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Tunneling and thermionic-field emission current in diode metal—isolator—metall

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An analytical solution of the one-dimensional Schrodinger equation with a potential in the form of a quadratic function of the coordinate and a fourth-order function of the coordinate is obtained. An analytical expression has been found for the transparency of the diode as a function of the electron energy and the anode voltage. The explicit analytical volt-ampere characteristic of the diode is determined as a function of the anode voltage and temperature. The tunneling current in the diode is calculated taking into account the temperature and its volt-ampere characteristics are constructed.

Keywords: thermionic-field emission, Schrodinger equation, tunneling, diode.

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Introduction

Although a flat diode is a simple structure, analytical expressions for the dependence of transparency $D(E, U_a)$ on energy and anode voltage during electron tunneling are not known for it. The current-voltage curves (CVC) and $J(U_a, T_c, T_a)$ are also not analytically known —the dependences of current density on the anode voltage U_a (electrostatic potential of the anode) and the temperatures of the cathode T_c and anode T_a. Although these values can be calculated in the [1–6] tunneling models used, they are important for vacuum electronics (including nanoelectronics), as well as for solid-state and semiconductor electronics. In a number of modeling tasks, the specified parameters are repeatedly changed and calculated. The analytical CVCs are critical in considering the diode interaction with the connection circuit. Modeling of tunnel devices has been continuously improved since the beginning of this concept (1928) (see [7–9] and the literature cited there). First, tunneling from a flat, remote metal cathode with an electric field set on it was considered. After that, the investigation of influence of the cathode surface structure and its material on tunneling was started [7–9]. The effect of field penetration into semiconductor and carbon structures, including nanoporous structures, was discovered. The shapes of the potential barrier and the effect of electrodes on it in nanoscale structures are obtained [1–4]. The classification of emission as auto-electronic (field) and thermoelectronic [8] was limited to a single thermal field emission [3].

We consider the simplest model of a metal-dielectric-metal diode (or metal-insulator-metal MIM) without field penetration into metal electrodes. Metals are considered to be highly conductive, i.e., the Debye penetration depth $L_D = \sqrt{\varepsilon_0 \varepsilon k_B T (e^2 N_e)}$ in them has an atomic layer size with the concentration of free electrons $N_e \sim 10^{29}\,\mathrm{m}^{-3}$, and the low-frequency permittivity (DP) of lattices $\varepsilon \sim 10$.

The purpose of this work is to obtain analytical relations for a diode. The structure of the work is as follows: First, we obtain accurate profiles of the quantum potential, then we obtain their parabolic approximations, on the basis of which we solve the Schrodinger equation (SE) and find transparency at a given energy. Then we calculate the integral current density as a function of voltage on the anode and approximately analytically calculate the integrals found in order to obtain explicit dependencies. Let's denote the cathode-related values by the indices „c" or „+", and the anode-related values we denote as „a" or „–", respectively. Next, the corresponding cathode indexes will sometimes be omitted. Tunneling, especially in resonant tunneling structures (RTS) at high current, is accompanied by heating of electrodes [1], so knowledge of the temperature dependences of CVC is also important. The theory of Fowler—Nordheim (FN) (or WKB approximation) is applicable for cold emission at a very remote anode and at energies at which the potential barrier is wide enough, which is not true for the nanostructures. In addition, the resulting transparency contains an unknown pre-exponential factor [10]. Therefore, for the diode it is necessary to solve a one-dimensional SE equation $(-\hbar\partial_{xx}^2/(2m_e) + V(x) - E)\psi(x) = 0$ with quantum potential $V(x)$ given in Fig. 1 and allowing for the electrodes effect [1–4]. Thus, $V(0) = E_{Fc}$, $V(d) = E_{Fc} - eU_a$, where U_a — anode voltage. If the work functions (WF) of $W_{c,a}$ cathode and anode differ then $V(d) = E_{Fc} - eU_a + W_c - W_a$. A vacuum diode may be considered as a source of electrons and as an element of an electron gun for electronic devices [2–4]. Solid-state diodes

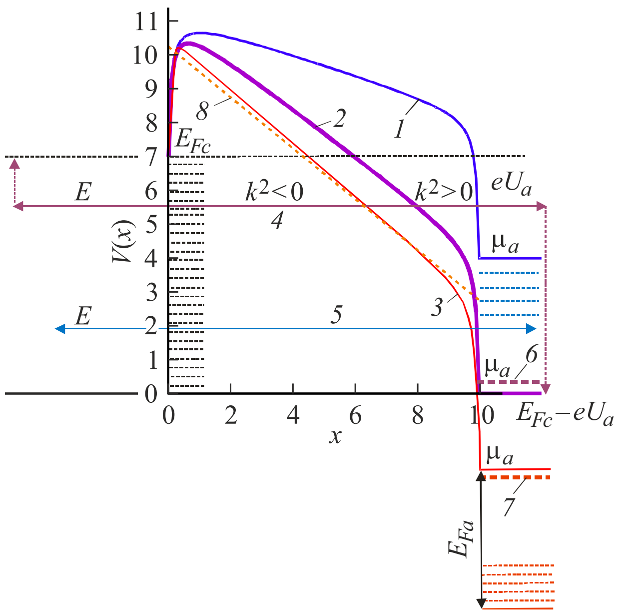

Figure 1. Potential barrier shape V [eV] and energy diagrams in vacuum diode $d = 10$ nm depending on coordinate x [nm] at different anode voltages (V): 3 (curve *1*), 7 (curve *2*), 9 (curve *3*). The electrodes are made of copper: $E_F = 7$, $W = 4.36$ eV. The lines *4* and *5* show the tunneling through the barrier 2 and 1, respectively. The levels 6 and 7 correspond to the curves *2* and *3* at $W_a < W_c$ (6) and $W_a > W_c$ (7). The dashed line *8* — is a triangular approximation of barrier 3.

are commonly used in generators of various frequency ranges. The transition to a vacuum diode in the obtained ratios occurs when substituting DP $\varepsilon = 1$. The model does not take into account semiconductor electrodes with a field penetration depth from fractions of nanometers to tens and hundreds of nanometers. It also does not apply to tunnel diodes, which consider tunnel and diffusion currents, i.e. there shall be a dielectric between the electrodes, which is assumed to be ideal. In the considered diode, at low temperatures, the current is mainly tunneling in nature, and taking temperature into account leads to the appearance of a usually small temperature component. However, at high voltages and currents, strong heating is possible, and the model takes into account thermal field emission with different electrode temperatures. We consider surfaces to be atomically smooth.

1. Parabolic approximation of potential

The exact potential for the diode included in SE is determined by the method of multiple images [1–4] and is given in appendix (P1) along with the legends. The calculations as per (P1) are shown in Fig. 1 together with energy diagrams. Next, the formula (P1) is approximated by a parabola of the second and fourth orders. The energy is counted from the bottom of the cathode conduction band. At large size d, the barrier relative to Fermi energy (FE) has a height of W_c/ε, and when the potential is applied, it decreases due to the Schottky effect. At small d, a stronger decrease occurs due to the mutual influence of the electrodes. This decrease is very strong at high anode voltage and low d, while the maximum of the barrier is shifted to the cathode. At a critical potential, the barrier relative to Fermi level (FL) of the cathode disappears when the maximum point hits the cathode. This critical potential is found from the condition $V'(0) = 0$ or $U_a = W_c d/(e\varepsilon\delta_c)$. For the considered case of a vacuum diode, this corresponds to the anode voltage $U_a = 44.4$ V at a critical field $4.4 \cdot 10^9$ V/m. At such fields, the barrier turns into an almost linear bevel to the anode, and for energies below FL, it becomes almost triangular on a small rectangular pedestal.

The potential (P1) is inconvenient for an analytical solution of SE. It is usually solved numerically using a piecewise constant approximation [2–4]. The barrier is also constructed using parabolic approximation [3,4], $s = 2$ in (1), as well as a more accurate approximation by a fourth-order parabola [4], $s = 4$:

$$V(x) = E_F + \frac{W_c}{\varepsilon}\left(1 - \frac{a}{d}\right)\left[1 - \left(\frac{2x}{d} - 1\right)^s\right] - \frac{eU_a x}{d}. \quad (1)$$

An even more accurate approximation, differing from (P1) by no more than 1 %, can also be constructed by [1–4], but it is inconvenient for an analytical solution. In jcite3, the exact formula (P1) is compared with the parabolic approximation according to formula (1) at $s = 2$ and 4 at $U_a = 0$, as well as with the more accurate approximation given there. Calculations show that approximation (1) with $s = 2$ describes a narrow barrier well enough and gives an error of about a few percent for a wide one. The formula with $s = 4$ has an error of about 1 %. It accurately takes into account the height of the barrier in the center and its values on the electrodes. Taking into account the anode potential in the form of adding an exact linear term $-eU_a x/d$ does not change the accuracy. The SE solution with a barrier (1) has the same margin of error as its shape itself. An approximate description of the barrier as a rectangular shape, triangular shape, triangular shape on a pedestal (trapezoid), often used in the literature, gives a significant error in the current. So, a triangular barrier greatly underestimates, and a rectangular barrier of the same width — overestimates the current by times. In formula(1), the materials of the electrodes are considered the same, the value $\widetilde{W} = W_c(1 - \alpha/d)$ means WF reduced due to the influence of electrodes, and the parameter $\alpha = \delta(2.7716 - 16\delta/(3d)) \approx 2.7716\delta$ that takes this into account is small. Next, we take WF and FE for the electrodes as having equal values, since the effect of different materials is simply limited to adding the term $(W_c - W_a)x/(\varepsilon d)$ to the potential V. We also introduce the value $W = \widetilde{W}/\varepsilon$, which determines the decrease in the barrier due to the dielectric. To get the analytical solution of SE we use approximation (1) at $s = 2$ and 4. In this case, when $s = 2$ and we make substitution of variables $\tau = 2x/d - 1$ in (1) we have a quantum potential

$$V(\tau) = E_F + W(1 - \tau^2) - eU_a(1 + \tau)/2,$$

as well as SE $\phi''(\tau) = (a\tau^2 + b\tau + c)\phi(\tau)$. Here the dimensionless constants are denoted

$$a = d^2 m_e W/(2\hbar^2),$$

$$\tilde{b} = d^2 m_e U_a/(4\hbar^2),$$

$$\tilde{c} = d^2 m_e(E - E_F - W + eU_a/2)/(2\hbar^2). \qquad (2)$$

Also

$$\tilde{c} = -d^2 m_e(E_F - E)/(2\hbar^2) - a + \tilde{b}.$$

Here at $0 \le x \le d$ the new variable changes within $-1 \le \tau \le 1$. It is convenient to make another substitution: $t = (\tau + 1)/2$, $\varphi(t) = \phi(2t - 1)$, $\varphi''(t) = 4\phi''(\tau)$. Then, variable t changes within $0 \le t \le 1$, and SE becomes $\varphi''(t) = \big(a(2t - 1)^2 + \tilde{b}(2t - 1) + \tilde{c}\big)\varphi(t)/4$. Let's rewrite it as

$$\varphi''(t) = (at^2 + bt + c)\varphi(t),$$

where

$$b = \tilde{b}/2 - a = d^2 m_e(eU_a/4 - W)/(2\hbar^2),$$

$$c = (\tilde{c} - \tilde{b} + a)/4 = d^2 m_e(E - E_F)/(8\hbar^2).$$

It should stressed that $a > 0$, $\tilde{b} > 0$, while $\tilde{c} > 0$, if $E > E_F + W - eU_a/2$ (over-barrier passing at low voltages). At low voltages, $E < E_F + W - eU_a/2$ corresponds to $\tilde{c} < 0$, with tunneling taking place mainly. At $E = E_F$ $c = 0$. Conditions $c < 0$ is consistent with tunneling, and $c > 0$ — corresponds to the over-barrier passing. If $0 < E < E_F - eU_a$, then tunneling to E level of the anode is possible if the electron from this level preliminary goes to FL $E_F - eU_a$ of the anode with absorption of the energy quantum $E_F - eU_a - E$. At the same time, due to the Nottingham effect, a quantum of energy is released at the cathode $E_F - E$, i.e., the total energy released during junction of one electron from the cathode to the anode is equal to eU_a. It is evolved due to the operation of the power supply source. If $eU_a > 2(E_F + W)$ (large anode voltages), then $\tilde{c} > 0$ for all energies. If $W = 0$, then $a = 0$, and the potential becomes linear. In this case SE has the most simple form at $E = E_F$ or $c = 0$: $\varphi''(t) = bt\varphi(t)$. Its solution satisfies the integral equation (IE)

$$\varphi(t) = \varphi(0) + \varphi'(0)t + b\int_0^t\int_0^\tau t'\varphi(t')dt'd\tau.$$

By substituting $\xi = b^{1/3}t$, $\varphi(t) = u(\xi)$ SE is normalized to $u''(\xi) = \xi u(\xi)$ and has its solutions in Bessel functions [4]: $u(z) = \sqrt{\xi}Z_{1/3}(2i\xi^{3/2}/3)$ or $u(b^{1/2}x/d) = \sqrt{(b^{1/3}x/d)}Z_{1/3}\big(2i(b^{1/3}x/d)^{3/2}/3\big)$. Here $Z_\nu(z) = C_1 J_\nu(z) + C_2 Y_\nu(z)$ — general solution of Bessel equation of index $\nu = \pm 1/3$, C_1 — arbitrary coefficients (integration constants). Using these functions or Airy functions, it is easy to solve a problem with a linear potential. Solutions in special functions for $a \ne 0$ are possible only in special cases, and in the general case are not known.

2. Solution of SE. Parabolic approximation

We are looking for a solution at a given energy E and a wavenumber (WN) $k_0 = \sqrt{2m_e E}/\hbar$ at the cathode in the form of $\psi(x) = \exp(ik_0 x) + R\exp(-ik_0 x)$. On the cathode at $x < 0$ we have $V(x) = 0$ (Fig. 1), i.e. the potential changes in a stepwise manner from 0 to E_{Fc}. From boundary conditions at $x = 0$ it follows that

$$1 + R = \varphi(0) = \alpha_0, \quad 1 - R = \varphi'(0) = \alpha_1/(ik_0 d),$$

$$Y = (1 - R)/(1 + R) = \alpha_1/(ik_0 d\alpha_0), \;\; 2R = \alpha_0 - \alpha_1/(ik_0 d),$$

$$2 = \alpha_0 + \alpha_1/(ik_0 d).$$

WN in the barrier region $k(x) = \sqrt{2m_e(E - V(x))}/\hbar$ may be imaginary (Fig. 1, area $k^2 < 0$ for the curve *2* up to its intersection with line E) or real (Fig. 1, region $k^2 > 0$ after intersection of curve *2* with the line E). The intersection points correspond to the turning points. Usually, regions $k^2 > 0$ are not taken into account during tunneling, i.e. movements up to the turning point x_{pt} are considered. However, the region $x_{pt} < x < d$ changes the phase of the wave function and shall be taken into account. In it the particle moves in a quasi-classical way. Let's denote a series of used wave numbers. On the cathode for energy E we have the wave number k_0. If the particle is moving to the FL of the cathode, then $k_c = \sqrt{2m_e E_c}/\hbar$. If it is moving to the FL of the anode, then (Fig. 1)

$$k_a = \sqrt{2m_e(E_{Fc} + W_c - W_a - eU_a)}/\hbar.$$

In the barrier region upstream the anode

$$k(d) = \sqrt{2m_e(E - E_{Fc} + W_a - W_c + eU_a)}/\hbar.$$

These ratios are simplified with identical electrodes. Electron with energy E moves from the cathode in a wave-like manner before scattering onto FL of the anode, i.e. until reaching the anode. Therefore, the FL on the anode shall be taken as $\psi(x) = \bar{T}\exp(ik_0(x - d))$. After scattering, the electron goes into the power supply with WF

$$\psi(x) = \bar{T}\exp(ik_a(x - d - \lambda_e)).$$

Here λ_e — the mean free path (MFP) of the electron on the anode. For copper $\lambda_e = 42$ nm, i.e. this region that doesn't obey SE may be significantly larger d. Junction from E level to $\mu_a = E_{Fc} + W_c - W_a - eU_a$ level of the anode may be accompanied by the release (if $E > \mu_a$) or absorption (if $E < \mu_a$) of a quantum of energy (Fig. 1), i.e., the anode either heats up or cools down due to the junction. Similarly, reverse tunneling to the cathode either cools it or heats it by $|E - \mu_c|$. On average, the electrodes heat up, and at high voltage, the anode heats up more. During reverse tunneling at the anode, the incident WF has the form $\psi(x) = R^- \exp(-ik_0(x-d))$, and the wave going to the source at the cathode has the form $\psi(x) = T^- \exp(-ik_0 x)$. If we need to solve the problem up to the turning point, then the coefficients of reflectance and transmission in both directions will coincide: $R^+ = R^- = R$, $T^+ = T^- = \widetilde{T}$, whereas $|R^{\pm}|^2 + |T^{\pm}|^2 = 1$. The turning point x_{pt} is found from the condition $E = V(x_{pt})$. If $eU_a \sim E_F$, then $x_{pt} \approx d$ (Fig. 1). If $eU_a = E_F$, then $x_{pt} = d$ equality is true, while reverse tunneling from the cold anode (at $T = 0$) is impossible: all energy levels on it become negative. From the level $E > 0$ of the anode, the electron tunnels to the level E of the cathode, and then moves to FL E_{Fc} (Fig. 1, lines *4* and *5*). Upon transition from the level E of any of the electrodes, the electron moves to its FL, giving or absorbing a quantum of energy, after which it goes to the power source. This is no longer a wave or ballistic process (like tunneling), but a diffusion process. It occurs on MFP and doesn't obey the law of conservation of energy $|R|^2 + |\widetilde{T}|^2 = 1$. In any case, when one electron jumps from the cathode to the anode, the source performs work eU_a. At $eU_a < E_{Fc}$, reverse tunneling for positive levels at the anode is also possible. Moving to the same cathode level, such an electron on MFP is replaced by an electron from the cathode's FL, moving to its level. Next, the hot electron moves from the cathode to the power source. During such a junction, a quantum of energy is absorbed at the cathode and carried away to the source, i.e., the cathode is cooled down. This is the opposite of the Nottingham effect that occurs for reverse tunnel current. Since the number of reverse tunneling electrons is significantly less than the number of direct tunnel junctions, the overall density of the total anode current J is positive, and the power supply as a whole heats both the cathode and the anode. When high-energy thermal electrons are tunneled, they cool the electrode from which they tunnel, and when they get to another electrode, they heat it, switching to its lower FL. These contributions are generally lower than the tunnel ones. In any case, the power of the source JU_a is spent on heating the electrodes. If there is an energy level on the anode E, then the transmission ratios in both directions also coincide, i.e. the transparency of the barrier is the same and can be calculated as $D(E) = 1 - |R(E)|^2$. If there is no such level (at zero temperature), then $D^-(E) = 0$, $D^+(E) = |\widetilde{T}|^2 = 1 - |R|^2 > 0$. At non-zero temperature $T > 0$, there are always such levels, so it is convenient to consider the same transparencies $D^+ = D^- = D$. In this case, there are jumps in wave resistances (WR) at both the cathode and the anode. Let's determine the normalized WRs as

$$\rho = k_0/k = k_0/\sqrt{2m_e(E-V)}/\hbar.$$

Then at the cathode $\rho = k_0/k_0 = 1$, in the near-cathode region $\rho = 1/\sqrt{1 - E_{Fc}/E}$ imaginary (with energy less than FE), in the near-anode region $\rho_a = 1/\sqrt{1 - E_{Fc}/E + eU_a/E}$ (with the same WF), and at the anode $\rho_a = \rho_0 = 1$.

We will integrate SE using the series method, taking the expansion $\varphi(t) = \alpha_0(1 + \varphi_0(t)) + \alpha_1\varphi_1(t)$ as a power series with coefficients $t^n\alpha_n/n!$:

$$\varphi''(t) = \sum_{n=2}^{\infty} t^{n-2}\frac{\alpha_n}{(n-2)!} = (at^2 + bt + c)\sum_{n=0}^{\infty} t^n \frac{\alpha_n}{n!}. \quad (3)$$

We obtain the solution by equating the coefficients at the same degrees. We have $\alpha_2 = c\alpha_0$, $\alpha_3 = c\alpha_1 + b\alpha_0$, and for $n \geq 4$ we have recurrent relation

$$\alpha_n = (n-2)!(c\alpha_{n-2} + b\alpha_{n-3} + a\alpha_{n-4}).$$

With its use we obtain the following ratios:

$$\alpha_4 = 2!(c\alpha_2 + b\alpha_1 + a\alpha_0) = 2!((c^2 + a)\alpha_0 + b\alpha_1),$$

$$\alpha_5 = 3!(c\alpha_3 + b\alpha_2 + a\alpha_1) = 3!(2bc\alpha_0 + (a + c^2)\alpha_1), \ldots.$$

Thus, the general solution is expressed as

$$\varphi(t) = \alpha_0 + \alpha_0\varphi_0(t) + \alpha_1\varphi_1(t),$$

where

$$\varphi_0(t) = ct^2/2 + bt^3/6 + (c^2 + a)t^4/12 + \ldots,$$

$$\varphi_1(t) = t + ct^3/6 + bt^4/12 + \ldots,$$

besides

$$\varphi_0(0) = \varphi_1(0) = 0, \quad \varphi_0'(0) = 0, \quad \varphi_1'(0) = 1.$$

If we use previous substitution and expansion in $\tau^n\tilde{\alpha}_n/n!$, then the recurrence relations and the type of solution will take the same form:

$$\tilde{a}_n = (n-2)!(\tilde{c}\tilde{\alpha}_{n-2} + \tilde{b}\tilde{\alpha}_{n-3} + a\alpha_{n-4}),$$

$$\phi(\tau) = \tilde{\alpha}_0(1 + \phi_0(\tau)) + \alpha_1\phi_1(\tau)$$

and

$$\phi(\tau) = \tilde{\alpha}_0 + \tilde{\alpha}_0\phi_0(\tau) + \tilde{\alpha}_1\phi_1(\tau),$$

where

$$\phi_0(\tau) = \tilde{c}\tau^2/2 + \tilde{b}\tau^3/6 + (\tilde{c}^2 + a)\tau^4/12 + \ldots,$$

$$\phi_1(\tau) = \tau + \tilde{c}\tau^3/6 + \tilde{b}\tau^4/12 + \ldots.$$

The reflectance and transmission coefficients are determined by imposing boundary conditions on WF and its derivative. The results are given in the Appendix (formulae (P2)−(P5)). Using a finite number of terms in the series, we may approximate the functions and their derivatives $\varphi_0'(1) = c + b/2 + (c^2 + a)/3 + \ldots$, $\varphi_1'(t) = 1 + c/2 + b/3 + \ldots$. Next, from (P4) and (P5) we determine the approximate value of G, linking α_1 and α_0, as well as the coefficient α_0, with $\alpha_1 = ik_0d(2 - \alpha_0)$. Moreover, $\alpha_1 = 2ik_0d/(1 + ik_0dG)$. Then, using the recurrent formula, we calculate all the coefficients α_n, $n+2, 3, \ldots$ up to those numbers when the terms $\alpha_n/n!$ become negligible. Using these coefficients we calculate $\varphi(1)$ and $\varphi'(1)$. We have the following formulae:

$$\widetilde{T} = \varphi(1) = \alpha_0\varphi_0(1) + \alpha_1\varphi_1(1),$$

$$\widetilde{T} = \varphi'(1)/(ik_0d) = [\alpha_0\varphi_0'(1) + \alpha_1\varphi_1'(1)]/(ik_0d),$$
$$R = \alpha_0 - 1.$$

The following discrepancies can be determined from them: (errors):

$$\Delta = \varphi(1) - \varphi'(1)/(ik_od),$$

$$\Delta_1 = \varphi(1) - \alpha_0\varphi_0(1) - \alpha_1\varphi_1(1),$$

$$\Delta_2 = \varphi'(1) - [\alpha_0\varphi_0'(1) + \alpha_1\varphi_0'(1)].$$

Now we may refine the coefficients from the conditions $\Delta_1 = \Delta_2 = 0$, which gives

$$\alpha_1 = \big(\varphi(1) - \alpha_0\varphi_0(1)\big)/\varphi_1(1),$$

$$\alpha_0 = [\varphi'(1)\varphi_1(1) - \varphi(1)\varphi_0'(1)]/(\varphi_0'(1)\varphi_1(1) - \varphi_0'(1)\varphi_0(1)).$$

Continuing the calculations with these coefficients, we determine the errors again, and so on until convergence. The accuracy is determined by the relative error of the solution $\delta_\varphi = |1 - \varphi'(1)/(ik_0d\varphi(1))|$. Since tunneling is a process without energy losses, the residual error $\widetilde{\Delta} = 1 - |R|^2 - |\widetilde{T}|^2 = 0$ shall also turn to zero to provide accurate solution. Accordingly, we have the transparency of the barrier $D = 1 - |R|^2$ or $D = |\widetilde{T}|^2$.

There is an analogy between SE and Helmholtz equation in optics when photons pass (tunnel) through a layer of an ideal dielectric [8]. $k^2 < 0$ stands for the electron tunneling, and negative DP $\varepsilon < 0$ (plasma) stands for the photon tunneling. We have the following consistency of the problems: $\varepsilon = 1 - V/E$. For the photon passing through the final non-absorbing layer, $|R|^2 + |\widetilde{T}|^2 = 1$ is also fulfilled. Both a photon in the layer and an electron in the potential are quasi-particles. Upon entering a dielectric, the velocity of a quasi-photon changes over a short length (on the order of) several atomic layers (offset theorem) due to collective interaction, and upon exiting the layer, it is restored. At $\varepsilon < 0$, the velocity becomes imaginary, as does the velocity of the electron inside the barrier. When passing through the barrier, the electron also retains its momentum and energy. The structure of the diode at large U_a corresponds to the movement of a photon through the junction of regions with $\varepsilon = 1$, $\varepsilon(x) < 0$ and $\varepsilon(d) > 1$. For $d = 0$ we have $1 + R = \bar{T}$, $R = (k_0 - k(d))/(k_0 + k(d))$ and for $\varepsilon \gg 1$ for the photon $R \approx -1$, i.e. it is completely reflected from the dielectric half-space. This is not true for an electron, i.e., the analogy is incomplete: the transition to FL with scattering disrupts the wave process.

The exact solution of the equations may be obtained by direct iteration by taking $\alpha_0^{(0)} = \alpha_0$, $\Delta_0 = \Delta$ and calculating $\alpha_0^{(k+1)} = \alpha_0^{(k)} - \tau_k\Delta_{(k)}$ until convergence $(k = 0, 1, 2, \ldots)$.

Table 1.

n	Coefficients in expansion $\varphi_0(t)$
1	0
2	c
3	b
4	$2!(c^2 + a)$
5	$3!2bc$
6	$4!(ac + 2!(ac + b^2 + c^3))$
7	$5!\lfloor ab + 2!b(c^2 + a) + 2 \cdot 3!bc^2 \rfloor$
8	$6!\lfloor 2!a(c^2 + a) + 3!2b^2c + 4!c(ac + 2!(ac + b^2 + c^3))\rfloor$

At each iteration, $\alpha_1 = ik_0d\big(2 - \alpha_0^{(k+1)}\big)$ should be recalculated to find the residual errors. Here τ_k — iteration parameter (for method of simple iteration all $\tau_k \equiv 1$). One may use the minimum residual error method by selecting τ_k from the minimum residual error condition at each step [11]. To calculate $\Delta_{(k+1)}$ let's determine $\alpha_1^{(k+1)} = ik_0d\big(2 - \alpha_0^{(k+1)}\big)$ and calculate all functions $\varphi_0(1)$, $\varphi_1(1)$, $\varphi_0'(1)$, $\varphi_1'(1)$. Another solution is to take into account a sufficient number of terms in the series when convergence of functions already takes place. Table 1 and 2 provides the first corresponding coefficients. Let's consider a method for numerically calculating coefficients from tables up to any values of n. For this, let's determine the functions

$$f_1(\alpha_1, \alpha_0) = \alpha_1, \quad f_2(\alpha_0, \alpha_1) = \alpha_0 c,$$

$$f_3(\alpha_0, \alpha_1) = \alpha_0 b + \alpha_1 c, \ldots,$$

$$f_n(\alpha_0, \alpha_1) = (n-2)!\big(cf_{n-2}(\alpha_0, \alpha_1) + bf_{n-3}(\alpha_0, \alpha_1) + af_{n-4}(\alpha_0, \alpha_1)\big).$$

Let us calculate all coefficients $\alpha_n = \alpha_n^{(0)} + \alpha_n^{(1)}$ up to the number n, where $\alpha_n^{(0)}$ — coefficients in φ_0, and $\alpha_n^{(1)}$ — coefficients in φ_1. Then, $\alpha_n^{(0)} = f_n(1, 0)$, $\alpha_n^{(1)} = f_n(0, 1)$. Thus, $f_5(1, 0) = 3!2bc$. The disadvantage for vacuum diodes is the need to define a large number of functions, or to use recursive calculations. However, for solid-state diodes with a low effective carrier mass and small d, the introduced coefficients become small, and the use of several coefficients leads to good accuracy, so analytical expressions for their parameters can be obtained.

Let us consider the examples. Let $d = 3$ nm, $E_F = 7$, $eU_a = 7$, $W_c = 2$, $W = 1.823$, $E = 5$ (eV), $\delta = 0.18$, $\alpha = 0.43$ (nm). This is a vacuum diode with copper electrodes. In this case $a = 108.2$, $\tilde{b} = 208$, $\tilde{c} = -38.4$, $b = -4.2$, $c = 18, 5$. Here $c^2 > a$. We see that major contribution to the even coefficients $\alpha_4^{(0)}$, $\alpha_6^{(0)}$, $\alpha_8^{(0)}$ is provided by the terms $2!c^2$, $4!2!c^3$, $6!4!2!c^4$, respectively. The odd coefficients are proportional to the powers of b and significantly less. The major contribution to $\alpha_3^{(1)}$, $\alpha_5^{(1)}$, $\alpha_7^{(1)}$ has the values of c, $3!c^2$, $5!3!c^3$, respectively, and the even coefficients are significantly smaller. For large numbers

Table 2.

n	Coefficients in expansion $\varphi_1(t)$
1	1
2	0
3	c
4	$2b$
5	$3!(a+c^2)$
6	$4!(2!+1)bc$
7	$5!\lfloor ca+2!b^2+3!c(a+c^2)\rfloor$
8	$6!\lfloor 2!ab+3!b(a+c^2)+4!(2!+1)bc^2\rfloor$

at $t=1$, the terms of the series for even n are approximately equal to $(n-2)!!c^{n/2}/n!$, and for odd n, respectively, $(n-2)!!c^{(n-1)/2}/n!$. Since $(n-2)!!=n!/(n-1)!!$, from the condition $(n-2)!!c^{n/2}/n!=1$ we obtain $n\sim 30$, i.e., for convergence it is necessary to take into account a very large number of terms in the series. Now let's $d=1\,\text{nm}$, $E_F=0.6$, $eU_a=1$, $W_c=4.2\,\text{eV}$, $\delta=0.086\,\text{nm}$, $\alpha=0.237\,\text{nm}$, $\widetilde{W}=3.02$, $W=0.53$, $E=0.5$, $E_F=0.6\,(\text{eV})$, $\varepsilon=5.7$ (the diode made of envelopes of n-InSb with the concentration of electrons $10^{24}\,\text{m}^{-3}$ and effective mass 0.013 m_e on a film of CVD-diamond). We have $a=0.0455$, $\tilde{b}=0.043$, $\tilde{c}=-0.0042$, $b=-0.024$, $c=-0.021$. In this case, all the terms are very small, and it is enough to take several (about 3−5) terms. In this case, we get very accurate analytical solutions. It follows from this that in order to obtain well-convergent expressions, the value d and the reduced mass shall be small. All dimensionless constants have the form of squares of size d multiplied by certain values of WN type associated with various combinations of energies. WN corresponds to certain wavelengths such as de Broglie waves for the corresponding energies. The constants are of the order of one if the corresponding wavelengths are d. The conditions when they are all modulo less than one have the form: $|c|<1$, if $E<E_F$ and $d<\hbar/\sqrt{m_eE_F/2}$, or $d<\hbar/\sqrt{m_eE/2}$ at $E>E_F$; $|b|<1$, if $eU_a>8W$ and $d<\hbar/(4\sqrt{m_eeU_a})$, or $d<\hbar/(\sqrt{m_eW/8})$ at $eU_a<8W$; $a<1$, if $d<\hbar/\sqrt{m_eW/2}$. Let us define

$$d_0=\min\big(\hbar/\sqrt{m_eW/2},\,\hbar/(4\sqrt{m_eeU_a}),\,\hbar/\sqrt{m_eE/2},\,\hbar/\sqrt{m_eE_F/2}\big).$$

Further, m_e will stand for the effective mass. If we consider the size of the diode $d=d_0$, then it is quite possible to limit ourselves to the eight terms given in the tables. As can be seen, all of them give decreasing contributions, each of which is less than one modulo. Moreover, these contributions can be alternating. Obviously, for such a diode, it is possible to associate all the dimensionless amplitudes $1+R$ and $ik_0d_0(1-R)$ on the left with the amplitudes $\widetilde{T}$ and $(ik_0d_0)\widetilde{T}$on the right with the transfer matrix $\hat{a}(d_0,E)$ in the form

$$\begin{pmatrix}1+R\\ ik_0d_0(1-R)\end{pmatrix}=\begin{bmatrix}a_{11}(d_0,E) & a_{12}(d_0,E)\\ a_{21}(d_0,E) & a_{11}(d_0,E)\end{bmatrix}\begin{pmatrix}\widetilde{T}\\ ik_ad_0\widetilde{T}\end{pmatrix}. \quad (4)$$

Since at $d=0$ (or $t=0$) $1+R=\widetilde{T}$ and $Y=k_a/k_0$ is true, then, it is necessary $a_{11}(d_0,E)=\varphi(1)$, $a_{11}(0,E)=\varphi(0)=\alpha_0=2k_0/(k_a+k_0)$. The other two parameters we find from the conditions

$$G=(a_{21}+ik_ad_0a_{11})/(a_{11}+ik_ad_0a_{12})$$

and

$$\widetilde{T}=2/[a_{11}+ik_ad_0a_{12}+(a_{21}+ik_ad_0a_{11})/(ik_0d_0)],$$

comparing them with (P4) and (P2). As a result, we obtain

$$a_{12}=\frac{1}{(ik_0d_0)[(1+\varphi_0(1))+(ik_0d_0)Y\varphi_1(1)]}-\frac{\varphi(1)}{ik_ad_0}, \quad (5)$$

$$a_{21}=(G-ik_ad_0)\varphi(1)+ik_ad_0a_{12}G. \quad (6)$$

Dividing the segment $(0,d)$ into n parts with dimensions $d_0=d/n$, we obtain coefficients a_n, b_n, c_n for the parabolic approximation of the potential $V(x)$ on these segments. The complete diode transfer matrix is the product of n matrices of the segments. In case of a triode, i.e., the presence of a grid d_g in size and grid voltage U_g instead of the anode, as well as the presence of a grid −anode area d_a in size, the complete triode matrix (transistor) is the product of three transfer matrices: cathode−grid matrix, transfer matrix grid and transfer matrix grid−anode. When constructing the first matrix, it is required to replace $U_a\to U_g$. When constructing the third matrix, it is required to replace $U_a\to U_a-U_g$ and $d\to d_a$. The second matrix in the grid area is associated with WF $\psi(x)=A^+\exp\big(ik_g(x-d)\big)+A^-\exp\Big(-ik_g(x-d)\Big)$ and has the form

$$\hat{a}(d_g,E)=\begin{bmatrix}\cos(\theta) & -i\rho\sin(\theta)\\ -i\rho^{-1}\sin(\theta) & \cos(\theta)\end{bmatrix}, \quad (7)$$

$\theta=k_gd_g$, $k_g=d_g\sqrt{2m_e(E-E_F+eU_g)}/\hbar$, $\rho=1/(k_gd_g)$.

3. Solution of SE. Approximation by a fourth-order parabola

This is the case $s=4$ in formula (1). Here it is more convenient to replace $\tau=2x/d-1$, $\phi(\tau)=\psi\Big(d(\tau+1)/2\Big)$, since replacing $t=x/d$ leads to a more complex recurrent formula with five terms. We have SE

$$\phi''(\tau)=(a\tau^4+b\tau+c)\phi(\tau),$$

where

$$a=d^2m_eW/(2\hbar^2),\quad b=d^2m_eeU_a/(4\hbar^2),$$

$$c = d^2 m_e(E - E_F - W + eU_a/2)/(2\hbar^2).$$

Now the recurrent formula takes the form

$$\alpha_n = (n-2)!(c\alpha_{n-2} + b\alpha_{n-3} + a\alpha_{n-6}).$$

According to this formula, the first several coefficients are expressed as:

$$\alpha_2 = c\alpha_0, \quad \alpha_3 = c\alpha_1 + b\alpha_0,$$

$$\alpha_4 = 2(c^2\alpha_0 + b\alpha_1), \quad \alpha_5 = 6(c^2\alpha_1 + 2cb\alpha_0),$$

$$\alpha_6 = 24\big((c^2 + a)\alpha_0 + b\alpha_1\big).$$

The boundary conditions lead to the relations (P6)–(P8) of the Appendix. They allow you to determine unknown coefficients:

$$\widetilde{G} = \frac{\phi_0'(1) - ik_0 d\phi_0(1)}{ik_0 d\phi_1(1) - \phi_1'(1)}, \tag{8}$$

$$\alpha_0 = \frac{2ik_0 d}{[ik_0 d\phi_0(-1) + \phi_0'(-1)] + G[ik_0 d\phi_1(-1) + \phi_1'(-1)]}, \tag{9}$$

wherein $\alpha_1 = \widetilde{G}\alpha_0$. In addition, these relations give two residual errors $\Delta_1 = 2 - \phi(-1) - \phi'(-1)/ik_0 d$ and $\Delta_2 = \phi(1) - \phi'(1)/ik_a d$. If the task is solved quite precisely, then $\Delta_1 \approx 0$, $\Delta_2 \approx 0$. It is convenient to use relative residual errors. $\delta_1 = |1 + \phi'(-1)/(ik_0 d\phi(-1))|$, $\delta_2 |1 - \phi'(1)/(ik_0 d\phi(1))|$. Further on, we have:

$$2R = \phi(-1) - \frac{\phi'(-1)}{ik_0 d} \approx \alpha_0\left[\phi_0(-1) - \frac{\phi_0'(-1)}{ik_0 d}\right] + \alpha_1\left[\phi_1(-1) - \frac{\phi_1'(-1)}{ik_0 d}\right], \tag{10}$$

$$2\widetilde{T} = \phi(1) + \frac{\phi'(1)}{ik_0 d} \approx \alpha_0\left[\phi_0(1) + \frac{\phi_0'(1)}{ik_0 d}\right] + \alpha_1\left[\phi_1(1) + \frac{\phi_1'(1)}{ik_0 d}\right]. \tag{11}$$

The reflectance and transmission coefficients are determined from these equations. Also, when substituting the coefficients found, these equations give two more residual errors:

$$\Delta_3 = 2 - \Delta_1 - \alpha_0\left[\phi_0(-1) - \frac{\phi_0'(-1)}{ik_0 d}\right] - \alpha_1\left[\phi_1(-1) - \frac{\phi_1'(-1)}{ik_0 d}\right], \tag{12}$$

$$\Delta_4 = \Delta_2 - \alpha_0\left[\phi_0(1) + \frac{\phi_0'(1)}{ik_0 d}\right] - \alpha_1\left[\phi_1(1) + \frac{\phi_1'(1)}{ik_0 d}\right]. \tag{13}$$

By substituting $\alpha_1 = \widetilde{G}\alpha_0$ in them it allows excluding the coefficients and get another one residual error.

$$\Delta = \frac{\Delta_2 - \Delta_4}{2 - \Delta_1 - \Delta_3} - \frac{ik_0 d\phi_0(1) + \phi_0'(1) + \widetilde{G}[ik_0 d\phi_1(1) + \phi_1'(1)]}{ik_0 d\phi_0(-1) - \phi_0'(-1) + \widetilde{G}[ik_0 d\phi_1(-1) - \phi_1'(-1)]}. \tag{14}$$

On the other hand, by imposing the conditions $\Delta_3 = \Delta_4 = 0$, we get two refinements

$$\alpha_1 = \frac{ik_0 d\Delta_2 - \alpha_0[ik_0 d\phi_0(1) + \phi_0'(1)]}{ik_0 d\phi_1(1) + \phi_1'(1)}, \tag{15}$$

$$\alpha_0 = \frac{ik_0 d[(2 - \Delta_1)(ik_0 d\phi_1(1) + \phi_1'(1)) - \Delta_2(ik_0 d\phi_1(-1) - \phi_1'(-1))]}{[ik_0 d\phi_0(-1) - \phi_0'(-1)][ik_0 d\phi_1(1) + \phi_1'(1)] - [ik_0 d\phi_0(1) + \phi_0'(1)][ik_0 d\phi_1(-1) - \phi_1'(-1)]}. \tag{16}$$

It should be noted that these refinements are determined by the residual errors Δ_1 and Δ_2 obtained by calculating the functions ϕ and ϕ' with any number of coefficients determined iteratively. Thus, SE solution algorithm may include the following. Let's determine α_0 by formula (P5) or (9) and $\alpha_1 = \widetilde{G}\alpha_0$. Iteratively we calculate the coefficients $\alpha_n = (n-2)!(c\alpha_{n-2} + b\alpha_{n-3} + a\alpha_{n-6})$ to the number when $|\alpha_n/n!|$ becomes less than the specified error. Let's calculate four values $\phi(\pm 1)$, $\phi'(\pm 1)$. We find Δ_1 and Δ_2. We determine new coefficients (16) and (15), as well as corresponding solution errors. If the errors are still significant, we calculate the values $\phi(\pm 1)$, $\phi'(\pm 1)$ again until convergence. Thus, we have $\widetilde{T}(E, U_a) = \phi(1) = \alpha_0 + \alpha_1 + \alpha_2/2! + \ldots \alpha_n/n!$. If all coefficients do not exceed modulo one, as above, it is possible to limit ourselves to several terms, i.e., to obtain an explicit form of transparency $D(E, U_a)$. The explicit form of this function is the sum of the relations of the polynomials with respect to E and U_a. Also the transfer matrix may be constructed.

4. Solution of integral equation

SE $\varphi''(t) = (at^2 + bt + c)\varphi(t)$ corresponds to IE

$$\varphi(t) = \varphi(0) + ik_0(2 - \varphi(0))t + \int_0^t\int_0^{t''}(at'^2 + bt' + c)\varphi(t')dt'dt'', \tag{17}$$

provided $\varphi(0) = 1 + R$,

$$\widetilde{T} = \varphi(0) + ik_0(1 - R) + \int_0^1\int_0^{t''}(at'^2 + bt' + c)\varphi(t')dt'dt'',$$

$$\widetilde{T} = 1 - R + \frac{1}{ik_0}\int_9^1(at'^2 + bt' + c)\varphi(t')dt'.$$

From this we find

$$\widetilde{T} = 1 + ik_0(1 - \varphi(0)) + \frac{1}{2ik_0}\int_0^1(at'^2 + bt' + c)\varphi(t')dt' + \frac{1}{2}\int_0^1\int_0^{t''}(at'^2 + bt' + c)\varphi(t')dt'dt'',$$

$$R=\frac{k_0^2+\int\limits_0^1(at'^2+bt'+c)\varphi(t')dt'-\\ -ik_0\int\limits_0^1\int\limits_0^{t''}(at'^2+bt'+c)\varphi(t')dt'}{ik_0(2-ik_0)}.$$

Taking the linear zero approximation $\varphi_{(0)}(t)=\varphi(0)+ik_0(2-\varphi(0))t$, in the first Born approximation we have WF in the form

$$\varphi(t)=\varphi(0)+ik_0(2-\varphi(0))t+\int\limits_0^t\int\limits_0^{t''}(at'^2+bt'+c)$$

$$\times[\varphi(0)+ik_0(2-\varphi(0))t']dt'dt'',$$

$$\varphi^{(1)}(t)=\varphi(0)+ik_0(2-\varphi(0))t+\varphi(0)(at^4/12+bt^3/6$$

$$+ct^2/2)+ik_0(2-\varphi(0))(at^5/20+bt^4/12+ct^3/6),$$

$$\varphi^{(1)}(1)=\varphi(0)+ik_0(2-\varphi(0))+\varphi(0)(a/12+b/6+c/2)$$

$$+ik_0(2-\varphi(0))(a/20+b/12+c/6),$$

$$\varphi^{(1)}=\frac{1+a/4+b/3+c/2-ik_0(1+a/20+b/12+c/6)}{1-ik_0(1+a/20+b/12+c/6)/2}. \quad (18)$$

From here we find that

$$\widetilde{T}=\varphi_{(1)}(1),\quad ik_0\widetilde{T}=\varphi'_{(1)}(1),\quad ik_0=\varphi'_{(1)}(1)/\varphi_{(1)}(1)$$

and

$$\varphi(0)=\frac{1+a/4+b/3+c/2-ik_0(1+a/20+b/12+c/6)}{1-ik_0(1+a/20+b/12+c/6)/2}. \quad (19)$$

The ratio (27) allows to determine the reflectance coefficient

$$R\approx\frac{a/2+2b/3+c-ik_0(1+a/20+b/12+c/6)}{2-ik_0(1+a/20+b/12+c/6)}. \quad (20)$$

It should be noted that for the function $\varphi^{(0)}(t)$ we get $R=0$. Substituting the function (18) into the IE (17), we obtain a more accurate approximation of $\varphi_{(2)}(t)$, which allows us to obtain a more accurate value of R. Such solution has good accuracy at small d. Another way to solve IE (17) may be to use quadrature formulas to calculate the integrals. This leads to a system of linear algebraic equations for determining the values of WF at specified points. This method doesn't require small d.

5. Current-voltage curves of diodes

The barrier profiles shown in Fig. 1 are obtained using the formula (P1) and are very close to the parabolic approximation (1) for $s=4$. Let the electrode materials be the same. The second-order parabola approximation is more suitable for small d. Figure 2 shows transparency D, calculated by numerically solving the SE by the wave impedance transformation method. Next, they are used to calculate the current density (Fig. 3), determined for thermal field emission in the form of $J(U_a,T_c,T_a)=J^+(U_a,T_c)-J^-(U_a,T_a)$

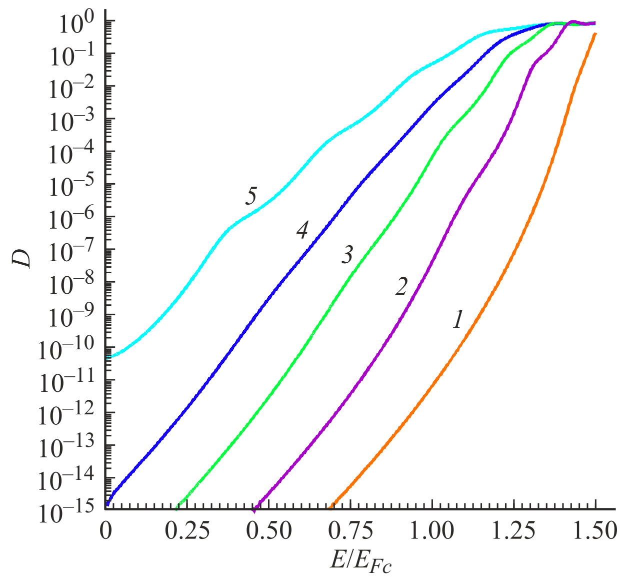

Figure 2. Transparency of vacuum diode barrier $d=2$ nm versus E/E_{Fc} under various voltages U_a, V: 1 (curve *1*), 4 (curve *2*), 7 (curve *3*), 10 (curve *4*), 15 (curve *5*).

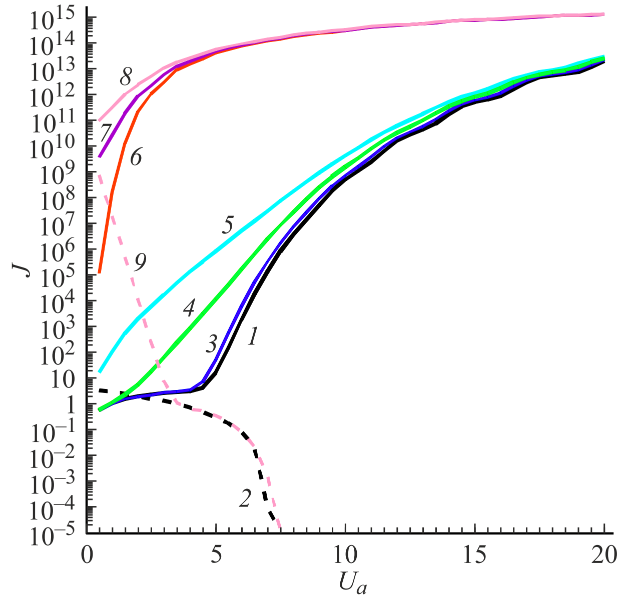

Figure 3. Current-voltage curve of the vacuum diode [Am^{-2}/V] with a length of $d=2$ nm (curves *1–5*) and the same diode with filling by CVD-diamond (curves *7–9*) at different temperatures [K]: $T_c=T_a=300$ (curves *1, 2, 6*), $T_c=T_a=800$ (curves *3, 7*), $T_c=1500$, $T_a=300$ (curve *4*), $T_c=T_a=1200$ (curves *5, 8, 9*). The dashed curves *2* and *9* show the inverse current densities for curves *1* and *8*, respectively. $E_{Fc}=E_{Fa}=7$, $W_c=W_a=4.36$ eV.

by integrals

$$J^{\pm}(U_a, T_{\pm}) = \frac{em_e}{2\pi^2\hbar^3} \int_0^{3E_F} D(E, U_a) f^{\pm}(E, T_{\pm}) dE. \quad (21)$$

Here

$$f^{\pm}(E, T_{\pm}) = k_B T_{\pm} \ln\big(1 + \exp((\mu_{\pm} - E)/(k_B T_{\pm}))\big),$$

$$\mu_+ = \mu_c = E_{Fc}, \quad \mu_- = \mu_a = E_F - eU_a$$

—electrochemical potentials, and instead of an infinite limit, the limit $3E_F$ is taken. This is more than sufficient to account for thermionic emission at the cathode temperature $T_c \sim 2000$ K. It's quite sufficient to use upper limit $2E_F$, since at $k_B T_c \sim 0.2$ eV the logarithm may be replaced by a small exponent and at $D(E, U_a) \approx 1$ for the remainder integral at $E_F = 7$ eV we'll obtain the value $1.26 \cdot 10^{-16}$. At zero temperatures $f^{\pm}(E, T_{\pm}) = (\mu_{\pm} - E)$. The density of current (21) is positive and determines the anodic current, although the negatively charged electrons from the cathode ($e > 0$) are tunneling. At $T_a = 0$ we have $D^-(E, U_a) = 0$ for $E > \mu_a$. The number of reverse electrons from the anode is proportionate to $f^-(E, T_a)$, i.e. significantly less than on the cathode. At low temperature this number is proportional to $E_F - eU_a - E$ whereas on the cathode it is proportional to $E_F - E$. The electron density near the bottom of the conduction band is maximum, therefore the value of $E_F - eU_a - E$determines higher energy levels relative to the conduction band bottom of the anode than $E_F - E$ relative to the same bottom of the cathode. At $eU_a = E_F$ and $T = 0$, there are no positive-energy electrons on the anode that could tunnel to the cathode (all existing levels are negative), $D^- = 0$, and there is no reverse current. When tunneling in a diode at low anode voltages or with a highly heated anode, the flow of electrons from it can be significant.

The analytical current-voltage curve of the diode is of interest. Considering the reverse current (tunneling from the anode), for it we get

$$J(U_a, T) = \frac{em_e}{2\pi^2\hbar^3} \int_0^{3E_F} D(E, U_a)[f^+(E, T) - f^-(E, T)] dE. \quad (22)$$

For simplicity we suggested that the temperatures of cathode and anode are the same are designated as T. Further we consider the temperature as high, i.e. $k_B T < 0.1$ eV. In this case, all the characteristic potentials and energies are significantly higher $k_B T$, the thermal current shall be taken into account, but it is small. At $T = 0$ the tunneling from the anode may occur only at $U_a < E_F/e$. At higher voltage, only a small thermal current is possible. The result of integration (22) is expressed as

$$J_3(U_a, T) = J_1(U_a, T) + J_2(U_a, T) + J_3(U_a, T), \quad (23)$$

where $J_1(U_a, T_c) = J_{11}(U_a) + J_{12}(U_a, T)$. The integrals are calculated in the Appendix (formulae (P9)–(P16)). The general view of the current-voltage curve (23) is not difficult to obtain at different temperatures of the cathode and anode.

Let's consider current-voltage curve (22) at zero temperature. At $U_a = 0$ from this it follows $J(O, t) = J(0, 0) = 0$. The current starts to rise with the growth of voltage. At low voltages, electrons from the levels at the cathode $E_F - eU_a < E < E_F$ contribute to the current, since these levels are absent at the anode. At lower levels, there is mutual tunneling, but the difference in density of states at the cathode $E_F - E$ and at the anode $E_F - eU_a - E$ begins to have impact. At $eU_a = E_F$, tunneling from the anode is impossible (all its energy levels are negative), and all electrons from the conduction band of the cathode can tunnel. At $eU_a > E_F$, the current continues to rise as the barrier narrows. At $eU_a \gg E_F$, the barrier turns into a linear bevel to the anode. At the same time, if d is small, then the problem can be approximately considered as the scattering of a wave $\psi(x) = \exp(ik_0 x) + R\exp(-ik_0 x)$ on a step. If no WF $\psi(x) = \widetilde{T}\exp(ik_0 x)$ is taken for it $1 + R = \widetilde{T}$, $R = 0$, i.e. the step is not scattering. If WF $\psi(x) = \widetilde{T}\exp(ik_0 x)$ is taken then $Y = k_a/k_0$, $R = (k_0 - k_a)/(k_0 + k_a)$. In this case at large voltage k_a — large value, and $R \approx -1$. Obviously, the latter option should be discarded, although there are analogues of wave diffraction in optics for it. The use of very strong fields theoretically leads to a value of $D = 1$ and to saturation of J. Theoretically possible limit is $J_{\max} = em_e E_F^2/(4\pi^2\hbar^3)$. It means tunneling all incoming electrons and is not achievable due to quantum properties, limitations related to spatial charge and temperature instability. Even at voltages $U_a = E_F/e$ and $d = 10$ nm we obtain the fields of 10^9 V/m. Further increase may lead to explosive emissions and is impractical. At an arbitrary temperature, all electrons with positive energies can tunnel, but the probability of tunneling is determined not only by transparency, but also by logarithmic dependencies in (22).

For small d and small coefficients a, b, c integrals (P11)–(P14) can be calculated using explicit expressions for $D(E, U_a)$ in the diode, while the integral function has the form of the ratio of polynomials in E and U_a or the ratio of polynomials multiplied by the exponent. To a first approximation, the ratio of polynomials can be replaced by a polynomial or even a linear term. For a fourth-order parabola approximation with small d and small coefficients in the first order in d^2, we have (see Appendix, formulas (P17)–(P19)):

$$J_1(U_a, T) = \frac{4em_e}{\pi^2\hbar^3}\left(1 + \frac{b}{12} - \frac{a}{15}\right)\Bigg\{g_1\bigg[f_{11}(E_F, T) - \frac{k_c}{k_a}k_B T \times \exp\left(-\frac{eU_a - E_F}{k_B T}\right) f_{12}(E_F, T)\bigg] - \frac{4d^2 m_e g_2}{15\hbar^2}\Big[(14W - 2E_F - eU_a) f_{13}(E_F, T) + f_{14}(E_F, T)\Big] + \frac{4d^2 m_e g_2}{15\hbar^2} k_B T \times \exp\left(-\frac{eU_a - E_F}{k_B T}\right)\Big[(14W - 2E_F - eU_a) f_{15}(E_F, T) + f_{16}(E_F, T)\Big]\Bigg\}. \quad (24)$$

The integrals (P9) and (P10) are found in a similar way. Since their calculation is not fundamentally different from the one carried out above, we do not give it here. Thus, the current-voltage curve was plotted. It has different representations depending on the relations between U_a, E_F, $k_B T$ and is described by functions of these values. A slightly more complex relationship can be constructed at different electrode temperatures.

Results and conclusions

The results of the current-voltage curve calculation using formula (22) for a vacuum diode at different electrode temperatures are shown in Fig. 3. The reverse and full current densities are also shown there. The current densities considered are such that the spatial charge can be neglected. If the current has large density (e.g., in RTS) the density of the spatial charge shall be taken into account. Within the framework of the considered approach, it can be found as

$$\rho_e(x) = \int_0^{3E_F} A^+(E) D^+(U_a, E) |\psi(x, E)|^2 dE$$

where $\psi(x, E)$ — the WF found above as a solution for SE, while the amplitude is expressed as

$$A^+(E) = m_e k_B T_c \ln\left(1 + \exp\left((\mu_c - E)/(k_B T_c)\right)\right)/(2\pi^2\hbar^3).$$

We limited ourselves to the electrons emitted by the cathode. In the general case, both emission streams should be considered. The maximum electron density will be near the cathode. It limits the escape of electrons and the current, which is equivalent to an increase in the work function W. This increase and the additional potential can be determined from the Poisson equation and added to (1). For a flat diode, it is solved analytically, for example, using the method of series in jcite4, so one may immediately adjust the parameters of the quantum potential and transparency. This is the advantage of an analytical solution. Fig. 4 shows a comparison of the results of cold emission from a diode using formula (22) at $T = 0$ with FN formula (formula (6.23) from [8]). The work function was taken as 4 eV. The results are also shown there without taking into account the Nordheim correction factor in the exponent. In this case, the electric field included in the formula was found as U_a/d. Since the results of FN have been widely compared with the experiment (see [7–9]), the calculations are consistent with them in terms of quality. It should be borne in mind that FN formula is determined up to a pre-exponential factor in the transparency of the barrier [10], and that experimental data for nanostructures are not available.

In conclusion, the following should be stressed. The above SE integration formulas work well at low d, low barriers and voltages, when there is good convergence and iterative methods do not need to be used. In this case, the parabolic approximation is significantly more efficient than the piecewise constant. The use of transfer matrices in parabolic approximation greatly reduces their number compared to piecewise constant approximation, where the required number is up to several hundred. In diode structures at small anode voltages, tunneling in both directions must be taken into account. The diode nanostructures with high current densities should be made using good dielectrics with high thermal conductivity such as diamond and BeO. This leads to a significant decrease in barrier and operating voltages, and an increase in current and higher stability to heating. In the general case, the formula (22) and numerical methods of SE integration should be used. The considered approach can be extended to both triode structures and RTS with quantum wells. However, for them, the relations become even more complex, which makes direct numerical modeling simpler. For modern computers, the counting time and the volume of the algorithm are not significant values in comparison with the accuracy of the model. Therefore, obtaining any approximations for the integral (22) can only make sense for clarity: how different parameters (anode voltage, temperature, electrode and dielectric properties) affect the anode current. If a sufficiently accurate nonlinear CVC is obtained for a nanoscale diode (which is possible with small sizes), then this allows us to simulate its inclusion in the circuit in the time domain, and then the counting time is reduced by orders of magnitude.

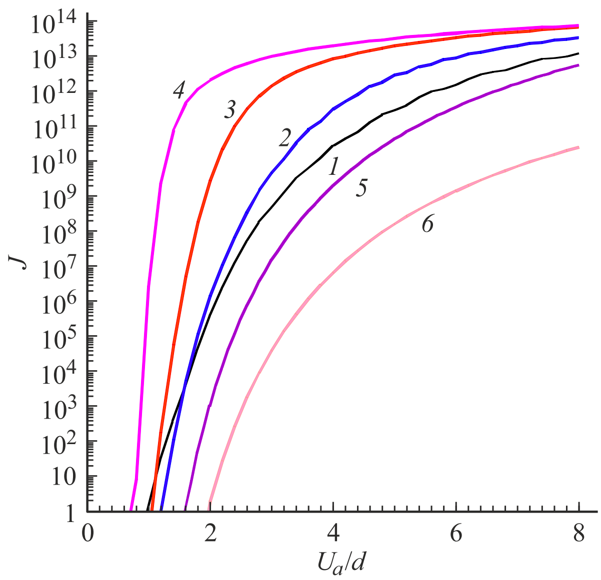

Figure 4. Density of tunnel current [A/m^2] from cathode by formula (22) at $T = 0$ for $d = 3$ nm (curve *1*), $d = 5$ nm (curve *2*), $d = 10$ nm (curve *3*) and $d = 20$ nm (curve *4*) depending on the density of electrical field [V/nm]. Curve *4* — calculated using FN formula, curve *5* — calculated by FN formula neglecting the correction multiplier.

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Conflict of interest

The author declares that he has no conflict of interest.

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Appendix

The potential obtained by the imaging method has the form [1–4]:

$$V(x)=E_{Fc}+\frac{W_c}{\varepsilon}-\frac{W_c}{\varepsilon}\delta_c\left\{\frac{1}{x+\delta_c}+\frac{2x^2}{d(d-x+\delta_a)(d+x)}+\frac{2x^2}{d^3}\sum_{n=2}^{\infty}\frac{1}{(n^2-(x/d)^2)n}\right\}-\frac{eU_a x}{d}. \tag{A1}$$

Here d — cathode–anode distance, ε — DP of the cathode–anode space, parameters $\delta_{c,a}$ are associated with the WF from the material of cathode $W_c = e^2/(16\pi\varepsilon_0\delta_c)$ and with the WF from the material of anode $W_a = e^2/(16\pi\varepsilon_0\delta_a)$. These parameters are entered based on experimental data. For $W_c = 4\,\text{eV}$ and $d = 10\,\text{nm}$ we have $\delta_c/d = 0.009$. On the cathode $V(0) = E_{Fc}$, on the anode $V(d) = E_{Fc} + (W_c - W_a)/\varepsilon - eU_a + \Delta$, where $\Delta = \delta_c/(d+\delta_c) + 2\delta_c/(3d)$. The error Δ of order $\delta_c/d \sim 1\,\%$ and occurs because in the high order images corresponding to the members of series in (1), the following is true $\delta_c = \delta_a = 0$. Of course, it is possible to achieve the absence of this error. To do this, it is enough to subtract from (1) the small term $\widetilde{\delta} = x\Delta/d$. However, this refinement is redundant. The series in (P1) converges extremely quickly, but convergence can be further increased by subtracting the asymptotic term n^{-3} from the sum and adding the result of the asymptotic summation $\xi(3) = 1.202$ to the sum. In such a sum it is sufficient to take into account two terms. However, this will not be necessary, since the expression (P1) will be approximated by parabolas. If the materials and, respectively, the WF of the cathode and anode match, then all energy levels at the anode are reduced by eU_a. Figure 1 also shows an energy diagram.

From the boundary conditions for SE at $x = d$ we have the equations (P2) and (P3):

$$\widetilde{T} = \varphi(1) = \alpha_0\Big[(1+\varphi_0(1)) + G\varphi_1(1)\Big], \tag{A2}$$

$$ik_0 d\widetilde{T} = \varphi'(1) = \alpha_0\Big[\varphi_0'(1) + G\varphi_1'(1)\Big], \tag{A3}$$

as well as the coupling $\alpha_1 = G\alpha_0$, where G is expressed by the equation (P4):

$$G = \frac{\varphi_0'(1) - ik_0 d(1+\varphi_0(1))}{ik_0 d\varphi_1(1) - \varphi_1'(1)} = (ik_0 d)Y. \tag{A4}$$

From these equations, the residual error $\Delta = ik_0 d - \varphi'(1)/\varphi(1)$ follows and the value is found

$$\alpha_0 = \frac{2ik_0 d}{ik_0 d + G} = \frac{2}{1+Y}. \tag{A5}$$

The solution is based on this value.

The boundary conditions in approximation at $s = 4$ result in the equations

$$\begin{gathered}1+R = \phi(-1) = \alpha_0\phi_0(-1) + \alpha_1\phi_1(-1),\\ 1-R = \frac{\phi'(-1)}{ik_0 d} = \frac{\alpha_0\phi_0'(-1)+\alpha_1\phi_1'(-1)}{ik_0 d},\\ \widetilde{T} = \phi(1) = \alpha_0\phi_0(1) + \alpha_1\phi_1(1),\\ \widetilde{T} = \frac{\phi'(1)}{ik_0 d} = \frac{\alpha_0\phi_0'(1)+\alpha_1\phi_1'(1)}{ik_0 d}.\end{gathered} \tag{A6}$$

In them the functions are used

$$\phi_0(\tau) = 1 + \frac{c\tau^2}{2!} + \frac{b\tau^3}{3!} + \frac{2c^2\tau^4}{4!} + \frac{12cb\tau^5}{5!} + \frac{4!(c^2+a)\tau^6}{6!} + \frac{5!(14c^2b+a)\tau^7}{7!} + \frac{6!(4!c^3+(4!+1)ca+3!2cb^2)\tau^8}{8!} + \ldots,$$

$$\phi_1(\tau) = \tau + \frac{c\tau^3}{3!} + \frac{2b\tau^4}{4!} + \frac{6c^2\tau^5}{5!} + \frac{24b\tau^6}{6!} + \frac{5!(2b^2+6c^3)\tau^7}{7!} + \frac{6!(4!cb+3!2bc^2)\tau^8}{8!}\ldots.$$

The derivatives of these functions are of the following form

$$\phi_0'(\tau) = c + b\tau^2/2! + 2c^2\tau^3/3! + \ldots,$$
$$\phi_1'(\tau) = 1 + c\tau^2/2! + 2b\tau^3/3! + \ldots.$$

Excluding, as above, from the relations (P6) R and $\widetilde{T}$, we obtain

$$\alpha_0\left[\phi_0(-1) + \frac{\phi_0'(-1)}{ik_0d}\right] + \alpha_1\left[\phi_1(-1) + \frac{\phi_1'(-1)}{ik_0d}\right] = 2 = \phi(-1) + \frac{\phi'(-1)}{ik_0d}, \tag{A7}$$

$$\alpha_0\left[\phi_0(1) - \frac{\phi_0'(1)}{ik_0d}\right] + \alpha_1\left[\phi_1(1) - \frac{\alpha_1\phi_1'(1)}{ik_ad}\right] = \phi(1) - \frac{\phi'(1)}{ik_ad} = 0. \tag{A8}$$

In the integral (22) let's break the integration into three areas: $E < E_F - k_BT$, $|E_F - E| < k_BT$ and $E > E_F + k_BT$. For the second area assuming that $eU_a \gg k_BT$ and $D(E, U_a) \approx 1$, the contribution in the current density is ($\tilde{e}$ — base of the natural logarithm)

$$J_2(U_a, T) \approx \frac{em_e(k_BT)^2}{2\pi^2\hbar^3}\left[2\ln\left(2 + \tilde{e} - \frac{1}{\tilde{e}}\right) - \exp\left(\frac{-eU_a}{k_BT}\right)\left(\tilde{e} - \frac{1}{\tilde{e}}\right)\right], \tag{A9}$$

since the first logarithm varies from $\ln(1+\tilde{e})$ to $\ln(1+1/\tilde{e})$, i.e. has an average value of $\ln(2+\tilde{e}+1/\tilde{e})/2$, and the second logarithm is approximately equalexp$\big((E_F - eU_a - E)/(k_BT_c)\big)$. This is a slightly overestimated value, since actually $D(E, U_a) < 1$. It can be adjusted by multiplying (P9) by the value $(1 - k_BT)/(1 + k_BT)$. For the third area we also assume that $D(E, U_a) = 1$ and replacing $x = (E_F - E)/(k_BT)$ we have

$$J_3(U_a, T) = \frac{em_e(k_BT)^2}{2\pi^2\hbar^3}\left(\frac{1}{\tilde{e}} - \exp\left(-\frac{2E_F}{k_BT}\right)\right) \times \left[1 - \exp\left(\frac{eU_a}{k_BT}\right)\right]. \tag{A10}$$

Small exponents can be omitted here. This contribution corresponds to the thermo-emission current. The first area corresponds to tunneling. If $eU_a > E_F - E$, then for it

$$J_1(U_a, T) = \frac{em_e}{2\pi^2\hbar^3}\int\limits_0^{E_F - k_BT} D(E, U_a)\left[(E_F - E) - k_BT\exp\left(-\frac{eU_a}{k_BT}\right)\exp\left(-\frac{E_F - E}{k_BT}\right)\right]dE. \tag{A11}$$

If $eU_a < E_F - E$, then the first integration area should be divided into two:

$$0 < E < E_F - eU_a + k_BT$$

and

$$E_F - eU_a + kB_T < E < E_F - k_BT.$$

We obtain two integrals:

$$J_1(U_a, T_c) = J_{11}(U_a) + J_{12}(U_a, T)$$

and

$$J_{11}(U_a) \approx \frac{e^2m_eU_a}{2\pi^2\hbar^3}\int\limits_0^{E_F - eU_a + k_BT} D(E, U_a)dE, \tag{A12}$$

$$J_{12}(U_a, T) = \frac{em_e}{2\pi^2\hbar^3}\int\limits_{E_F - eU_a + k_BT}^{E_F - k_BT} D(E, U_a) \times \left[E_F - E - k_BT\exp\left(\frac{E_F - eU_a}{k_BT}\right)\exp\left(\frac{-E}{k_BT}\right)\right]dE. \tag{A13}$$

Finally, for very small voltages $eU_a < k_BT$, when replacing $x = (E_F - E)/(k_BT)$, we have

$$J_1(U_a, T) = \frac{em_e(k_BT)^2}{2\pi^2\hbar^3}\int\limits_1^{E_F/k_BT} D(x, U_a) \exp(x)\left[1 - \exp\left(-\frac{eU_a}{k_BT}\right)\right]dx. \tag{A14}$$

To calculate the integrals (P10)–(P14), it is necessary to know the explicit dependences of transparency on energy. In case of high voltages, the barrier becomes close to triangular, and for the latter, an approximation takes place [10]:

$$D(E, U_a) \approx \exp\left(-\frac{4d\sqrt{2m_e}}{3\hbar eU_a}(E_F + W - E)^{3/2}\right).$$

This is a very rough formula obtained in WKB approximation with an accuracy of an unknown pre-exponential factor and not for too narrow barriers. At $E \approx E_F + W$ it gives $D(E, U_a) \approx 1$, and at $E > E_F + W$ it stops working. Yet, it may be used to calculate the integral (P11). At high voltages $W \approx 0$, and in this case, when replacing $x = (E_F - E)/(k_BT)$, it is needed to calculate the integral

$$J_1(U_a, T) = \frac{em_e(k_BT)^2}{2\pi^2\hbar^3}\int\limits_1^{E_F/k_BT}\exp\left(-\frac{4(k_BT)^{3/2}d\sqrt{2m_e}}{3\hbar eU_a}x^{3/2}\right) \times \left[x - \frac{k_c}{k_a}\exp\left(-\frac{eU_a}{k_BT}\right)\exp(x)\right]dx.$$

Denoting $g = 4(k_BT)^{3/2}d\sqrt{2m_e}/(3\hbar eU_a)$, we divide it into two, and for the first integral, replacing $y = x^{3/2}$ and assuming a large upper limit equal to infinity, we obtain

$$I_1(U_a, T) = \int_1^{E_F/k_BT} \exp(-gx^{3/2})x\,dx = (2/3)\int_1^{\infty} \exp(-gy)y^{1/3}dy.$$

This integral is calculated by integration in parts, obtaining the expansion

$$I_1(U_a, T) = \frac{2\exp(-g)}{3}\left[\frac{1}{g} + \frac{1}{3g^2} - \frac{2}{9g^3} + 3\sum_{n=4}^{\infty}\frac{(-1)^n}{(3g)^n}(n+1)!!!\right].$$

Here we denote the triple factorial: $n!!! = n(n-3)!!!$, $0!!! = 1$, $1!!! = 1$, $2!!! = 2$. The second integral after replacing $y = x^{3/2}$ is represented as

$$I_2(E_F, T) = \int_0^{(\frac{E_F}{k_BT}^{3/2} - \frac{E_F}{k_BT})} \frac{\sqrt{E_F/(k_BT)}}{\sqrt{x + eU_a/(k_BT)}}\frac{\exp(-y)}{3\sqrt{x}/2 - 1}dy$$

$$\approx -\sqrt{E_F/(eU_a)} + \frac{2\sqrt{kBT}}{\sqrt{E_F + eU_a}}\exp\left(-(E_F/(k_BT))^{3/2}\right). \quad \text{(A15)}$$

Here we applied partial integration once, removing the remaining integral, since this integral is preceded by a small exponential. The second term with an exponent of (P15) is small and may be removed. For the large upper limit we take $y \approx x^{3/2} = (E_F/k_BT)^{3/2}$. Then, we get

$$J_1(U_a, T) = \frac{em_e(k_BT)^2}{2\pi^2\hbar^3}\left[I_1(U_a, T) - \exp\left(-\frac{eU_a}{k_BT}\right)I_2(E_F, T)\right]. \quad \text{(A16)}$$

When approximating by a fourth-order parabola with small d and small coefficients in the first order with respect to d^2, we have

$$\phi_0(\tau) \approx 1 + c\tau^2/2 + b\tau^3/6 + a\tau^6/30,$$

$$\phi_1(\tau) = \tau + c\tau^3/6 + b\tau^4/12 + b\tau^6/30.$$

Let all the coefficients be small: $a \ll 1$, $b \ll 1$, $|c| \ll 1$ and $k_ad \ll 1$, $k_0d \ll 1$. This is possible for the semiconductor diodes GaAs-Al_xGa_{1-x}AS-GaAs at 77 K and doping of electrodes. For such a diode the low-frequency DP $\varepsilon = 12.9$, FE values, eU_a and W below 1 eV, and for the effective masses less than $0.1m_e$ and $d < 1$ nm we obtain right the needed small coefficients. Next, we consider all values in the first order by coefficients, neglecting the powers d above 2. We have

$$G \approx \frac{ik_0d(1 + c/2 + b/6 + a/30) - (c + b/2 + a/5)}{(1 + c/2 + 8b/15) - ik_0d(1 + c/6 + 2b/15)},$$

or, in a more rough approximation,

$$G \approx 2ik_0d - (c + b/2 + a/5) \approx 2il_0d.$$

Further on, we have:

$$ik_0dY \approx \frac{-c + b/2 - a/5 + G(1 + c/2 - b/3 - b/5)}{1 + c/2 - b/6 + a/30 + G(-1 - c/6 + b/12 + b/30)}.$$

Having taken $G \approx 2ik_0d$, we transform this expression into

$$Y \approx \frac{-c + b/2 - a/5 + 2ik_0d}{ik_0d(1 + c/2 - b/6 + a/30) + 2k_0^2d^2},$$

From where we find

$$|R|^2 \approx \frac{d^2k_0^2(-1 + c/2 - b/6 + a/30)^2 + [2k_0^2d^2 + c - b/2 + a/5]^2}{d^2k_0^2(3 + c/2 - b/6 + a/30)^2 + [2k_0^2d^2 - c + b/2 - a/5]^2}.$$

All coefficients are proportional to d^2, therefore, omitting the terms from d^4, we find

$$D \approx \frac{8(1 + b/12 - a/15)}{9}\left[1 - \frac{2k_0(c/2 - b/6 + a/30)}{3k_0}\right]. \quad \text{(A17)}$$

Here, the round bracket in the numerator does not depend on energy, and the square bracket in our approximation can be replaced by unit. If we replace the parenthesis with one, we get approximate transparency $D \approx 8/9$. Using (P17), we need to integrate with the function

$$D(E, U_a) \approx \frac{8\sqrt{E(E + eU_a - E_F)}}{(\sqrt{E} + 2\sqrt{(E + eU_a - E_F)})^2}.$$

The fraction in brackets in (P17) is represented as

$$\frac{d^2m_e}{30\hbar^2}\sqrt{E}\frac{14W - 2E_F - eU_a + E}{\sqrt{E} + 2\sqrt{(E + eU_a - E_F)}}.$$

It is required to substitute these values in the integrals (P11)–(P14). For an approximate calculation of integrals, consider the second mean value theorem using sub-integral functions $g_{1.2}(E)f(E)$, where $f(E) = \sqrt{E}$, $f(E) = E$, $f(E) = E^2$, $f(E) = E\exp(-E/k_BT_c)$, $f(E) = E^2\exp(-E/k_BT_c)$, and weight functions have the form

$$g_1(E) = \frac{\sqrt{E + eU_a - E_F}}{\left(\sqrt{E} + 2\sqrt{(E + eU_a - E_F)}\right)^2},$$

$$g_2(E) = \frac{\sqrt{E + eU_a - E_F}}{\left(\sqrt{E} + 2\sqrt{(E + eU_a - E_F)}\right)^3}.$$

The change from $g_1(0) = 1/(4\sqrt{eU_a - E_F})$ and $g_2(0) = 1/(8(U_a - E_F))$ to respectively

$$\sqrt{eU_a - k_BT_c}/(\sqrt{E_F} + 2\sqrt{eU_a - k_BT_c})^2$$

and

$$\sqrt{eU_a - k_BT_c}/(\sqrt{E_F} + 2\sqrt{eU_a - k_BT_c})^3$$

with the upper limit. We'll take the values in the middle point $E_F/2$:

$$g_1 = \sqrt{eU_a - E_F/2}/(\sqrt{E_F/2} + 2\sqrt{2eU_a - E_F/2})^2,$$

$$g_2 = \sqrt{eU_a - E_F/2}/(\sqrt{E_F/2} + 2\sqrt{eU_a - E_F/2})^3.$$

Now transparency will take the form

$$D \approx 8\left(1 + \frac{b}{12} - \frac{a}{15}\right)\left[\sqrt{E}g_1 - \frac{4d^2m_eg_2}{15\hbar^2} \times \left((14W - 2E_F - eU_a)E + E^2\right)\right]. \quad \text{(A18)}$$

To calculate integrals with a square root, we replace $x = \sqrt{E}$. In case of (P11) we have integrals

$$\int\limits_0^{\sqrt{E_F - k_BT_c}} 2x^2(E_F - x^2)dx = \frac{2(E_F - k_BT_c)^{3/2}(6k_BT_c - E_F)}{15} = f_{11}(E_F, T_c),$$

$$\int\limits_0^{\sqrt{E_F - k_BT_c}} 2x^2 \exp\left(-\frac{x^2}{k_BT_c}dx\right) = -k_BT_c\sqrt{E_F - k_BT_c} \times \exp\left(1 - \frac{E_F}{k_BT_c}\right) + \frac{\sqrt{\pi}}{2}(k_BT_c)^3\mathrm{erf}\left(\sqrt{E_F/(k_BT_c) - 1}\right) = f_{12}(E_F, T_c). \quad \text{(A19)}$$

The last integral is taken from table and is represented by the formula 1.3.3.8 from [12] through the Gauss error function. If we replace the upper limit with infinity, then for the second integral we get a simple result $\sqrt{\pi}(k_BT_b)^{3/2}/2$. Now we only need to calculate the integrals with linear and quadratic dependencies in D. For the linear term we have two integrals

$$\int\limits_0^{E_F - k_BT_c} (E_F - E)EdE = (E_F - k_BT_c)^2(E_F/6 + k_BT_c/3) = f_{13}(E_F, T_c),$$

$$\int\limits_0^{E_F - k_BT_c} E\exp\left(-\frac{E}{k_BT_c}\right)dE = (k_BT_c)^2 - k_BT_c(E_F - k_BT_c) \times \exp\left(1 - \frac{E_F}{k_BT_c}\right) = f_{14}(E_F, T_c).$$

For the quadratic we have, respectively

$$\int\limits_0^{E_F - k_BT_c} (E_F - E)E^2dE = E_FE^3/3 - E^4/4 = (E_F - k_BT_c)^3 \times (E_F/12 + k_BT_c/4) = f_{15}(E_F, T_c),$$

$$\int\limits_0^{E_F - k_BT_c} E^2\exp\left(-\frac{E}{k_BT_c}\right)dE = -2(k_BT_c)^3 + k_BT_cE_F \times \exp\left(1 - \frac{E_F}{k_BT_c}\right)\left(E_F^2 - 2k_BT_cE_F + 3(k_BT_c)^2\right) = f_{16}(E_F, T_c).$$

By reconstructing the integral (P11), we have formula (24).