SiC contact, if $R_1 = 0$, it means that the contact is the single layer MS contact (Au-SiC) with barrier height 1.52 eV. Similarly, if $R_1 = 1$, the single layer MS contact will be formed (Pt-SiC) with barrier height 1.03 eV. If $0 < R_1 < 1$, then the contact will be formed by the combination of two metals and the effective barrier height of Au-Pt-SiC contact will change according to the variation of the ratio R_1.

Fig. 2 shows the strong dependendence of effective barrier height on ratio of the area, occupied by component metals. It is interesting to stress that strong influence occours only, when the ratio is in avarage less than 10% (in case Au-Pt alloy ca. 2%). The crystal direction (anisotropy) has practically zero influence on effective barrier height ($\phi_{Bi\parallel}/\phi_{Bi\perp} \rightarrow 1$). The reason arises from the behaviour of the crystal structure, which affects strongly on transport.

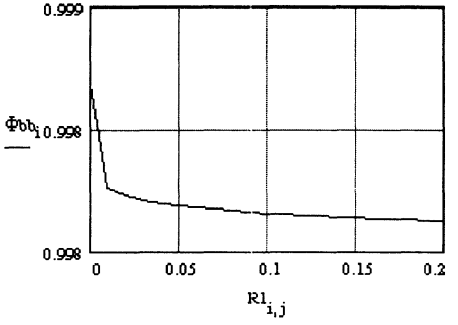

Figure 2: The relationship of the barrier heights of different crystal directions versus persentage of the area of one component metal for Au-Pt alloy contact to SiC, where $\phi_{bbi} = (\phi_{bi\parallel} / \phi_{bi\perp})$ and $R1_{i,j}$ = (% of Pt area).

Fig. 3-5 show the current density dependence on applied voltage for different metallizations, taking into account the anisotropy of the crystal. As in previous case, the strong influence occours only, when the ratio is in avarage less than 10% (in our example ca. 2%). As one can see, the difference of current density could reach 4-5 orders in magnitude. It means that the strong redistribution of the current should take place only by alloys, where the metal, having higher potencial barrier, forms in avarage 90% (in our case already 98%) of alloy. It is correct, because the specific resistance of the contact caused by the barrier height, drops drastically in these spots, where the metal with lower potential barrier forms the contact. More than 10 % (ca. 2% in our example) of the metal in alloy, which has lower barrier height, practically doesn't influence the current flow through the contact compared to single metal contact with lower barrier.

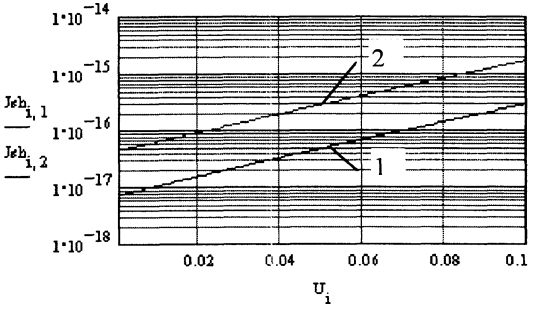

Figure 3: Logplot of thermionic current versus applied voltage for pure Au (100%) contact to SiC, $N_D = 10^{18}$, (1 - $\varepsilon_\perp$, 2 - $\varepsilon_\parallel$), $T = 300$.

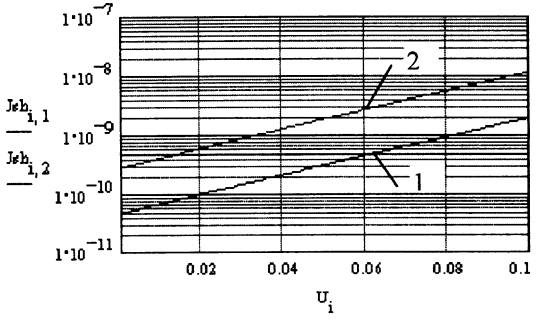

Figure 4: Logplot of thermionic current versus applied voltage for Au (95%) Pt (5%) alloy contact to SiC, N_D=10^{18}, (1 - $\varepsilon_\perp$, 2 - $\varepsilon_\parallel$), T=300.

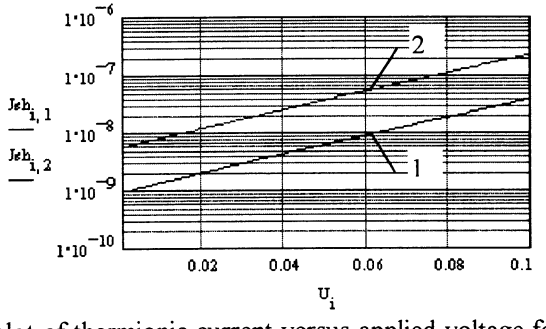

Figure 5: Logplot of thermionic current versus applied voltage for Au (5%0 Pt (95%) alloy contact to SiC, N_D = 10^{18}, (1 - $\varepsilon_\perp$, 2 - $\varepsilon_\parallel$), T = 300.

4 Conclusions

Very often the contacts will be fabricated from metal alloys or the single metal contact has additional components (eg. silicides, or O, etc.) at the interface, which both change the effective barrier height. Therefore, the modeling of effective barrier height for the multilayer MS contacts is very important activity area for electronics and microsystems design.

The results obtained from this model for MS contacts allow us to determine the effective barrier height for optional metallization schemes. For example, for the single layer contacts Au-SiC and Pt-SiC the barrier heights were found to be 1.03 and 1.52 eV respectively [10]. According to the model, the calculated effective barrier height of $Au_{22}Pt_{78}$-nSiC should be 1.05 eV. This number is relative close to barrier height of single Pt contact, which is in agreement with statement, made already earlier.

To investigate the variation of barrier height and the electrical properties of the MS contacts with the inhomogeneous interface arises because the MS barriers formed simultaneously by the different metals with the surface atoms of

semiconductor could be not planar and is spatially inhomogeneus [10]. In this case at the interface of the contact the barrier has the so called local characteristics, which lead to the formation of different local barriers at the different subregions with different contact properties and current flows through the different subregions having different resistances. Therefore, the effective height of the MS contact barrier will be a combination of sevral local barrier heights. These local spots, having lower barrier height, will conduct the majority of current and the failure of the contact can occour.

This model does not include the tunneling part in the whole current. As it is shown for example in [8, 9], the tunneling current will dominate ($J^T > J^{ED}$) at higher doping and lower temperature levels. Therefore, the ideality factor n will depend also on current, slightly different from this one, calculated from our model. Due to this fact the model becomes slightly unexact. So, it will be our next task to complete the model with tunnelling term. Later it should be very important to connect these ideas and ideology with numerical simulation programmes of semiconductor devices.

References

1. Braslau, N. Interfaces and contacts. pp. 247-248, Proc. of the Materials Research Society Symp., v. 18, 1983.
2. Ohdomari, J. & Tu, K.N. Parallel silicide contacts. *J. Appl. Phys.*, 1980, **51**, 3735 - 3739.
3. Freeouf, J.L., Jackson, T.N., Laux, S. E. & Woodall, J.M. Effective barrier heights of mixed phase contacts. Size effects. *Appl. Phys. Lett.*, 1982, **40**, 634 - 636.
4. Freeouf, J.L., Jackson, T.N., Laux, S.E. & Woodall, J.M. Size dependence of "effective" barrier heights of mixed phase contacts. *J. Vac. Sci. and Technol.*, 1982, **21**, (9. Annual Conf. Phys. and Chem. semicond. Interfaces, Pacific Grove, Calif. 27 - 29 Jan. 1982), 570 - 573.
5. Tung, R.T. Electron transport of inhomogeneous Schottky barriers. *Appl. Phys. Lett.*, 1991, **58**, 2821 - 2823.
6. Tung, R.T., Sullivan, A.F.J. & Schrey, F. Schottky barrier inhomogenity at epitaxial NiSi interfaces on Si (100), *Phys. Rev. Lett.*, 1991, **66**, 72 - 75.
7. Tuy, T.Q., Mojzes, I. & Szentpáli, B. The dependence of Schottky barrier height on the ratio of different metal components. *Periodica Polytechnica, ser. El. Eng.*, 1993, **37**, 3 - 19.
8. Rang,T. Tunnel current in metal-semiconductor junctions. *Trans. of TTU*, 1983, No. 558, 69-74.
9. Sze, S.M. *Physics of Semiconductor Devices*. 2-nd Ed., J.Wiley and Sons, 1981.
10. Waldrop, J.R. & Grant, R.W. Schottky barrier height and interface chemistry of annealed metal contacts to alpha 6H-SiC. Crystal face dependence. *Appl. phys. Lett.*, 1993. **62**, 2685-2687.