PERIODICA POLYTECHNICA SER. EL. ENG. VOL. 37, NO. 1, PP. 3–19 (1993)

THE DEPENDENCE OF SCHOTTKY BARRIER HEIGHT ON THE RATIO OF DIFFERENT METAL COMPONENTS[1]

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Received: December 10, 1992

Abstract

In order to understand the variation of the barrier height of different metal-semiconductor contacts, a model for common effective contact (CEC) was proposed. The CEC consists of several primary diodes prepared or formed by different metals on the same semiconductor substrate. The smallest interfacial area of each primary diode was assumed to be the smallest limitation of area on which the Schottky contact's properties exist. The results of the investigation show that all electrical properties – the barrier height especially – of the CEC depend on the ratio of the interfacial area occupied by each metal component in the common effective interface. This result may be applied to the metal compound-semiconductor contact to investigate the variation of potential barrier height, as well as the electrical characteristics of multilayer metal-semiconductor contacts.

Keywords: contact, Schottky barrier, interface multilayer contacts.

1. Introduction

The most important current transport mechanisms through the metal-semiconductor contact (MSC) are: thermionic emission over the top of the barrier, thermionic field emission of hot carriers through the barrier. The variation of the transport mechanism is generally determined by the control of the height and the thickness of the potential barrier at the interface of Schottky contacts having ultrathin interface metal layer [1].

The variation of the potential barrier of contacts can be realized using different methods, including reactions to form new interfacial phases with different electric properties, as well as outdiffusion of a component of a compound semiconductor and metal indiffusion and alloying and/or sintering to form metal contact layer with new effective work function [2, 3].

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[1] This work was supported by a grant N° T4171 from the Hungarian Research Foundation (OTKA)

In practice, the MSC multilayer metallizations are used for influencing the potential barrier height [4, 5]. In our present work only single metal-semiconductor contacts (SMSC) and bi-metal-semiconductor contacts (BMSC) will be treated. In our paper all calculations were carried out for n-type semiconductors, but the theory is valid for p-type material, too.

The results reviewed above show a wide variation of potential barrier height and thickness from those of Schottky contacts to ohmic ones [5] with the variation of the composition of metal or by incorporating highly doped surface layer realized using ion implantation. Many experimental data show the common result that the variation of Schottky barrier height and thickness may occur partially, or simultaneously when there is a simultaneous interaction of some type of metals (or those of metal and semiconductor elements) on semiconductor substrate in both microscopic and macroscopic aspects.

For thermionic emission current, the barrier height of metal compound-semiconductor contacts strongly depends on the composition of the metallic film [6, 7, 8, 9], and on the inhomogeneity of the area occupied by each metal in the interface of contact. The first model for these structures was proposed in Ref. [10]. The authors of this paper assumed that ideality factors for both phases were the same. This model was extended to parallel diodes with lateral dimensions comparable to the Debye length of the given semiconductor where the diodes are no longer independent and the potential, and hence the electron transport, of each individual patch may be no longer treated independently [11]. The first attempt to describe this structure was made very recently [12].

The determination of the barrier height for different MSC is one of the most important problems for the electrical description of these systems. The exact solution of this problem is not yet complete. This paper presents a simple common effective contact (CEC) model consisting of several primary diodes formed by two different metals on the same semiconductor substrate to investigate the influence of the distribution of the area occupied by each metal component in the effective interface of contact on the electrical properties of CEC. Numerical results concerning the I-V, and C-V characteristics of some typical contacts formed n-GaAs and n-Si are presented. The results of the investigation can be extended to other MSC as it is presented in Part 3.

2. Theory

The CEC consists of several primary diodes formed by two different metals on the same semiconductor substrate. The smallest interfacial area of each elementary diode was assumed to be the smallest area on which the Schottky contact's properties still existed.

From the point of view of the device technology the noble metals should be used. which do not react significantly with each other. So that each primary diode formed by the same metal has almost identical electrical characteristics, and has a local potential barrier in the CEC.

For the CEC the interface is inhomogeneous both in the real structure and in the energy one. The influence of the primary diodes on each other at the interface is supposed to be very small, and may be neglected. Then the electrical properties of the CEC can be characterized by the macroscopic parameters such as the effective barrier height, the ideality factor, the I-V, C-V characteristics.

We use the following notations:

S is the total interfacial area of the CEC, S_1 is the part of the interfacial area occupied by all primary diodes of the first metal, and n_{mi}, s_{mi} are the number and the interface area of i-th primary diode formed by the first metal. Then

$$S_1 = \sum_0^{N_1} n_{mi} S_{mi}, \tag{1}$$

where N_1 is the number of elementary diodes of the first type metal in the CEC.

Similarly, for the second type of the elementary diodes we have

$$S_2 = \sum_0^{N_2} n_{mj} S_{mj}. \tag{2}$$

S_2, n_{mj}, s_{nj}, N_2 are the corresponding indices for the second metal-semiconductor diode.

In practice we have

$$S = S_1 + S_2 \tag{3}$$

and if we delineate

$$P = S_1/S \qquad \text{and} \qquad 1 - P = S_2/S \tag{4}$$

as the ratios of the area of the first metal and those of the second metal to total effective interface area then almost every electrical parameter of the

CEC depends on this ratio. On the basis of this assumption we perform the investigations of the I-V, and C-V characteristics of CEC. Other parameters such as noise, reliability are out of the scope of the present paper. The pinch-off effect was not included in our calculation.

2.1. I-V Characteristics

If J_1 and J_2 are the apparent current densities across the interfacial areas formed by each metal component, and J is the total current density across the CEC, then

$$JS = J_1S_1 + J_2S_2. \tag{5}$$

(It should be mentioned that *Eq.* (5) is the same as *Eq.* (1) in Ref. [10]).

Using thermionic emission theory [8] the current densities are expressed as

$$J_1 = A_1 * T^2 \exp(-q\phi_1/kT)[\exp(qV/kTn_1) - 1]. \tag{6}$$

and

$$J_2 = A_2 * T^2 \exp(-q\phi_2/kT)[\exp(qV/kTn_2) - 1], \tag{7}$$

where $A_1* = A_2*$ are the effective Richardson constants, ϕ_1 and ϕ_2 are the barrier heights, n_1 and n_2 are the ideality factors of each SMSC. V is the applied voltage, T is the absolute temperature, k is the Boltzmann constant, q is the magnitude of electronic charge.

The saturation current densities and the ideality factors of each SMSC are given as

$$J_{10} = A_1 * T^2 \exp(-q\phi_1/kT), \tag{8}$$

$$J_{20} = A_2 * T^2 \exp(-q\phi_2/kT) \tag{9}$$

and

$$n_1 = (q/kT)\frac{dV}{d(\ln J)}, \tag{10}$$

$$n_2 = (q/kT)\frac{dV}{d(\ln J)}. \tag{11}$$

For the CEC we have

$$J = J_s[\exp(qV/kTn) - 1], \tag{12}$$

$$J_s = A * T^2 \exp(-q\phi/kT), \tag{13}$$

$$n = (q/kT)\frac{dV}{d(\ln J)}. \tag{14}$$

Here J_s is the saturation effective current density.

The *Eq.* (5) means that the total current through the total interfacial area of CEC is equal to the sum of currents through the area S_1, S_2 and the electrical parameters of CEC can be described by the own parameters of elementary contacts.

Solving the system of the *Eqs.* (4)–(14), the barrier height and the ideality factor of the CEC can be described by the following expression:

$$\phi = \phi_1 - (kT/q)\ln\{(1/A)[PB + (1-P)C\exp(q(\phi_1 - \phi_2)/kT)]\} \qquad (15)$$

and

$$\begin{aligned} 1/n = 1/n_1 + &(1-P)\exp(q(\phi_1 - \phi_2)/kT) * \\ &* [(B/n_2)\exp(qV/kTn_1) - (C/n_1)\exp(qV/kTn_2)]/ \\ &/\{B[PB + (1-P)C\exp(q(\phi_1 - \phi_2)/kT]\}, \end{aligned} \qquad (16)$$

where

$$\begin{aligned} A &= \exp(qV/kTn) - 1, &(17)\\ B &= \exp(qV/kTn_1) - 1, &(18)\\ C &= \exp(qV/kTn_2) - 1. &(19) \end{aligned}$$

From *Eqs.* (15) and (16), it can be seen that the barrier height and the ideality factor of the CEC depend on parameters of all single diodes. They especially depend on the interfacial areas occupied by each type of metal at the interface of CEC and in the general case the barrier height and the ideality factor also depend on the applied voltage.

A) The ideal case: The ideality factors are $n_1 = n_2 = 1$.

From *Eqs.* (15) and (16) the barrier height and the ideality factor of the CEC are obtained as

$$\phi = \phi_1 - (kT/q)\ln[P + (1-P)\exp(q(\phi_1 - \phi_2)kT)], \qquad (20)$$

and

$$n = 1. \qquad (21)$$

In this case, the ideality factor of the CEC is also equal to the unity as in the ideal contact.

B) The nonideal simple case: The ideality factors are $n_1 = n_2 \neq 1$.

The formulas of the effective barrier height also from *Eqs.* (15) and (16) coincide with those of the ideal CEC and:

$$n = n_1 = n_2. \tag{22}$$

This means that the barrier height of the CEC only depends on the areas occupied by each type of metal and on the barrier heights of single metal.

Generally, *Eqs.* (15) and (20) are the basic equations to calculate the variation of the Schottky barrier height vs the area occupied by each metal at the interface of the CEC.

C) In the general case: $n_1 \neq n_2 \neq 1$.

In this case, from *Eq.* (15) the following approximating expression can be deduced for the effective barrier heights

$$\phi = \phi_1 - (kT/q)\ln\{(1/n_1)[Pn + (1-P)n_2\exp(q(\phi_1 - \phi_2)/kT)]\}. \tag{23}$$

In obtaining *Eq.* (23), the expansion $e^x \approx 1+x$ was used, where $x = qV/kT$. The barrier height is always determined at very small applied voltages, $V \approx 0$.

In the *Eq.* (23) n is the ideality factor of the CEC and in the general case it is determined by *Eq.* (16), but ideality factor of the SMSC is determined at the linear part of I-V characteristics, therefore it can be also determined from *Eq.* (16) in the voltage range from 0.2 to 1.0 volts. Generally, the ideality factor, i.e. *Eq.* (16) of the CEC depends on the applied voltage in a complicated way.

The expressions for the barrier height ϕ, i.e. *Eqs.* (15), (20) and (22), and for the ideality factors, i.e. *Eqs.* (16), (21) and (22) of the CEC all depend on the interfacial area occupied by each metal component at the interface. Then the corresponding total current density and the saturation current density of the CEC also have the similar dependencies.

To introduce the theoretical results of some electrical properties of the CEC, the numerical application was realized on the Schottky barrier diodes fabricated on Al, Ag, Au and Cr/GaAs [13] published by NEWMAN et al. In the course of these experiments, the metal-n-GaAs diodes were fabricated by in situ deposition. The data of the barrier heights and the ideality factors of all the single metal-n-GaAs diodes are presented in the *Table 1.* Based on these results, a calculation was carried out using our model.

Fig. 1 shows the barrier height of the CEC of AuAl, AuAg, AuCr, AlAg and Au on GaAs surface depending on the ratio of interfacial areas occupied by Au, Ag, Al, Cr to total area of effective interface in the case of unannealed samples. It is clear that for each BMSC, the value of

Table 1

The results of I-V and C-V electrical measurements. Diodes were formed on UHV-cleaned (110) GaAs [13]

		ϕ_B I-V ± 0.02 [eV]	n	ϕ_B C-V ± 0.02 [eV]
Al	unannealed	0.83	1.06	0.89
	370°C anneal	0.90	1.05	0.92
Ag	unannealed	0.89	1.06	0.94–0.97
	370°C anneal	0.91	1.07	0.92–0.99
Au	unannealed	0.92	1.05	1.00
	370°C anneal	0.80	1.06	0.88
Cr	unannealed	0.66	1.06	0.74
	370°C anneal	0.67	1.06	0.74

the effective barrier heights is situated in the range of barrier heights of corresponding single metal-GaAs contacts which formed the CEC. For the AuAl-GaAs contact, if $P = 0$, this means that the effective contact becomes a SMSC-Au/GaAs one, the barrier height is ϕ(Au/GaAs)$=$ 0.92 eV. Similarly, if $P = 1$, the CEC will be a single component Al/GaAs one, and the barrier height of it is ϕ(Al/GaAs)$=$ 0.83 eV. If $0 < P < 1$, then the contact was formed by the combination of two metals, and the barrier heights of AuAl-GaAs CEC will change according to the variation of the ratios P of the interfacial area occupied by each metal to the total area of the interface.

The AuCr-GaAs CEC demonstrates the situation when about 15 % interfacial area of the AuCr-GaAs CEC is occupied by Cr, and the barrier height of CEC has decreased significantly. It may be interpreted as a 'window' for the electrical conductance, and the saturation current of the effective contact will be changed. The area of this SMSC increases the current across this interfacial area and it will dominate in the total current of the CEC. After that, with the increase of the interfacial area of the SMSC having the low barrier height, the saturation current density will be increased slowly. Therefore, the effective barrier height of the CEC will be changed simultaneously with the variation of the saturation current density according to ratio of the area occupied by each metal as mentioned above.

It means that the Schottky barrier height of the CEC can be increased or decreased depending on the ratio of metal components in the CEC.

Using the data of ARIZUMI et al [6], [7], the similar variations of the effective barrier heights of the CEC contacts AuAg-Si, AuCu-Si, AgCu-Si and Au-Si were presented in *Fig. 2*. *Fig. 3* shows the corresponding variations of the saturation current densities.

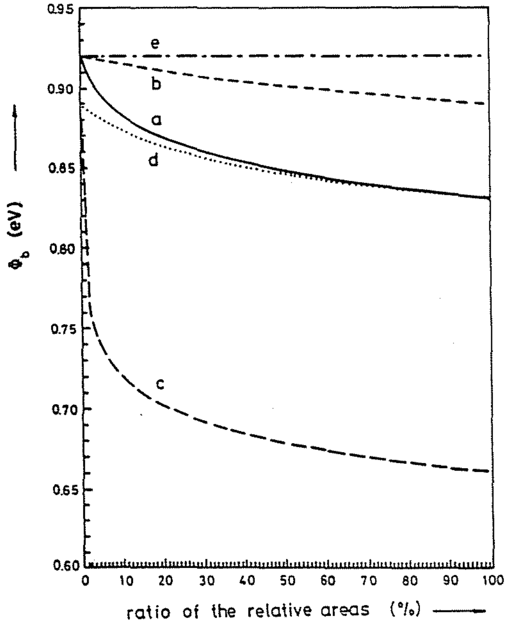

Fig. 1. Barrier height of metal-n-GaAs contacts obtained from I-V measurements. a) AuAl, b) AuAg, c) AuCr, d) AlAg, e) Au

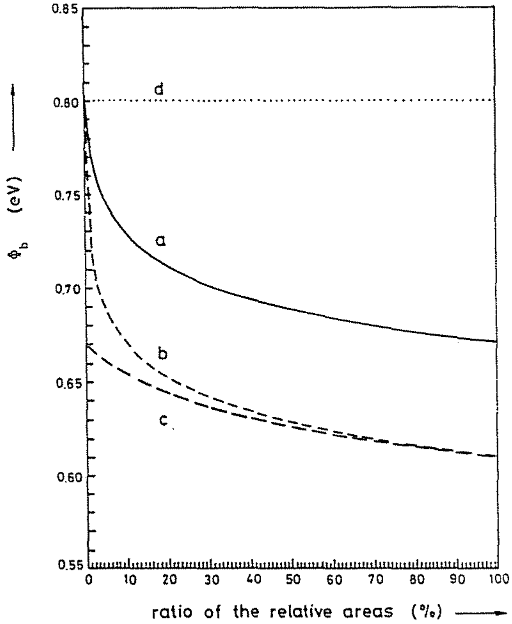

Fig. 2. Barrier height of metal-n-Si contacts obtained from I-V measurements. a) AuAg, b) AuCu, c) AgCu, d) Au

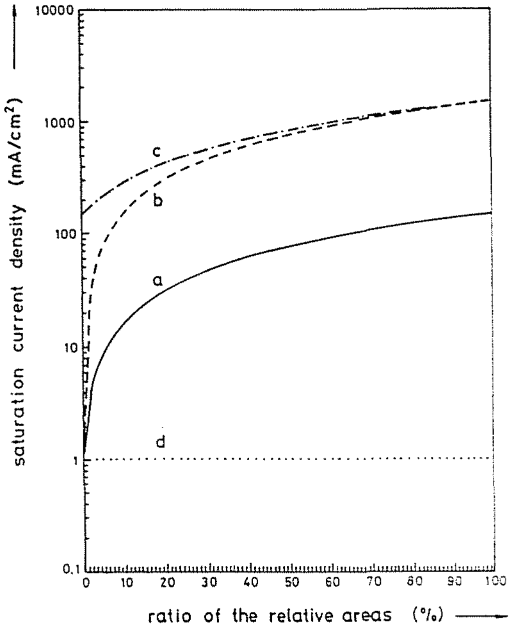

Fig. 3. Saturation current density of metal-n-Si contact
a) AuAg, b) AuCu, c) AgCu, d) Au

Figs. 4a, b, c present the log I-V characteristics of corresponding CEC mentioned above, and it is clear that the family of the logarithmic forward I-V curves is situated between the two lines corresponding to forward I-V curves is situated between the two limes corresponding to forward I-V characteristics of two SMSC. The density of the curves reflects the dependence of the barrier heights of the CEC on the areas of the single contacts at the interface.

If the area ratio as mentioned above corresponds with the atomic percentage of the different metals in the metal film on semiconductor substrate, then the obtained results may be applied to the real BMSC. This problem will be discussed in Part 3.

2.2. C-V Characteristics

The total capacitance (C_t) of the CEC will be the sum of the capacitances of the primary diodes. In the case of the CEC made of two different metals, the total capacitance will be

$$C_t = C_1 + C_2, \tag{24}$$

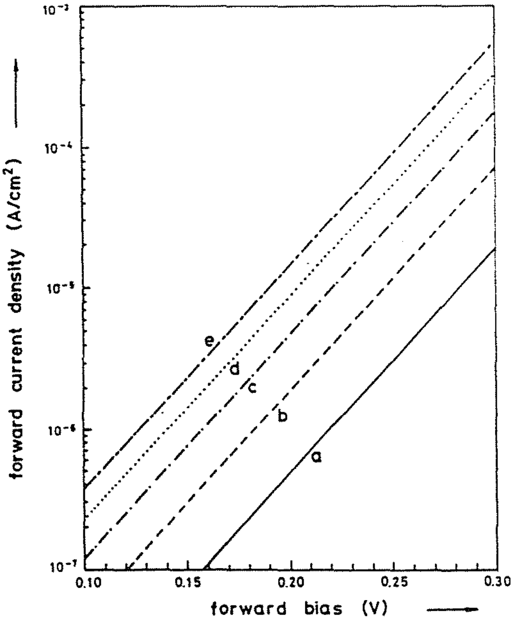

Fig. 4a. Forward I-V characteristics of AlAu-n-GaAs contact
a) 100 % Au, b) 90 % Au, c) 70 % Au, d) 40 % Au, e) 0 % Au

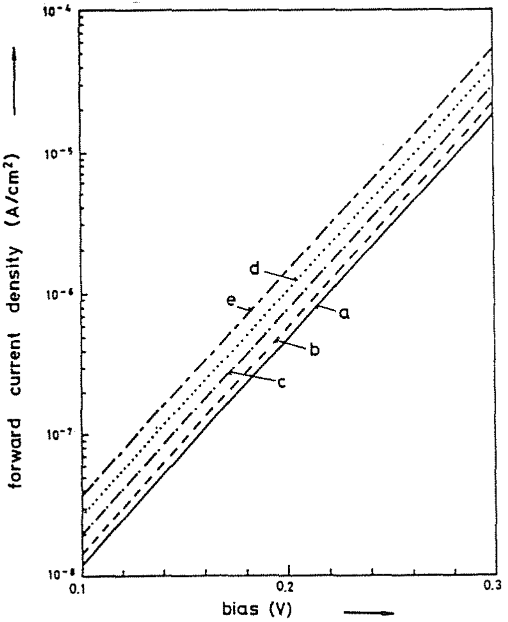

Fig. 4b. Forward I-V characteristics of AgAu-n-GaAs contact
a) 100 % Au, b) 90 % Au, c) 70 % Au, d) 40 % Au, e) 0 % Au

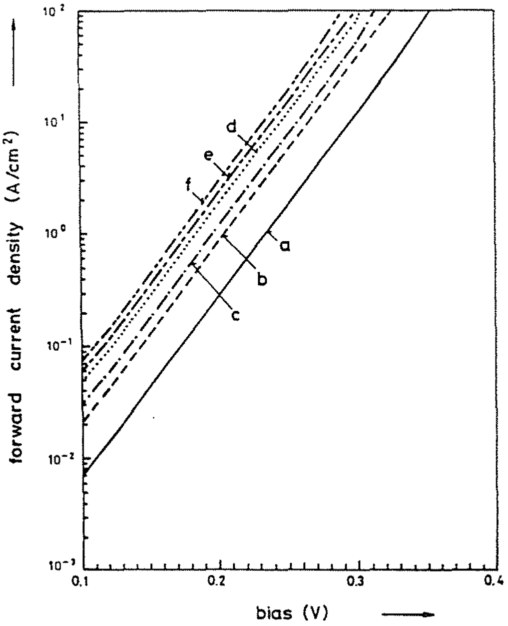

Fig. 4c. Forward I-V characteristics of AgAu-n-Si contact
a) 100 % Au, b) 78 % Au, c) 64 % Au, d) 35 % Au, e) 22 % Au, f) 0 % Au

where C_1, C_2 are the capacitances of the two SMSC, respectively, and [8]

$$C_1 = S_1\left[\frac{q\epsilon N_d}{2(V_{b1} - V - kT/q)}\right]^{1/2}, \tag{25}$$

$$C_2 = S_2\left[\frac{q\epsilon N_d}{2(V_{b2} - V - kT/q)}\right]^{1/2}, \tag{26}$$

where $N_d =$ constant is the donor density throughout the depletion region of semiconductor substrate, ϵ is the permittivity of the semiconductor, V_{b1}, V_{b2} are the built-in potentials of the two SMSC, respectively.

For the CEC,

$$C_t = S\left[\frac{q\epsilon N_d}{2(V_b - V - kT/q)}\right]^{1/2}. \tag{27}$$

From *Eq.* (24 to 26) the capacitance of the CEC can be written as

$$C_t = \left[\frac{q\epsilon N_d}{2(V_{b1} - V - kT/q)}\right]^{1/2}\left\{S_1 + S_2\left[\frac{V_{b_1} - V - kT/q}{V_{b2} - V - kT/q}\right]^{1/2}\right\}. \tag{28}$$

Table 2

Barrier height and ideality factor for metal-Si contacts [6, 7]

Contact	Barrier height [eV]	Ideality factor
Au-n-Si	0.80 ± 0.02	1.05 ± 0.02
Ag-n-Si	0.67 ± 0.02	1.02 ± 0.02
Cu-n-Si	0.61 ± 0.02	1.02 ± 0.02

The depletion layer capacitance of the CEC per unit area is given by:

$$C_0 = \left[\frac{q\epsilon N_d}{2(V_{b1} - V - kT/q)}\right]^{1/2} \left\{P + (1-P)\left[\frac{V_{b1} - V - kT/q}{V_{b2} - V - kT/q}\right]^{1/2}\right\}. \quad (29)$$

From *Eq.* (29), the C-V characteristics of the CEC can be presented by plotting $1/C_0^2$ versus applied voltage V, and

$$\begin{aligned} 1/C_0^2 &= 2(V_b - V - kT/q)/q\epsilon N_d = \\ &= \frac{2(V_{b1} - V - kT/q)(V_{b2} - V - kT/q)}{q\epsilon N_d\{P(V_{b2} - V - kT/q)^{1/2} + (1-P)(V_{b1} - V - kT/q)^{1/2}\}^2}. \end{aligned} \quad (30)$$

The relationship between C_0 and V (*Eq.* (30)) gives the possibility to determine the barrier height of the CEC contact [8]

$$\phi_{bn} = V_i + V_n + kT/q - \delta\phi, \quad (31)$$

where V_i is the voltage corresponding to the intercepted point on the voltage axis, and from *Eq.* (30):

$$V_b - V - kT/q = \frac{(V_{b1} - V - kT/q)(V_{b2} - V - kT/q)}{\{P(V_{b2} - V - kT/q)^{1/2} + (1-P)(V_{b1} - V - kT/q)^{1/2}\}^2}. \quad (32)$$

If the barrier height lowering $\delta\phi$ is so small that it can be neglected and if $1/C_0^2$ is zero, i.e.

$$V_b - V - kT/q = 0, \quad (33)$$

then

$$\phi_{bn} = V_i + V_n + kT/q = V_b + V_n, \quad (34)$$

where V_n is the depth of the Fermi level below the conduction band. On the basis of these results, one may determine the Schottky barrier height of the CEC with the variation of the area ratio.

Using data from results of ARIZUMI et al. [6], [7] for some AuAg-Si, CuAu-Si, CuAg-Si and Au-Si CEC, the similar variations of the electrical properties of the CEC can be calculated. The barrier heights of the single metal-Si contacts according to the cited papers are presented in *Table 2*.

Based on the results presented in *Table 1* and *Table 2*, *Figs. 5*, *6a* and *6b* show the results, where $1/C_0^2$ was plotted against the applied voltage using *Eq.* (30) for AlAg-GaAs, CuAu-Si and AgAu-Si CEC. The family of plots of C-V characteristics is situated between two plots corresponding to SMSC-Si contacts. The distribution of plot family depends on the ratio of interfacial area occupied by each metal in CEC at the interface.

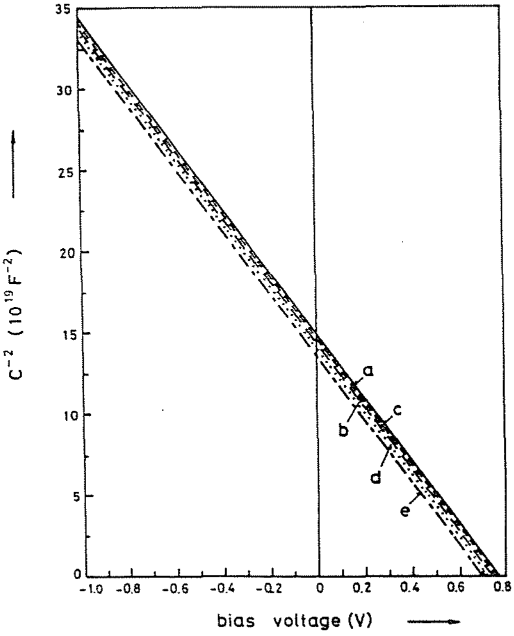

Fig. 5. C-V characteristics of AlAg-n-GaAs contact
a) 100 % Ag, b) 90 % Ag, c) 70 % Ag, d) 40 % Ag, e) 0 % Ag

Using the method determining the barrier heights from the C-V characteristics, the variation of the barrier heights according to the area ratio occupied by the different metals at interface of CEC was presented in *Figs. 7* and *8*.

The barrier heights of AgAu-Si CEC obtained from the C-V characteristics depend almost linearly on the ratio of the interfacial area, but from the I-V characteristics this dependence is not totally linear.

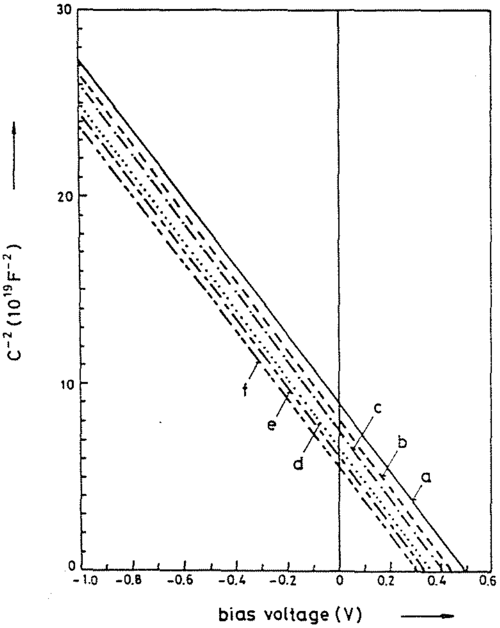

Fig. 6a. C-V characteristics of CuAu-n-Si contact
a) 100 % Au, b) 78 % Au, c) 64 % Au, d) 35 % Au, e) 22 % Au, f) 0 % Au

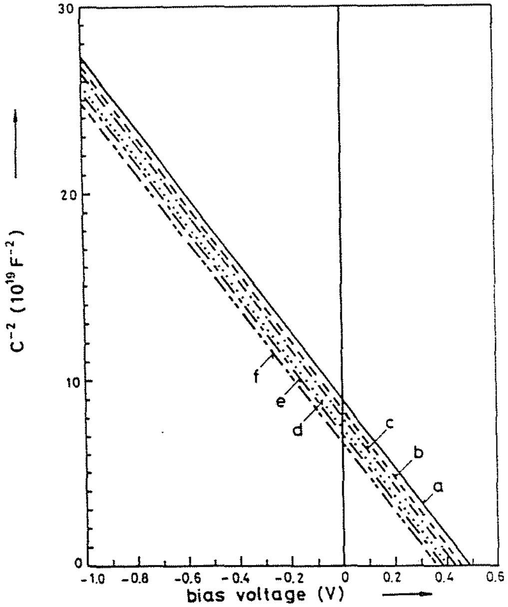

Fig. 6b. C-V characteristics of AgAu-n-Si contact
a) 100 % Au, b) 78 % Au, c) 64 % Au, d) 35 % Au, e) 22 % Au, f) 0 % Au

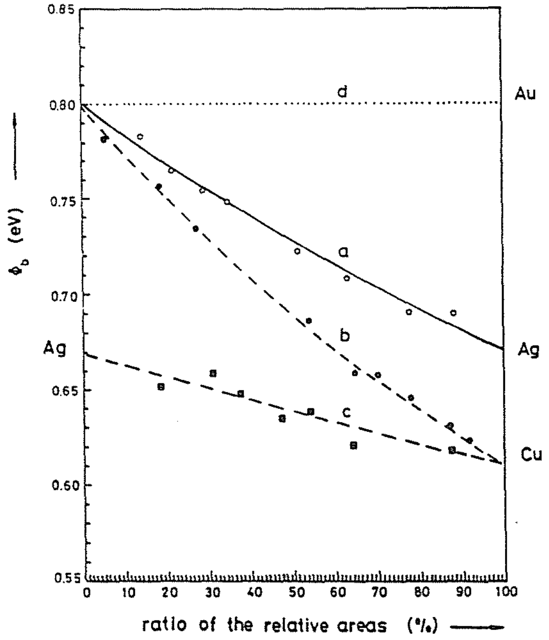

Fig. 7. Calculated and experimental values of barrier height of corresponding metal-n-Si contacts. The experimental results were obtained from [6, 17]. a) AuAg, b) AuCu, c) AgCu, d) Au

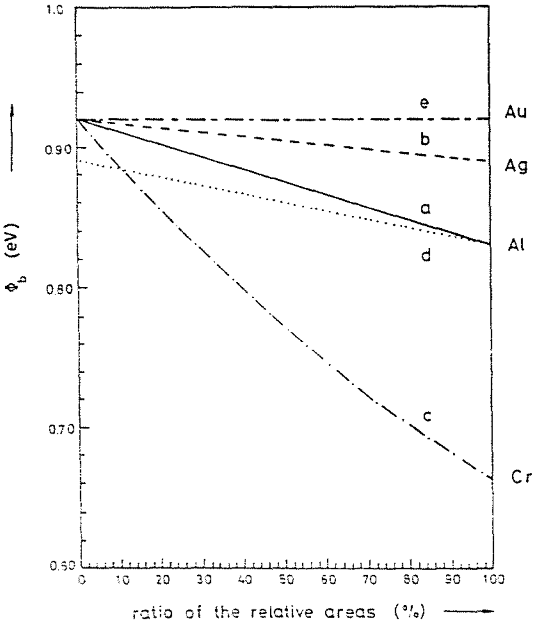

Fig. 8. Barrier height of metal-n-GaAs contacts obtained from C-V measurements a) AlAu, b) AgAu, c) CrAu, d) AlAg, e) Au

3. Discussion and Conclusion

1. The results obtained from the model of the CEC as proposed in some case nearly coincided with those of the MSC. If the SMSC Ni-Si, and W-Si the Schottky barrier heights were found to be 0.61 and 0.67 eV, respectively [8] then according to the *Eqs.* (15), 20 and (23) for the I-V characteristics the calculated barrier height of $Ni_{36}W_{64}$-nSi should be 0.63±0.01 [eV]. The value of this barrier height almost coincided with the experimental result presented by Lien et al. [14]. The results calculated by our model from C-V characteristics are in good agreement with results obtained for AuAg, AuCu and AgAu-Si systems (*Fig. 7*) investigated by ARIZUMI et al. [6], [7]. These results suggest that in this case the results of the dependence of the Schottky barrier heights on the ratio of the interfacial area occupied by each metal component of the CEC can be applied to the MSC.

2. The simple model of CEC still suggests a method to investigate the variation of the barrier height and the electrical properties of the BMSC with the inhomogeneous interface. The reason is that when the Schottky barrier is formed only by the simultaneous and direct interaction between the atoms of the different metals with the surface atoms of semiconductor [9], [15], and the interface is not planar, but spatially inhomogeneous [4], then at the interface of contact the barrier has the local characteristics [15], [16], [17], [18]. This means that the interaction of several metals on the semiconductor will lead to the formation of different local barriers at different subregions with different contact properties and the current flows through the matrix of subregion having different resistances. Thus, the height of the CEC entire contact will be a combination of several local barrier heights. So that the distribution of the different metal atoms along the interfacial area of MSC will play an important role in forming the effective Schottky barrier.

3. The weakness of the model is that there is a discrepancy between the calculated barrier heights from I-V and C-V characteristics of the same CEC. This discrepancy is not explained until now. However, the simultaneous interaction of different metals on the same semiconductor substrate can result in different transport mechanisms including both the thermionic emission and the tunnelling.

The present results indicated that neglecting the influences of simultaneous presence and the distribution of the different metal atoms, or the different atomic groups along the inhomogeneous interface could lead to some error in the evaluation of the electrical properties of the metal semiconductor contacts.

Acknowledgements

The authors wish to thank Dr. B. Pődör, Dr. B. Kovács, Ms. Németh–Sallay, Dr. A. Nagy, Mr. Zs. J. Horváth and Mr. V. V. Tuyen for the helpful and stimulating discussions.

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