

7.4 The Energy Zone Distortion in an External Electric Field

The metal-semiconductor or semiconductor-semiconductor interface phenomena are thoroughly discussed in semiconductor device courses. In that section, the basic interface phenomena while the electric current runs through a substance are under investigation.

The mechanisms of the interface processes for metal-semiconductor and semiconductor-semiconductor contact are very like.

In these processes, the charge carriers of the interface boundary region are redistributed. It leads to distortion of energy zones of a semiconductor.

The contact phenomena can be explained by generation of an electric field across the contact. For simplicity it can be modeled by an external electric field.

Let an electric field be applied across an electron semiconductor (Fig.7.1). The electric charge distribution is violated and a negative volume charge $\rho(\mathbf{r})$ is produced. The generated electric field is described by:

$$\operatorname{div}\mathbf{E}(\mathbf{r}) = \rho(\mathbf{r}) / \varepsilon_0 \quad (7.18)$$

The potential energy:

$$U(\mathbf{r}) = U_0(\mathbf{r}) + U_1(\mathbf{r}) \quad (7.19)$$

$U_0(\mathbf{r})$ is a potential energy of the volume charge when there is no external field.

$U_1(\mathbf{r})$ is a potential energy when the field is switched in.— потенциальная энергия при действии поля;

$$U_1(\mathbf{r}) = -e\varphi(\mathbf{r}), \quad (7.20)$$

The electrostatic potential $\varphi(\mathbf{r})$ and the electric field strength are related by:

$$\mathbf{E} = -d\varphi(\mathbf{r}) / dr. \quad (7.21)$$

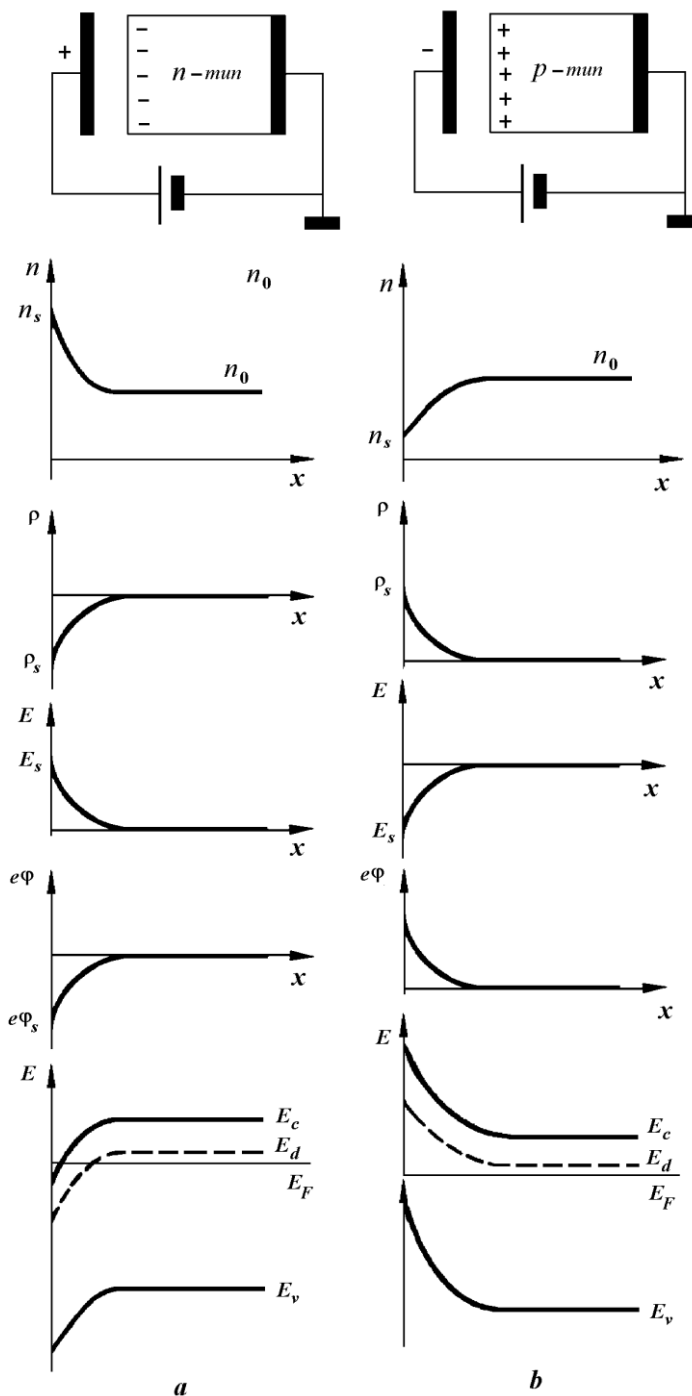
It follows from (7.18) that the redistribution of charges changes the potential energy and reinstalls the energy levels. The electric field is mainly located in boundary (contact) zone. It is not greater than $10^6 \text{ V}\cdot\text{cm}^{-1}$ and is weak in comparison with atomic field ($10^8 \text{ V}\cdot\text{cm}^{-1}$) and can not change the structure of energy zone. It only distorts (curves) the energy levels near the interface.

All levels are distorted, thus the energy interval $E_c - F$ and $F - F_v$ transforms into:

$$E_c + U_1(\mathbf{r}) - F; \quad F - [E_v + U_1(\mathbf{r})] \quad (7.22)$$

In the state of the thermodynamic equilibrium, the position of the Fermi level is stationary. Hence the distance between the level and boundaries of allowed zones can change.

Fig.7.1. The energy zone distortion in an external field. Generation of the volume charge and additional



In accordance with (6.38)—(6.47) when the position of Fermi level relative the forbidden zone boundary is shifted, the electrons are redistributed and the properties of a semiconductor can change. In the interface region, a non-degenerated electron semiconductor can transform into a degenerated one because the Fermi level is located inside the conduction zone. Direction of the zone bending (Fig.7.16) depends of the sign of $U_1(\mathbf{r})$ (for given condition it bends downward).

If the polarity of an applied voltage is changed the concentration distribution (in interface region) changes too. The additional positive electric charge $\rho(\mathbf{r})$ is produced.

The intrinsic field polarity is changed and the direction of bending also changes (Fig.7.16).

Thus at sufficient great bending, we can speak about reversing of the conduction type (from n -type into p -type). The layer with changed type of conduction is called the **inverse layer**. Moving in the depth of a semiconductor we can find a layer with $p \approx n = n_i$, i.e. the layer of the intrinsic conductivity. That layer is called the **i -layer**. The region of a semiconductor where the type of electric conductivity is changed is called the **p - n transition**. It is caused by an external field and vanishes when the field is switched off.

All those changes occur at small depth and we can speak about an effective penetration depth of the field in a crystal (or about a region of an additional volume charge). Let us evaluate that quantity using the Poisson equation (7.18) and formula (7.21). For an one-dimensional case:

$$d^2\varphi(x)/dx^2 = -\rho(x)/\varepsilon_0 \quad (7.23)$$

In accordance with (3.39) and (7.22) in a n -type semiconductor, the concentration of the basic charge carriers:

$$n = N_c e^{-\frac{E_c(x)+U(x)-F}{k_0T}} = N_c e^{-\frac{E_c(x)-F}{k_0T}} e^{-\frac{U(x)}{k_0T}} = n_0 e^{-\frac{U(x)}{k_0T}} \quad (7.24)$$

The quantity n_0 is the equilibrium concentration.

In an electron semiconductor, the volume charge of the interface region is dominated by positive charges of donor impurity $N_d^+ = p_d$:

$$\rho = e[p_d - n(x)]. \quad (7.25)$$

At room temperature $N_d = p_d = n_0$:

$$\rho = e[n_0 - n(x)]. \quad (7.26)$$

Introducing (7.24) into (7.26) we get:

$$\rho = [n_0 - n_0 e^{-U/k_0T}] = en_0(1 - e^{-U/k_0T}). \quad (7.27)$$

The equation (7.23) can be written as follows:

$$d^2\varphi/dx^2 = -en_0/\varepsilon_0(1 - e^{-U/k_0T}). \quad (7.28)$$

Equation (7.28) is valid as for negative so for positive volume charges at the interface. Indeed if $\varphi > 0$, then $\mathbf{E} < 0$ and the positive volume charge is produced when the electrons leave the interface region and move in the depth of a semiconductor. The concentration at the surface is zero and increases up to the equilibrium one in the depth. In transitional region, the non-compensated positive charge is produced (due to donor ions), which follow the Poisson equation.

If we assume that $|U| \ll k_0T$ and use the series approximation, we get [see (7.20)]:

$$\frac{d^2\varphi}{dx^2} = \frac{en_0\varphi}{\varepsilon_0 k_0T}. \quad (7.29)$$

The solution of (7.29) is:

$$\varphi(x) = \varphi_1(x_0) e^{-\frac{x}{\sqrt{\frac{\varepsilon\varepsilon_0 k_0 T}{e^2 n_0}}}} + \varphi_2(x_\infty) e^{-\frac{x}{\sqrt{\frac{\varepsilon\varepsilon_0 k_0 T}{e^2 n_0}}}} \quad (7.30)$$

The quantities $\varphi_2(x_\infty)$ and $\varphi_1(x_0)$ are defined by the boundary condition. $\varphi_1(x_0) = \varphi_s$ is the potential at the interface.

$\varphi_2(x_\infty) = 0$ – the potential inside the semiconductor. In (7.30), it is convenient to designate

$$l_D = \sqrt{\frac{\varepsilon\varepsilon_0 k_0 T}{e^2 n_0}}, \quad (7.31)$$

The quantity (7.31) is a relaxation length and is called sometime the **Debye screen length**.

$$\varphi(x) = \varphi_s e^{-x/l_D}. \quad (7.32)$$

It should be noted that in the length interval of the order the screen length from the interface, the field and carrier concentration changes considerably. At a distance of the order of the screen length, the electric neutrality is practically reestablished. In metals there is the screen effect too. In metals, the electron concentration is great, $n \approx 10^{23} \text{ cm}^{-3}$. The screen length is small, $\sim 10^{-8} \text{ cm}$, i.e. less than the atomic size. Thus the additional charge is distributed on the surface of the metal.

The screen length in semiconductors is greater than that one in metals. In silicon ($n_0 = 10^{14} \text{ cm}^{-3}$ and $\varepsilon = 12$) the field penetrates inside the sample through the distance of 4mm. According (7.32), the potential energy $U(x)$ and volume charge density $\rho(x)$:

$$U(x) = -e\varphi(x) = U_s e^{-x/l_D}; \quad (7.33)$$

$$\rho(x) = -\frac{e^2 n_0}{k_0 T} \varphi(x) = -\frac{e^2 n_0}{k_0 T} \varphi_s(x) e^{-x/l_D} = \frac{e^2 n_0}{k_0 T} U, \quad (7.34)$$

The index 's' means the surface.

Using equation (7.24) and (7.34) we find:

$$\rho_s = U_s e^{-x/l_D}; \quad (7.35)$$

$$n_s = n_0 e^{U_s/k_0 T}. \quad (7.36)$$

A glance at equation (7.35) shows that the sign of the surface charge depends on the sign of the potential energy. The curvature of energy zone also depends on the potential energy sign. Hence when $\rho_s(x) > 0$ zones are screwed upward, when $\rho_s < 0$ zones are screwed downward.

It follows from (7.36) that the surface carrier concentration can be greater than the volume carrier concentration. It leads to greater electric conductivity of the surface layers [see equation (4.4)] The phenomenon is called the **field effect**.

7.5 Contact Voltage

The electron energy in a crystal is negative. Electrons can not leave the crystal. Thus there is a potential barrier at the interface (Fig.7.2). To pass through the barrier, certain energy (the work of exit) is needed. It is convenient to measure that quantity from the bottom of a conduction zone:

$$\chi_0 = E_B - E_C. \quad (7.37)$$

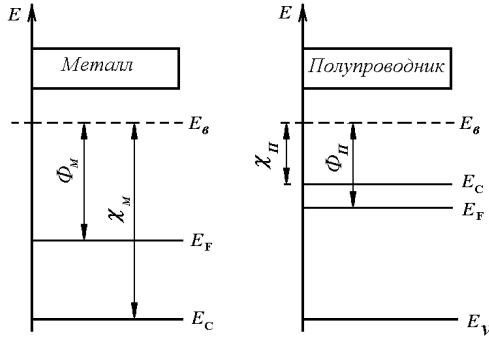


Fig.7.2. The solid – vacuum electric diagram

The quantity E_B is the free electron energy.

If the energy is measured from the Fermi level, the exit work is called the **thermodynamic work of exit**:

$$\Phi = \chi_0 + E_C - F = E_B - F. \quad (7.38)$$

The exit work χ_0 is about 1-6eV. Heat, radiation or others can transmit the energy needed for an electron to leave a crystal. The thermionic emission is the simplest. The thermionic current depends on thermodynamic work of exit:

$$j = AT^2 e^{-\frac{\Phi}{k_0 T}}, \quad (7.39)$$

$$A = \frac{4\pi k_0^2 e^* m}{h^3}$$

The counting of energy from the Fermi level is very profitable because the semiconductor properties strongly depend on the level position (see section 3). In accordance with (3.35) for an intrinsic semiconductor:

$$\Phi_i = \chi_0 + \frac{E_C + E_v}{2} + \frac{k_0 T}{2} \ln \frac{N_c}{N_v}. \quad (7.40)$$

At low temperature for a donor semiconductor:

$$\Phi_d = \chi_0 + \frac{E_C - E_d}{2} + \frac{k_0 T}{2} \ln \frac{N_d}{2N_c}. \quad (7.41)$$

In the region of impurity exhaustion:

$$\Phi_d = \chi_0 + k_0 T \ln \frac{N_d}{N_c}. \quad (7.42)$$

There are analogue formulas for an acceptor semiconductor:

$$\Phi_a = \chi_0 + \Delta E + \frac{E_a - E_v}{2} + \frac{k_0 T}{2} \ln \frac{N_a}{2N_v}; \quad (7.43)$$

$$\Phi_a = \chi_0 + \Delta E + k_0 T \ln \frac{N_a}{2N_v}. \quad (7.44)$$

The exit work of an acceptor semiconductor is greater than that of a donor semiconductor more than ΔE .

At the interface of two solids (there is a small vacuum slit) with different energy barriers, the **contact voltage** is generated. If the exit work of the first metal is less than that of the second metal, the current from the first metal would be greater [see (7.39)]. The interface region of the first metal becomes positive and vice versa. The contact voltage U_K would be generated. The process stops when the thermodynamic equilibrium is established ($\mathbf{j}_{10} = \mathbf{j}_{20}$). In accordance with (7.39):

$$AT^2 e^{\frac{\Phi_1}{k_0 T}} = AT^2 e^{\frac{\Phi_2 + eU_K}{k_0 T}}; \quad (7.45)$$

$$U_K = \frac{1}{e} (\Phi_2 - \Phi_1). \quad (7.46)$$

The quantity U_K is called the **external contact voltage**.

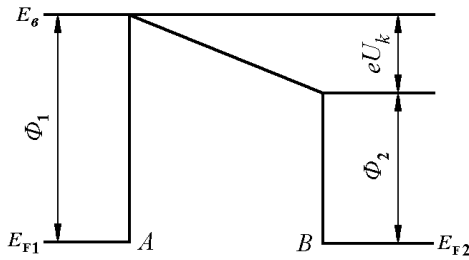


Fig.7.3. Generation of an external contact voltage in the equilibrium state

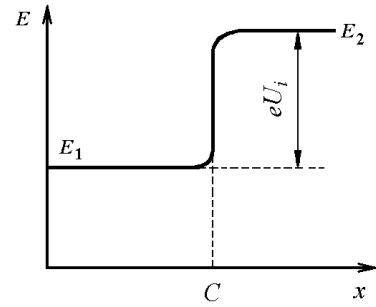


Fig.7.4. Generation of an intrinsic contact voltage

If the distance between metals is sufficiently great the depth of the contact field penetration depends on the screen length. If $\Phi_2 - \Phi_1 \approx 1\text{eV}$ that distance is $d \approx 1\text{ cm}$.

If the metals are brought in close contact, we arrive to concept of the **intrinsic contact** U_i . In the equilibrium state:

$$E_2 = E_1 + eU_i. \quad (7.47)$$

$$E_2 = E_1 - F = E_2 - F_2 = E_1 + eU_i - F_2 \quad (7.48)$$

$$U_i = \frac{1}{e} (F_2 - F_1). \quad (7.49)$$

It follows from (7.49) that an intrinsic contact voltage depends on the difference of the initial Fermi energy level (Fig.7.4). The energy of the Fermi level depends on the effective carrier mass and concentration. The intrinsic contact voltage is about 0.001 – 0.01eV.

7.5 The Metal – Semiconductor Contact

The charge carrier concentration of metals can change in great range that leads to specific phenomena in a metal – semiconductor contact.

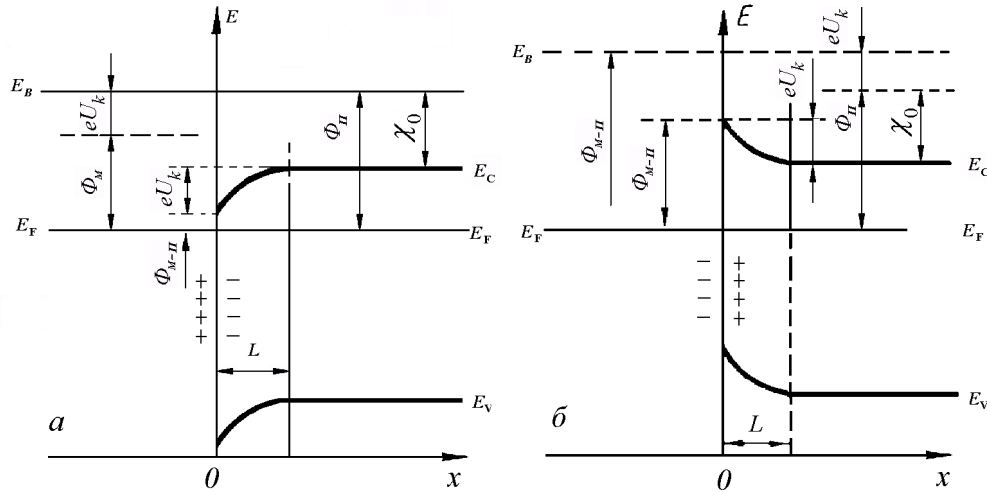


Fig.7.5. The energy diagram of a metal-electron semiconductor contact; a- $\Phi_s > \Phi_m$ and b- $\Phi_s < \Phi_m$

If the exit work of an electron semiconductor is greater than that of the metal [$\Phi_{II} \gg \Phi_M$ (Fig.7.5)] the electron flux from the metal dominates. In the contact region of the metal, the positive charge is generated. In the contact region of the semiconductor, the negative charge is generated. Thus the contact voltage is produced which hinders the transition of electrons from the metal into the semiconductor:

$$eU_K = \Phi_{II} - \Phi_M \quad (7.50)$$

The electron concentration of the metal is much greater than that of the semiconductor and the external electric field penetrates only into the depth of the semiconductor. If the volume charge is negative, electrons saturate the contact layer. The electric conductivity of the semiconductor contact region becomes greater.

If the exit work of a metal is greater than that of the semiconductor [$\Phi_M > \Phi_{II}$ (Fig.7.5b)] the semiconductor energy zones bend upwards and it will be enriched by holes (non-basic charge carriers of an electron semiconductor). The electric conductivity becomes smaller. In the equilibrium state of a non-degenerated semiconductor $n_i^2 = n_0 p_0$ [see (6.51)]. Thus increasing of the non-basic charge carrier concentration p_0 leads to decreasing of the basic carrier concentration n_0 .

Hence the electron semiconductor conductivity, depends on the basic carrier concentration $\sigma = en\mu$. The layer with a small quantity of basic carriers is the region of

high resistance. It is called the **barrier layer**. The layer of great conductivity is called the **conducting layer**. Thus at a metal-semiconductor interface the barrier and conducting layers can be produced. That contact is not linear because it depends what is the voltage direction.

There can be an analogue situation in a metal-hole semiconductor pair (Fig.7.6.). When $\Phi_s > \Phi_m$ the barrier layer is produced; when $\Phi_m > \Phi_s$ the conducting layer is generated.

In an electron semiconductor $\Phi_m > \Phi_s$. The generated contact field would push free electrons in the depth of the semiconductor and almost entire volume charge would be caused by ionized donor ions when $p_d = n_0$.

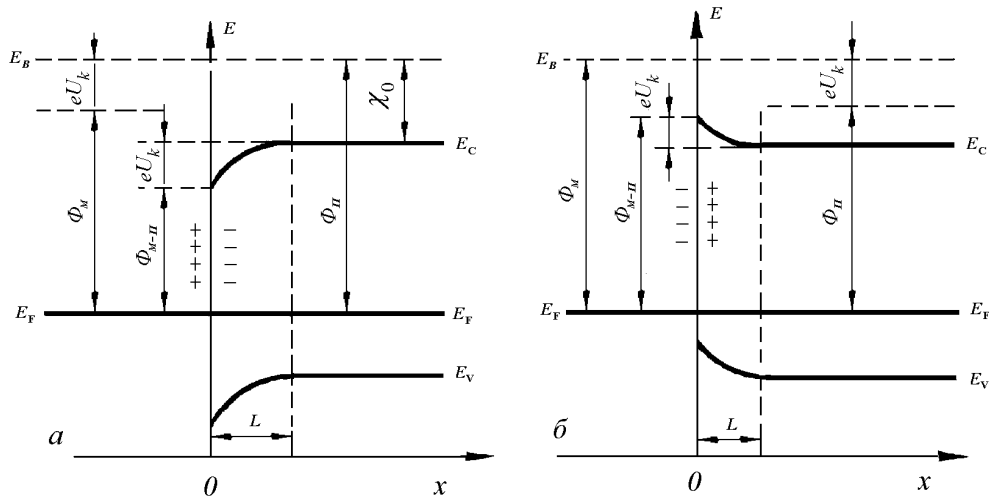


Fig.7.6. The energy diagram of a metal –hole semiconductor contact; a- $\Phi_s > \Phi_m$ and b- $\Phi_s < \Phi_m$

The volume charge density in the contact region can be considered as constant:

$$\rho = en_0. \tag{7.51}$$

Calculations prove that if $U > k_0 T$. When $U > 2,3 k_0 T$ the input of the quantity $n(x)$ in ρ (7.26) is less then 0.1.

The Poisson equation (taking into account the condition (7.51)) in the volume charge region is:

$$d^2\varphi / dx^2 = -n_0 / \epsilon_0. \tag{7.52}$$

It follows that:

$$d\varphi / dx = -n_0 / \epsilon_0 (\zeta - x). \tag{7.53}$$

At the layer boundary ($x = \zeta$):

$$\varphi(\zeta) = 0 \quad \text{u} \quad E = - \left. \frac{d\varphi}{dx} \right|_{x=\zeta}. \quad (7.54)$$

At the contact ($x=0$):

$$\varphi(0) = eU_K = \Phi_M - \Phi_{II}. \quad (7.55)$$

Equation (7.53) transforms into:

$$d\varphi(x) = \frac{e^2 n U_K}{2\epsilon_0} (\zeta - x)^2. \quad (7.56)$$

The contact field penetration depth:

$$\zeta = \sqrt{\frac{2\epsilon_0 U_K}{n_0 e}} = \sqrt{\frac{2\epsilon_0 (\Phi_M - \Phi_{II})}{n_0 e^2}}. \quad (7.57)$$

Comparing the quantity (7.57) with screen length (7.31) we see that the penetration depth of a contact field can be considerably greater than the screen length. It is due to the fact that the contact voltage is usually greater than $k_0 T$ and depends on the exit work, which in its turn depends on the Fermi level position in a metal and semiconductor. The Fermi level of a semiconductor can be controlled. Hence we can control the penetration depth [see (7.57)] of a contact field in the semiconductor.

The less is alloyed a semiconductor (the Fermi level is lower) and greater is the difference of the exit thermodynamic work of the metal and semiconductor, the greater is the penetration depth of a contact field in the semiconductor. For silicon (the difference is about 1eV, the impurity concentration $N_d = 10^{17} \text{ cm}^{-3}$) the penetration depth is about 15mkm, which is greater then the screen length by the factor of fifteen. The penetration depth in intrinsic semiconductor is greater then that one in an impurity semiconductor.

A metal-semiconductor contact with the barrier layer can be used as the current rectifier. In the equilibrium state, the diffuse current of basic carriers is compensated by the drift current of the non-basic charge carriers in contact field. When an electric field is applied through contact, the equilibrium is violated and an electric current produced. Almost entire applied voltage is needed to overcome the barrier layer.

When an electric current runs through a metal-semiconductor contact, the thermodynamic equilibrium of the semiconductor becomes violated. The carrier concentration depends on the Fermi quasi-level. In a contact between a metal and non-degenerated electron semiconductor metal $\Phi_m > \Phi_s$:

$$n = N_c e^{-\frac{E_c - F_n^* + eU(x)}{k_0 T}}. \quad (7.58)$$

Let us find a new position of the Fermi level (in the interval between two points of x-axis) in the volume charge region ($0 < x < \zeta$).

The current density:

$$j = en\mu_n \mathbf{E} + eD_n dn / dx . \quad (7.59)$$

It follows from (7.58):

$$\mathbf{j} = en\mu_n dF_n^* / dx , \quad (7.60)$$

$$\Delta F_n^* = \int_{x_1}^{x_2} dF_n^* = \int_{x_1}^{x_2} \frac{\mathbf{j}}{n\mu_n} dx . \quad (7.61)$$

The voltage across the interval:

$$V_2 - V_1 = j \int_{x_1}^{x_2} \frac{dx}{\sigma} = j \int_{x_1}^{x_2} \frac{dx}{en\mu_n} . \quad (7.62)$$

Comparing (7.61) and (7.62) we see that changing in position of the Fermi level depends mainly on the quantity:

$$\Delta F_n^* = e(V_2 - V_1) . \quad (7.63)$$

Thus a barrier at the metal-semiconductor interface would increase or decrease depending on polarity of an external voltage.

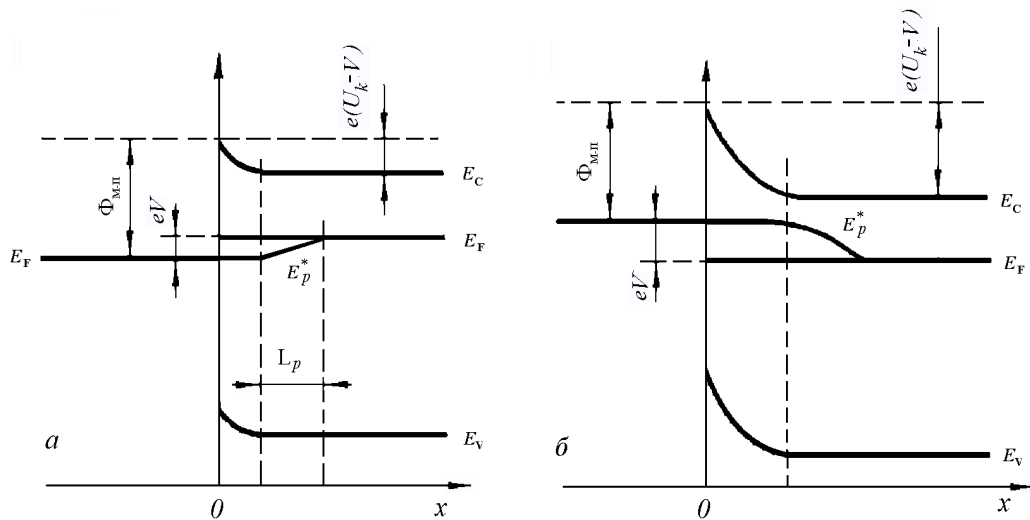


Fig.7.7. The energy diagram of a contact between a metal and electron semiconductor when the direct (a) and barrier (b) voltage is applied through the contact

JI

When a negative voltage is applied through the barrier layer of an electron semiconductor and a positive voltage is applied through a metal ($\Phi_m > \Phi_s$), the electrons would pass from the semiconductor into metal. The thickness of the contact layer with a small concentration of basic carriers would decrease (Fig.7.7a).

The interface barrier decreases by the quantity eV : $e(U_K - V)$. Such voltage is called **direct**: $V < 0$. When polarity of an external voltage is reversed electrons flow into a semiconductor. The thickness of the contact layer increases (see Fig.7.7b). The barrier

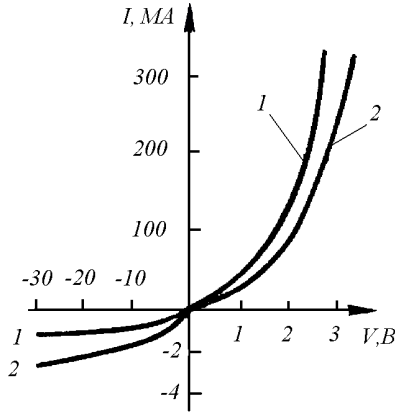


Fig.7.8. The volt-ampere characteristic of a metal-semiconductor contact for a thin (1) and thick (2) barrier layer

height becomes greater: $(U_K + V)$ and the current stops. Such voltage is called the **blackout voltage**: $V > 0$.

An analogue phenomenon is observed when a voltage is applied through the barrier layer of a p -type semiconductor. When the polarity of the semiconductor is positive it corresponds to a direct voltage. If at the metal-semiconductor interface there is a barrier layer, and the voltage polarity initiates the increase of non-basis carrier concentration in the contact layer, the contact resistance increases and the current is small.

If the concentration of non-basic carriers becomes smaller, the current through a metal-semiconductor contacts increases. The contact can be used as a rectifier (see Fig.7.8). The thickness of a blackout layer:

$$\zeta = \sqrt{\frac{2\epsilon\epsilon_0(U_K + V)}{n_0 e}}. \quad (7.63)$$

A glance at equation (7.63) shows that at the direct voltage $V \ll 0$ the layer thickness decreases, at blacking $V \gg 0$ the layer thickness becomes greater. Using equation (7.45) and (7.46) we get the saturated current density through the contact as follows:

$$j = AT^2 e^{\frac{eU_K + eV}{k_0 T}} - AT^2 e^{\frac{eU_K}{k_0 T}} = j_s \left(e^{\frac{eV}{k_0 T}} - 1 \right), \quad (7.64)$$

$$j_s = AT^2 e^{\frac{eU_K}{k_0 T}} \quad (7.65)$$

The blackout layer is considered as thick when:

$$\zeta \gg \lambda \quad (7.66)$$

(λ — the free path). The charge carrier motion through the blaking layer is dominated by diffusion.

That theory of rectification is called the **diffuse theory**. The criterion of its validity is:

$$k_0 T / 2eU_K \lambda \gg 1. \quad (7.67)$$

The equation (7.67) holds if the energy acquired in a contact field at a free path is greater then the thermal energy. For hole semiconductor p -Cu₂O with $\mu_p = 60$ V/(cm² c), equilibrium concentration $p_0 = 10^{14}$ cm⁻³, free path of holes $\lambda = 4 \cdot 10^{-7}$ cm, contact

voltage energy $eU_K = 0.5\text{eV}$, and the thickness of a blackout layer $\zeta = 2,2 \cdot 10^{-4}$ cm, condition (7.66) and (7.67) is true because:

$$\frac{k_0 T \zeta}{2eU_K \lambda} = 15 \gg 1, \quad (7.68)$$

The theory is not valid for germanium, silicon, compounds of A^{II}B^{VI} and A^{III}B^V type with a great carrier concentration and mobility. For example, for n -Si $m_n^* = 0,26m$; $\mu_n = 1300$ V/(cm² c); $\varepsilon = 12$; $n_0 \approx 10^{14}$ cm⁻³; $eU_K = 0,3\text{eV}$; $\zeta = 2 \cdot 10^{-4}$ cm, and $\lambda = 1,5 \cdot 10^{-5}$ cm.

Then:

$$\frac{k_0 T \zeta}{2eU_K \lambda} \approx 0.5 < 1, \quad (7.69)$$

For semiconductors when the following condition holds:

$$\frac{k_0 T \zeta}{2eU_K \lambda} < 1 \text{ or } \zeta < \lambda \quad (7.70)$$

The **diode rectification theorem** is true.

According to the diffuse theory:

$$\mathbf{j} = en_s \mu_n \mathbf{E}_0 \left(e^{-eV/k_0 T} - 1 \right), \quad (7.71)$$

$\mathbf{j}_s = en_s \mu_n \mathbf{E}_0$ is the saturation current density at the external boundary of the blacking layer.

$$E_0 = \frac{2e(U_K - V)}{\zeta}.$$

In accordance with the diode theory:

$$\mathbf{j} = en_s \mathbf{v}_T \left(e^{-eV/k_0 T} - 1 \right), \quad (7.72)$$

$\mathbf{v}_T = \sqrt{8k_0 T / \pi m^*}$ is a mean thermal speed.

Comparing of equation (7.71) and (7.72) shows that there is a difference between the diode and diffuse theory. The saturation current density (diode theory) does not depend on the blackout voltage. In accordance with diffuse theory, (for thick blacking layer) the current density increases with the blackout voltage and decreases when the voltage is direct. Besides the saturation current density in a thin blackout layer is greater than that one in a thick layer so times as the mean thermal speed \mathbf{v}_T is greater than the drift speed of the charge carriers \mathbf{v}_d . Thus the characteristic is asymmetric (Fig.7.8).