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Application Notes

Tunnel Current in MIM System

John G. Simmons Formula

Now, using the Sommerfeld model (see chapter "Metal Energy-Band Structure") and WKB approximation (see chapter "Tunneling Effect in Quasiclassical Approximation") and assuming that $T = 0$, potential barrier is of arbitrary shape and the mass of electrons is isotropic in space, we can derive an expression for the tunneling current flowing in a metal-insulator-metal (MIM) system.

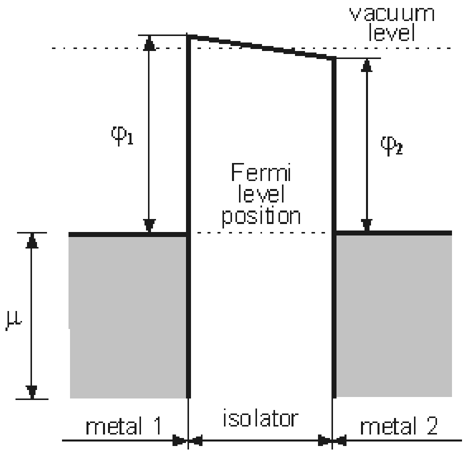

Fig. 1. Diagram of MIM system in equilibrium.
j1 and j2 – work function of the left and right metals, respectively

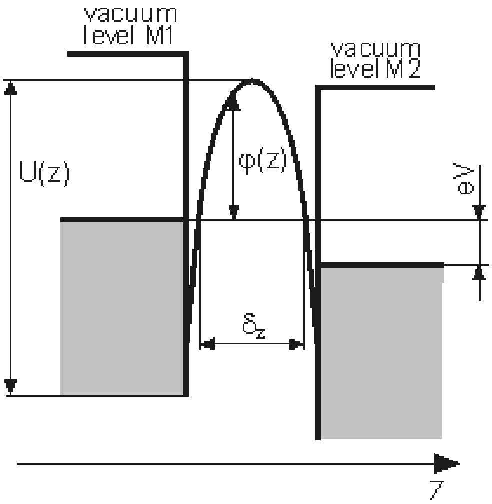

Fig. 2. Model of MIM system with an arbitrary shape potential barrier. Positive potential is applied to the right metal

Consider two metal electrodes with an insulator of thickness L between them. If electrodes are under the same potential, the system is in thermodynamic equilibrium (see chapter "Metal Energy-Band Structure") and Fermi levels of electrodes coincide (Fig. 1). However, if electrodes are under different potentials, current flow between them is available. Fig. 2 shows the energy diagram of electrodes with applied bias energy eV. Potential barrier width for electrons occupying the Fermi level is denoted as $\delta_z = z_2 - z_1$. Consider that all the current flowing in the system is due to the tunneling effect.

Probability $D(E_z)$ of the electron transmission through the po-tential barrier of height $U(z)$ is given by expression (4) in chapter "Tunneling Effect in Quasiclassical Approximation". For the number of electrons N_1 tunneling through the barrier from electrode 1 into electrode 2, we can write [1], [2]

$$N_1 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{p_z}{4\pi^3\hbar^3 m} f_1(E)(1-f_2(E+eV))D(E_z)\,dp_x dp_y dp_z = \int_0^{E_m} D(E_z)n(p_z)\,dE_z \quad (1)$$

where

$$n(p_z) = \frac{1}{4\pi^3\hbar^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_1(E)(1-f_2(E+eV))\,dp_x dp_y \quad (2)$$

and Em – maximum energy of tunneling electrons.

Integration of expression (2) can be performed in polar coordinates. Because in the model under consideration $p_r^2 = p_x^2 + p_y^2$, $E_r = p_r^2/2m$ and total energy is $E = E_z + E_r$, changing variables $p_x = p_r\cos\theta$, $p_y = p_r\sin\theta$, we get

$$n(p_z) = \frac{1}{4\pi^3\hbar^3}\int_0^{2\pi}\int_0^{\infty} f_1(E)(1 - f_2(E + eV))p_r dp_r d\theta =$$

$$= \frac{m}{2\pi^2\hbar^3}\int_0^{\infty} f_1(E)(1 - f_2(E + eV))dE_r$$

(3)

Substituting (3) in (1), we obtain

$$N_1 = \frac{m}{2\pi^2\hbar^3}\int_0^{E_\infty} D(E_z)dE_z \int_0^{\infty} f_1(E_z + E_r)(1 - f_2(E_z + E_r + eV))dE_r$$

(4)

The number of electrons N2 tunneling back from electrode 2 into electrode 1 is calculated in the same way. According to (4) from chapter "Tunneling Effect in Quasiclassical Approximation", the potential barrier transparency in the given case will be such as if positive voltage V is applied to electrode 1 relative to electrode 2. In this case

$$N_2 = \frac{m}{2\pi^2\hbar^3}\int_0^{E_\infty} D(E_z)dE_z \int_0^{\infty} f_2(E_z + E_r + eV)(1 - f_1(E_z + E_r))dE_r$$

(5)

Net electrons flow N through the barrier is obviously N = N1 – N2. Let us denote

$$\xi_1(E_z) = \frac{me}{2\pi^2\hbar^3}\int_0^{\infty} f_1(E)(1 - f_2(E + eV))dE_r$$

$$\xi_2(E_z) = \frac{me}{2\pi^2\hbar^3}\int_0^{\infty} f_2(E + eV)(1 - f_1(E))dE_r$$

$$\xi(E_z, eV) = \xi_1 - \xi_2 = \frac{me}{2\pi^2\hbar^3}\int_0^{\infty} [f_1(E) - f_2(E + eV)]dE_r$$

(6)

Then, the tunneling current density J is

$$J = \int_0^{E_\infty} D(E_z)\xi(E_z, eV)dE_z \qquad (7)$$

According Fig. 2, U(z) can be written in the form $U(z) = \mu + \varphi(z)$. Then, integrating (4) from chapter "Tunneling Effect in Quasiclassical Approximation" and using expression (A5) from Appendix, we get

$$D(E_z) \infty \exp\left\{-A\delta_z\sqrt{\mu + \overline{\varphi}(z) - E_z}\right\} \qquad (8)$$

where $\overline{\varphi}$ – average barrier height relative to Fermi level of the negative electrode; $\overline{\phi} = \frac{1}{\delta_z}\int_{z_1}^{z_2}\phi(z)dz$;

$A = 2\beta\sqrt{\frac{2m}{\hbar^2}}$, β – dimensionless factor defined in the Appendix (A6).

At $T = 0$ K

$$\xi(E_z) = \frac{me}{2\pi^2\hbar^3}\begin{cases} eV, & npu\ E_z \in [0; \mu - eV]; \\ \mu - E_z, & npu\ E_z \in [\mu - eV; \mu] \\ 0, & npu\ E_z > \mu \end{cases} \qquad (9)$$

Introducing (8) and (9) into (7), we obtain

$$J = \frac{me}{2\pi^2\hbar^3}\left\{eV\int_0^{\mu - eV}\exp\left[-A\delta_z\sqrt{\mu + \overline{\phi} - E_z}\right]dE_z + \right.$$

$$\left. + \int_{\mu - eV}^{\mu}(\mu - E_z)\exp\left[-A\delta_z\sqrt{\mu + \overline{\phi} - E_z}\right]dE_z\right\} \qquad (10)$$

Integrating (10), we get

$$J = \frac{\alpha}{\delta_z^2}\left\{\overline{\phi}\exp\left(-A\delta_z\sqrt{\overline{\phi}}\right) - \left(\overline{\phi} + eV\right)\exp\left[-A\delta_z\sqrt{\overline{\phi} + eV}\right]\right\}$$

(11)

where $\alpha = e / 4\pi^2\beta^2\hbar$.

Thus, expression (11) approximates the tunneling current in the MIM system for arbitrary barrier shape.

Summary

- The general expression (7) to calculate the tunneling current in the MIM system was derived in this chapter.
- The analytic approximate solution (11) of tunneling current in the MIM system was calculated.

References

1. Burshtein E., Lundquist S. Tunneling phenomena in solid bodies. Mir, 1973 (in Russian)
2. John G. Simmons. J. Appl. Phys. - 1963. - V. 34 1793.
3. John G. Simmons. J. Appl. Phys. - 1963. - V. 34 238.

- Appendix

Let us integrate an arbitrary function $\sqrt{f(z)}$ from z_1 to z_2.

$$\int_{z_1}^{z_2} \sqrt{f(z)}dz \qquad \text{(A1)}$$

Defining $\bar{f}$ as

$$\bar{f} = \frac{1}{\delta_z} \int_{z_1}^{z_2} f(z)dz \qquad \text{(A2)}$$

where $\bar{f}$ – average value of a function f on the interval from z_1 to z_2, $\delta_z = z_1 - z_2$. Then equation (A1) can be rewritten as

$$\int_{z_1}^{z_2} \sqrt{f(z)}dz = \sqrt{\bar{f}} \int_{z_1}^{z_2} \sqrt{1 + \frac{\left[f(z) - \bar{f}\right]}{\bar{f}}}dz \qquad \text{(A3)}$$

Considering a Taylor series expansion of the integrand (A3) in and neglecting $\left[(f(z) - \bar{f})/\bar{f}\right]^3$ and higher order members, we get

$$\int_{z_1}^{z_2} \sqrt{f(z)}dz = \sqrt{\bar{f}} \int_{z_1}^{z_2} \left\{1 + \frac{\left[f(z) - \bar{f}\right]}{2\bar{f}} - \frac{\left[f(z) - \bar{f}\right]^2}{8\bar{f}^2}\right\}dz$$

(A4)

The second term in (A4) vanishes upon integration, therefore (A4) can be expressed as

$$\int_{z_1}^{z_2} \sqrt{f(z)}dz = \beta\sqrt{\bar{f}}\delta_z \qquad \text{(A5)}$$

where the correction factor is

$$\beta = 1 - \frac{1}{8\bar{f}^2\delta_z} \int_{z_1}^{z_2} \left[f(z) - \bar{f}\right]^2 dz \qquad \text{(A6)}$$

John G. Simmons Formula in a Case of Small, Intermediate and High Voltage (Field Emission Mode)

According chapter John G. Simmons Formula, the approximate expression for the tunneling current in the MIM system can be written as [1]:

$$J = \frac{\alpha}{\delta_z^2}\left\{\bar{\phi}\exp(-A\delta_z\sqrt{\bar{\phi}}) - (\bar{\phi} + eV)\exp\left[-A\delta_z\sqrt{\bar{\phi} + eV}\right]\right\}$$

(1)

where $\alpha = e/4\pi^2\beta^2\hbar$, $A = 2\beta\sqrt{\frac{2m}{\hbar^2}}$, $\bar{\phi}$ – average barrier height, δ_z – barrier width, V– voltage between electrodes.

Small voltage

At low voltages $\bar{\phi} >> eV$, expression (1) can be simplified [1]

$$J = \frac{\gamma\sqrt{\bar{\phi}}V}{\delta_z}\exp(-A\delta_z\sqrt{\bar{\phi}}) \qquad (2)$$

where $\gamma = \frac{e\sqrt{2m}}{4\beta\pi^2\hbar^2}$. Since $\bar{\phi} >> eV$, we can consider that $\bar{\phi}$ doesn't depend on V. Thus, in the case of small applied voltage, the tunneling current proportionate to V. Energy diagram of the MIM system then $\bar{\phi} >> eV$ is shown on Fig. 1.

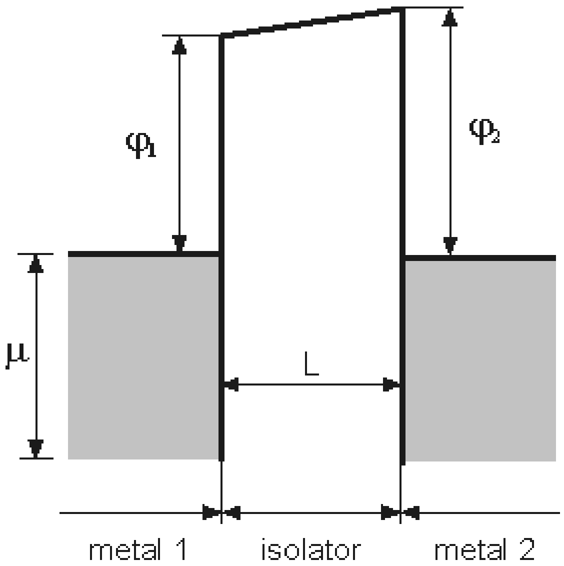

Fig. 1. Potential barrier in the MIM system then V ~ 0. ϕ_1 and ϕ_2 – work function of the left and right metals, respectively

In this case, as shown on Fig. 1, $\delta_z = L$ and $\bar{\phi} = (\phi_1 + \phi_2)/2$

Intermediate voltage

If $eV < \phi_2$, then $\delta_z = L$ and $\bar{\phi} = (\phi_1 + \phi_2 - eV)/2$ (Fig. 2).

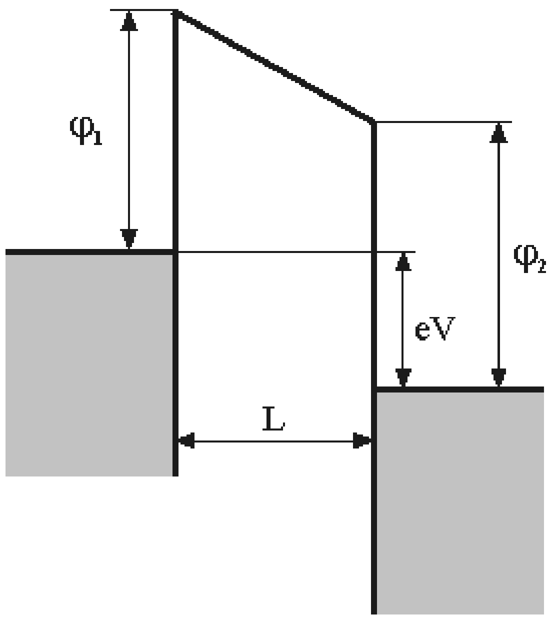

Fig. 2. Potential barrier in the MIM system then $eV < \phi_2$. ϕ_1 and ϕ_2 – work function of the left and right metals, respectively

In [2] it is shown, that for this case the tunneling current-voltage relation is given by

$$J = \frac{\gamma\sqrt{\bar{\phi}}}{\delta_z}\exp(-A\delta_z\sqrt{\bar{\phi}})(V + \sigma V^3) \quad (3)$$

where $\sigma = \dfrac{(Ae)^2}{96\bar{\phi}\delta_z^2} - \dfrac{Ae^2}{32\delta_z\bar{\phi}^{3/2}}$

High voltage – Field emission mode

The case when $eV > \phi_2$ corresponds to energy diagram shown in **Fig. 3** and to the following $\delta_z = L\phi_1/(\phi_1 - \phi_2 + eV)$, $\bar{\phi} = \phi_1/2$.

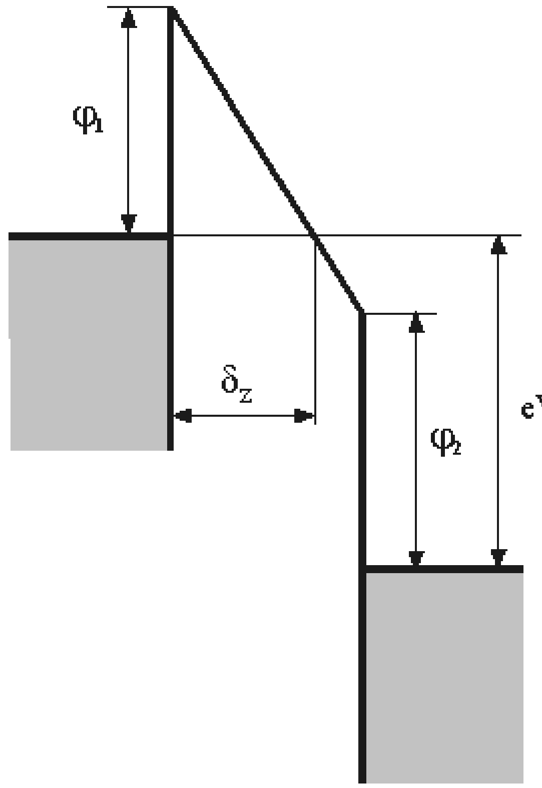

Fig. 3. Potential barrier in the MIM system then $eV > \phi_2$. ϕ_1 and ϕ_2 – work function of the left and right metals, respectively.

Substituting δ_z and $\bar{\phi}$ into equation (1), we obtain

$$J = \frac{e^3F^2}{8\pi^2\hbar\phi_1\beta^2}\left\{\exp\left[-\frac{2\beta}{eF}\phi_1^{3/2}\frac{\sqrt{2m}}{\hbar}\right] - \left(1 + \frac{2eV}{\phi_1}\right)\exp\left[-\frac{2\beta}{eF}\phi_1^{3/2}\frac{\sqrt{2m}}{\hbar}\sqrt{1 + \frac{2eV}{\phi_1}}\right]\right\} \quad (4)$$

where $F = V/L$ – electric field strength.

At high applied voltage $(eV > \phi_1 + \mu)$ the Fermi level of electrode 2 is lower than the conduction band bottom of electrode 1. Under such conditions, electrons can not tunnel from electrode 2 into electrode 1 because of lack of empty states. An inverse situation is for electrons tunneling from electrode 1 into empty states of electrode 2. This process is similar to autoelectronic emission from a metal into vacuum. Thus, since $eV > \phi_1 + \mu$, the second summand in (4) can be neglected and for the current we get

$$J = \frac{e^3}{8\pi^2 \hbar \beta^2} \frac{F^2}{\phi_1} \exp\left[-\frac{2\beta}{e} \frac{\sqrt{2m}}{\hbar} \frac{\phi_1^{3/2}}{F} \right] \qquad (5)$$

where coefficient β = 23/24. This result agrees qualitatively with an analytical expression for the field emission current density [3].

Thus, using formulas (2)–(5), we can compute the tunnel current at given system parameters and plot current-voltage characteristics. Fig. 4 shows theoretical tunneling current-applied voltage plot in case of carbon electrode 1 (ϕ_1 = 4,7 эВ) and platinum electrode 2 (ϕ_2 = 5,3 эВ) at δ_z = 5 Å and contact area $S = 10^{-17}$ m^2.

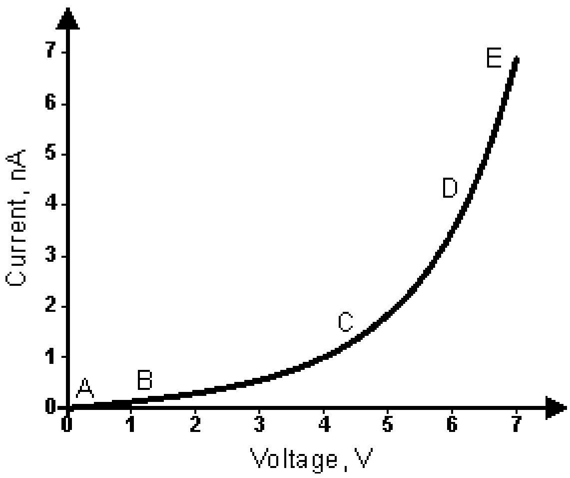

Fig. 4. Current-voltage characteristic for carbon electrode 1 and platinum electrode 2 at δ_z = 5 Å and contact area 10–17 m2. Parts of J(V) curve correspond to the following expressions: AB – (22), BC – (23), CD – (24), DE – (25).

Summary

- Depend upon magnitude of applied voltage, formula (1) can be simplified (2)–(5).
- It is possible to describe the experimental tunneling current dependences by approximated expressions (2)–(5) in accordance with magnitude of applied voltage.

References

1. John G. Simmons. J. Appl. Phys. - 1963. - V. 34 1793.
2. John G. Simmons. J. Appl. Phys. - 1963. - V. 34 238.
3. Dobretzov L.N., Gomounova M.V. Emission electronics. Nauka, 1966 (in Russian)

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