RECTIFYING PROPERTIES OF A METAL–SEMICONDUCTOR CONTACT

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We calculate the current-voltage characteristics of a metal–semiconductor contact model with regard for the metal–semiconductor gap and surface states at the semiconductor–gap interface. The corresponding analytical expressions are derived in the approximation, in which only the majority charge carriers are taken into consideration. In the case of the forward bias voltage, the current-voltage characteristics are shown to be described as $i = i_s e^{\alpha V}$. Analytical expressions for the parameter α are derived. We show that the existence of the gap leads to the condition $\alpha \leqslant \frac{e}{kT}$. The parameter α can also be affected by surface states. For the forward bias voltage, the results of theoretical calculations with allowance for surface states are in agreement with the experimental current-voltage characteristics for low-resistivity silicon diodes.

Although the problem of rectifying properties of a metal–semiconductor contact belongs to the oldest problems in semiconductor physics, it has not lost its significance. There are two underlying reasons for that. First, of importance are a variety of devices which are based on rectifying properties of a metal–semiconductor contact (e.g., microwave point-contact diodes). Second, the vast majority of semiconductor devices require reliable nonrectifying contacts, the absence of which can considerably complicate and even worsen the device functioning.

At the same time, the mechanism of metal–semiconductor contact functioning remains, to a large degree, open to discussion. Indeed, the actual current-voltage characteristics of metal–semiconductor contacts, which are described rather satisfactorily by the expression

$$i = i_s \left(e^{\alpha V} - 1\right), \tag{1}$$

differ substantially from the theoretical characteristics $i = i_s(e^{\frac{eV}{kT}} - 1)$ obtained in basic diode and diffusion theories [1–3], namely, by the value of $\alpha < \frac{e}{kT}$ and by the strong dependence of i_s on the voltage.

To explain such discrepancies, some authors considered the effect of tunneling through the barrier in the space charge region [1–3], image forces [4], presence of multiple contacts [5], metal–semiconductor gap [6–9], and surface electron states [9].

However, although the allowance for all those factors does improve the qualitative agreement between theoretical and experimental results, theoretical expressions either include plenty of unknown parameters or have the form which does not enable them to be compared with expressions of type (1). Moreover, owing to a great number of parameters, no theoretical model can be adopted for specific devices prior to a detailed experimental verification.

In this paper, we report the results of our calculations in the framework of a metal–semiconductor contact model with allowance for a gap between the electrodes and the presence of surface states. The validity of the proposed model is confirmed by comparing between theoretical expressions and experimental data.

Theoretical Calculations

The model of a metal–semiconductor contact with a gap between the electrodes is shown in Fig. 1. A vacuum gap or a gap formed by an intermediate phase (e.g., an oxide film) is an appropriate example. In the case of a narrow gap, electrons pass through by tunneling. The model also takes into account the presence of surface electron states in the contact region. Two systems of surface states are known to exist at the free surface of semiconductors such as germanium and silicon, namely, the internal and external states which are related to the semiconductor–oxide interface and the external side of the oxide, respectively. We consider only internal electron states, which should have a stronger effect on rectifying properties. Figure 1 shows four discrete levels peculiar to a free germanium surface [11]. Our technique can be used for an arbitrary system of surface levels as well.

In work [10], we derived an expression for the current-voltage characteristic with allowance for the gap and with surface states taken into account by means of

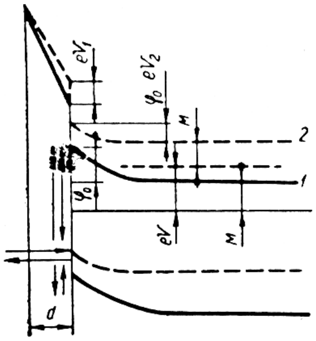

Fig. 1. Model of the metal–semiconductor contact (*1*) without external voltage and (*2*) with forward bias voltage

the parameter φ_0:

$$i = i_s \left(e^{\frac{eV_2}{kT}} - e^{-\frac{eV_1}{kT}} \right). \tag{2}$$

Here, V_1 and V_2 are the fractions of the total voltage V across the gap and the semiconductor, respectively. In the framework of the diode and diffusion theories for low transparency factors $\bar{D} \ll \frac{4E_2^0 U}{\bar{v}}$, we have

$$i_s = \frac{en_0 \bar{v}}{4} \bar{D} e^{-\frac{\varphi_0}{kT}}. \tag{3}$$

For high transparency factors, the diffusion theory yields

$$i_s = eU_n E_2^0 e^{-\frac{\varphi_0}{kT}}. \tag{4}$$

Here, n_0 is the number density of electrons, U_n is the electron mobility, $\bar{v}$ is the average thermal velocity of electrons, and E_2^0 is the field strength in the semiconductor with the gap at the interface.

At sufficiently large currents, when $e^{\frac{eV_2}{kT}} \gg e^{-\frac{eV_1}{kT}}$, expression (2) is reduced to the relation $i = i_s e^{\alpha V}$ which is observed experimentally [see Eq. (1)]. The parameter α not being too small, the diode and diffusion theories both give the expression

$$\alpha = \frac{e/kT}{1 + \frac{d}{\varepsilon_1} \sqrt{\frac{2\pi n_0 \varepsilon_2 e^2}{\varphi_0 - eV_2}}}, \tag{5}$$

where ε_1 and ε_2 are the permittivities of the gap and the semiconductor. One can see that the effect of the gap with thickness d is such that the parameter α is smaller than $\frac{e}{kT}$.

A thorough account of surface electron states includes, first of all, the account of the metal–surface states–semiconductor currents (possible transitions for one of the levels are shown in Fig. 1). In the framework of the diode theory, these currents can be taken into consideration by the addition of the current i_n through the surface levels to the current over the barrier in the space charge region. The total current is

$$i = i_s \left(e^{\frac{eV_2}{kT}} - e^{\frac{eV_1}{kT}} \right) + i_n. \tag{6}$$

In the framework of the diffusion theory, the current through surface levels can be taken into account in boundary conditions, so that the current-voltage characteristic can be written as

$$i = \frac{U_n E_2^0 \bar{D} \bar{v}}{\bar{D} \bar{v} + 4U_n E_2^0} \left[en_0 e^{-\frac{\varphi_0}{kT}} \left(e^{\frac{eV_2}{kT}} - e^{-\frac{eV_1}{kT}} \right) + \frac{4i_n}{\bar{D} \bar{v}} \right]. \tag{7}$$

The density of the current through surface levels is required for the current-voltage characteristic to be determined in the framework of both theories. Generally, it can be written as

$$i_n = e \sum_i \left[k_{im} m_i - k_{mi} \left(n_i - m_i \right) \right], \tag{8}$$

where k_{im} and k_{mi} are the kinetic coefficients which characterize the transition from the i-th surface level into a metal and backward, respectively, n_i is the number density of the i-th level, and m_i is the corresponding electron density.

With regard for the electron exchange between the surface levels and the minority charge carrier band, we get

$$i_n = e \sum_i \frac{n_i \left[k_{im} \left(k_{ci} n_f + k_{vi} \right) - k_{mi} \left(k_{ic} + k_{iv} p_f \right) \right]}{k_{mi} + k_{im} + k_{ci} n_f + k_{ic} + k_{iv} p_f + k_{vi}}, \tag{9}$$

where k_{ci}, k_{ic}, k_{vi}, and k_{iv} are the kinetic coefficients which characterize the electron exchange between level i and the conduction and valence bands; n_f and p_f are the number densities of electrons and holes on the interface, respectively.

When the electron exchange with the minority charge carrier band can be ignored and the exchange with the metal prevails, the forward current through the i-th level can be written in the framework of the diode theory as

$$i_n = en_0 \bar{v} n_i C_n^i e^{-\frac{\varphi_0}{kT}} e^{\frac{eV_2}{kT}}, \tag{10}$$

C_n^i being the electron capture cross-section. One can see that surface levels affect the current strength without any change in the character of its dependence on V_2.

On the other hand, when the electron exchange with the semiconductor is dominant, we have

$$i_n = en_i k_{im}. \tag{11}$$

The coefficient k_{im} grows with voltage, so that the total current strength and its dependence on voltage change.

When the density of the current through surface levels is much lower than the density of overbarrier currents, these levels should be taken into consideration in calculating the parameter α.

Let us consider two our examples in the case of the Schottky barrier layer. The electron exchange with the metal being dominant, we get

$$\alpha = \frac{e/kT}{1 + \frac{d}{\varepsilon_1}\sqrt{\frac{2\pi n_0 \varepsilon_2 e^2}{\varphi_0 - eV_2}} + \frac{4\pi d e n_i}{\varepsilon_1}\frac{d}{dV_2}\left(\frac{k_{mi}}{k_{im}}\right)}. \tag{12}$$

This expression differs from formula (5) by an extra term in the denominator. This term is negative because it decreases with increasing V_2. Therefore, surface levels lead to an increase of the parameter α in this case.

When the electron exchange with the semiconductor prevails, we have

$$\alpha = \frac{e/kT}{1 + \frac{d}{\varepsilon_1}\sqrt{\frac{2\pi n_0 \varepsilon_2 e^2}{\varphi_0 - eV_2}} + \frac{4\pi d e n_i}{\varepsilon_1}\frac{d}{dV_2}\left(\frac{k_{ci} n_f}{k_{ci} n_f + k_{ic}}\right)}. \tag{13}$$

The presence of surface levels lowers the parameter α.

Thus, taking the metal–semiconductor gap into account leads to a decrease of the parameter α in comparison with $\frac{e}{kT}$ and its dependence on gap thickness, charge carrier density, potential barrier height, and voltage. The potential barrier height, as well as the current strength and the character of its dependence on voltage, are affected by surface states in this case.

The contact model and all its features related to the presence of the gap and surface levels were tested experimentally.

Experimental Results

The model was tested experimentally using silicon diodes with a pressed point contact. Attention was mainly focused on forward current. We investigated the effect of surface states on current-voltage characteristics, as well as the dependence of the parameter α on the gap width, number density of majority charge carriers, potential barrier height, and voltage.

The diodes were made from low-resistance silicon for which, as seen from formulas (5), (12), and (13), the above-mentioned dependences can be defined more clearly.

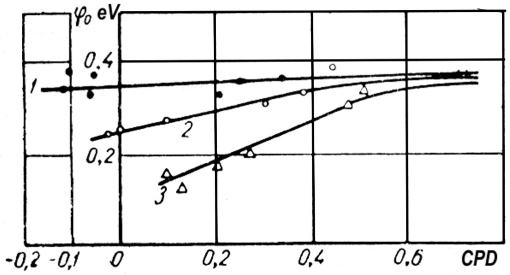

Fig. 2. Potential barrier height as a function of the contact potential difference (CPD). The potential difference across the gold–silicon contact is (*1*) 0.23, (*2*) 0.11, and (*3*) −0.05 V

Effect of surface levels

To establish the factor which determines the potential barrier height φ_0, we investigated the height of the potential barrier in the space charge region as a function of the contact potential difference [12]. Figure 2 demonstrates typical results obtained for one of our samples at various surface conditions (dots near the curves correspond to different contact needle materials). The dependence of the potential barrier height on the contact potential difference is seen to be governed by the initial work function of silicon. The barrier height depends on the contact potential difference slightly at low work functions (large contact potential differences), whereas this dependence is well-defined at high work functions. These results can be explained with the assumption of the considerable influence of a single discrete surface level. The barrier height changes with the contact potential difference (curves *2* and *3*), when the near-surface Fermi level is located below the surface level. When the Fermi level lies close to the surface level, a change in its occupation leads to the barrier height stabilization (curve *1*). The solid curves in Fig. 2 represent the results of theoretical calculations for the surface level located at a distance of $-9kT$ from the middle of the forbidden band, the number density ranging from 10^{12} to 10^{13} cm^{-2}.

Thus, our experiments indicate that the potential barrier height is determined by surface levels and the contact potential difference.

To test the role of currents through surface levels and the effect of these levels on the parameter α, we compared the differential resistances of a diode at low and ultrahigh frequencies. The differential resistances at

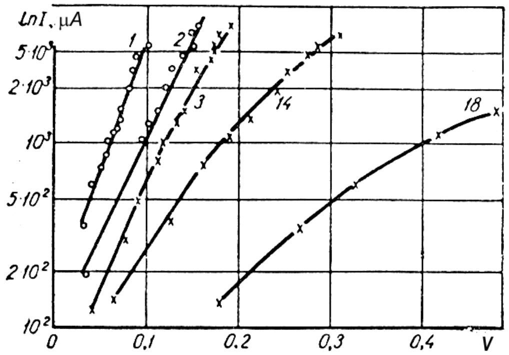

Fig. 3. Current-voltage characteristics for time intervals of (*1*) 5, (*2*) 15, and (*3*) 30 min after the specimen cleavage and (*14*) 48 h and (*18*) 4 h after the tube was filled with air

such frequencies can be supposed to be different in the case of a substantial effect of surface levels. Indeed, the quantity $R = 1/i\alpha$ should change due to the effect of surface levels on the parameter α. So, this parameter is given by expression (12) or (13) at low frequencies and by expression (5) at ultrahigh frequencies. For forward-biased diodes, we found no difference between the differential resistances at frequencies of 10^2 and 10^9 Hz, to within the experimental accuracy. In our opinion, this result testifies that the surface electron states can be ignored, in the first approximation, when considering the questions related to the origin of additional currents and to the variation of α due to their recharging.

Gap effect

The above-described experiments as well as other similar experiments [13] point to the existence of a metal–semiconductor gap (the absence or diminishment of the effect of the metal contact material on the barrier height is just caused by a drop in the contact potential difference across the gap). However, we considered it necessary to carry out direct experiments which would confirm the presence of the gap and its influence on the parameter α.

For this purpose, we compared the current-voltage characteristics of diodes held in an ultrahigh vacuum with ordinary ones [14]. The experiments were performed in a special sealed-off tube with a vacuum of about 10^{-9} mmHg. The tube design allowed us to acquire cleaved surfaces of semiconductors, to clean a metal needle by heating, and to put the needle and the cleaved surface into contact.

Figure 3 shows the semilog plots of the current-voltage characteristics obtained for various time moments after the specimen cleavage and after the tube was filled with air. Note two features of these characteristics. First, the dependence of ln i on V cannot be fitted by a line for large time intervals after the surface cleavage and in the case of air environment. Hence, the parameter $\alpha = d\mathrm{ln}i/\mathrm{d}V$ is not constant and has properties of a differential quantity. It decreases as the voltage increases, just as formula (5) predicts. So, we used the constant value eV_2 (or $\alpha V = eV_2/kT$) when comparing the effects of various factors on parameter α. Second, the parameter α is maximum for the first measurements after the cleavage, and it diminishes with time as the surface stays in a vacuum or in air. For the first measurements after the cleavage, the parameter α is close to the estimate e/kT, which should be obtained when there is no gap. For example, in 5 min after the cleavage, the parameter α was equal to 38.2 V^{-1} for a specimen with $\rho = 3 \times 10^{-1}$ $\Omega\,\mathrm{cm}$) and to 32.6 V^{-1} for a specimen with $\rho = 2 \times 10^{-2}$ $\Omega\,\mathrm{cm}$.

The fact that the parameter α decreases while the cleaved surface stays in vacuum or, especially, in air environment is caused by the enlargement of the layer of adsorbed gases and by surface oxidation. Such a decrease cannot be related to variations in other parameters of the contact, e.g., to variations in the potential barrier height. Indeed, the control experiments showed that the barrier height increases as the cleaved surface stays in vacuum. In this case, the parameter α would increase, but, in reality, it decreases (as was proved experimentally).

The experimental data suggest that the gap, whose characteristics are mainly determined by adsorbed gases and an oxide film, plays a significant role in the rectifying properties of the pressed metal–semiconductor contact.

We also investigated thoroughly the dependence of the parameter α on the gap thickness d (various time intervals, on which the specimen was exposed to air, as well as a low-temperature heating). Figure 4 demonstrates the parameter α as a function of the oxide layer thickness, which can be identified with the gap width in the case of weak pressure forces. We used a silicon specimen with $\rho = 2 \times 10^{-2}$ $\Omega\,\mathrm{cm}$. The data were obtained by the optical method [15]. The parameter α is seen to decrease with increase in the oxide layer thickness. Such a decrease is described by expression (5), provided that other parameters present in formula (5) are constant (solid curve in Fig. 4).

Figure 5 shows the average values of the parameter α as a function of the number density of majority charge carriers. Dots represent experimental data, and the solid curve represents the theoretical calculations by formula

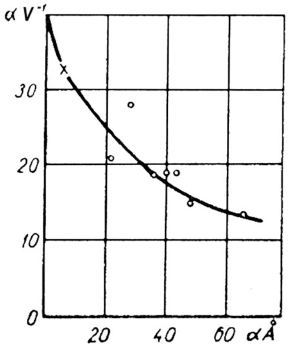

Fig. 4. Parameter α as a function of the thickness of an oxide film on the silicon surface (the point marked by × was obtained in an ultrahigh vacuum)

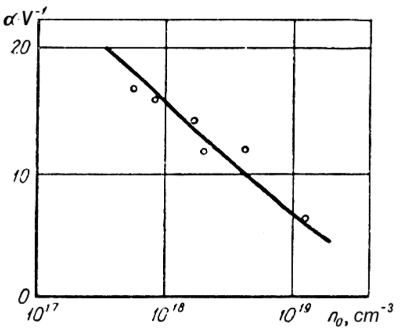

Fig. 5. Parameter α as a function of the number density of current carriers

(5) made using an appropriate fit of the quantity $\frac{\sqrt{\varphi_0-eV_2}}{\varepsilon_1}d$. One can see that the agreement between theoretical and experimental data can be achieved by one-parameter fitting only.

By testing the dependence of the parameter α on the potential barrier height, we found that α increases with the barrier height, in accordance with formula (5).

Thus, the main conclusions drawn from formula (5), which takes into account the metal–semiconductor gap, were confirmed experimentally.

Our results indicate that the model which allows for the metal–semiconductor gap and surface states is valid for low-resistance silicon diodes with a pressed metal contact. In this case, the potential barrier height is determined by surface states and the contact potential difference.

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STRIKHA VITALIY ILARIONOVYCH (30.05.1931–08.02.1999)

The scientific activity of Vitaliy I. Strikha was focused on studying the physical principles of the operation and applications of contact structures and, essentially, metal–semiconductor contacts with a Schottky barrier. The physical model of real contacts with allowance for a metal–semiconductor gap and surface states at the contact interface was justified experimentally for the first time. This model was used as a basis for developing the theory of real contacts. A variety of new physical effects were predicted: variation of current-voltage characteristics with frequency, weak dependence of the capacity on the voltage, the existence of sections with negative resistance in current-voltage characteristics, etc. They found practical applications in the semiconductor device fabrication. V.I. Strikha had also developed the theory of the operation of superhigh-frequency devices with a Schottky barrier and of solar cells based on metal–semiconductor contacts. His theories were used for the device parameter optimization. A new class of devices—biosensors—was created and studied on the basis of semiconductor multilayer contact structures.