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Field emission in nanotubes with the length of several nanometers

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We consider the problem of field emission based on carbon nanotubes (CNT), which length differs from several nanometers up to dozens of nanometers. The particle transmission function is obtained, considering the difference of potentials on the ends of CNT to be $U = 2{-}3.5\,\mathrm{V}$. The value of the emission current is calculated according to the obtained transmission function. We establish the dependence of the Nordheim function on the length of nanoparticles. We consider the limiting transition for the transmission coefficient for field emission from the cathode surface in the absence of nanoparticles on it. Linear dependence of the electrical current envelopes I on the field strength W is obtained.

Keywords: field emission, nanotubes, Nordheim functions.

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In the case of field emission large electric field strengths (about $E = 10^9{-}10^{10}\,\mathrm{V/m}$) are required, which leads to the appearance of strong mechanical stresses. Therefore, in the case of field emission, the needle material must be mechanically strong in order to remain intact. As such mechanically strong materials, one can consider elongated carbines [1–4], two-dimensional structures: nanotubes and nanoribbons [5–7], where the transverse dimensions of elongated carbines can be by three to four orders of magnitude smaller than the longitudinal ones. This leads to small values of the depolarization factor along the nanoparticles (to a high aspect ratio — the ratio of the length L to the nanotube diameter $2R$), which in turn leads to the fact that the electric field near the tip of carbon nanotubes (CNTs) by $\beta \approx L/(2R)$ times exceed the mean value of the field [8]. When studying field emission, bundles of single-walled CNTs [9,10] are used. Modern theories of field electron emission originate in the study of Fowler and Nordheim (FN) 1928 [11,12]. Today, the FN theory is described by a whole family of different forms of the Fowler–Nordheim [13] equations.

In this paper, based on the electron transmission function obtained on the basis of theoretical results and the results of numerical calculations, we calculated the current through a single CNT with a metallic type of conductivity (corresponding to the case of loosely packed CNTs). A linear dependence of the current I on the field strength W, as well as a linear dependence of the envelopes of the function I/W^2 on the inverse value of the field strength $1/W$ are established.

To determine the current during field emission from the tip of nanoparticles, based on the Landauer formula, it is necessary to know the functions of particle passage from the anode to the cathode. The transmission function was obtained on the basis of theoretical results (Fig. 1, *a*) and the results of numerical calculations (Fig. 1, *b*) under the assumption that a nanotube of length L_1 is on the surface of a metal cathode with a Fermi level $U = U_1 = E_F$ (for more details see [14]). In the calculations shown in Fig. 1, the solid curves correspond to CNTs of length $L_1 = 3.5$ (*1*), 3.0 (*2*), 2.5 (*3*), 2.0 nm (*4*) at field strength $W = 10^9\,\mathrm{V/m}$; dashed curves correspond to CNTs of length $L_1 = 7$ (5), 6 (*6*), 5 (*7*), 4 nm (*8*) at field strength $W = 0.5 \cdot 10^9\,\mathrm{V/m}$; dotted curves correspond to CNTs of length $L_1 = 14$ (*9*), 12 (*10*), 10 (*11*), 8 nm (*12*) at field strength of $W = 0.25 \cdot 10^9\,\mathrm{V/m}$ (the voltages at the ends of the nanotubes were equal to $U = WL_1 = 3.5$, 3.0, 2.5, 2.0 V). When changing the length of nanotubes in the interval $2 \leqslant L_1 \leqslant 14\,\mathrm{nm}$, the aspect number in the case of nanotubes $(m, 0)$ of the „zigzag“type, where $m = 7$, will lie in the interval $3.65 \leqslant \beta \leqslant 25.5$. Neglecting the presence of mirror image forces, we assume that the potential energy $U(z)$ in the presence of electric field $W \neq 0$ in the region $z \geqslant L_1$ will have the form $U_{ext} = -|e|Wz$, and inside the nanotube $(0 \leqslant z \leqslant L_1)$ the potential energy (inside the shallow potential well) is approximated by a rectangular shape (for more details see [14])

$$U(z) = \begin{cases} U_1, & z < 0, \\ U_{2a}, & 0 \leqslant z \leqslant L_1, \\ -|e|Wz, & z > L_1. \end{cases} \qquad (1)$$

It was assumed in the calculations that $U_1 = -4\,\mathrm{eV}$, $U_2 = -6.4\,\mathrm{eV}$. Based on the potential (1), we write the solution of the Schr'dinger equation

$$\psi(z) = \begin{cases} A_1 e^{ik_1 z} + B_1 e^{-ik_1 z}, & z < 0, \\ A_2 e^{ik_2 z} + B_2 e^{-ik_2 z}, & 0 \leqslant z \leqslant L_1, \\ C\chi(z), & z \geqslant L_1, \end{cases} \qquad (2)$$

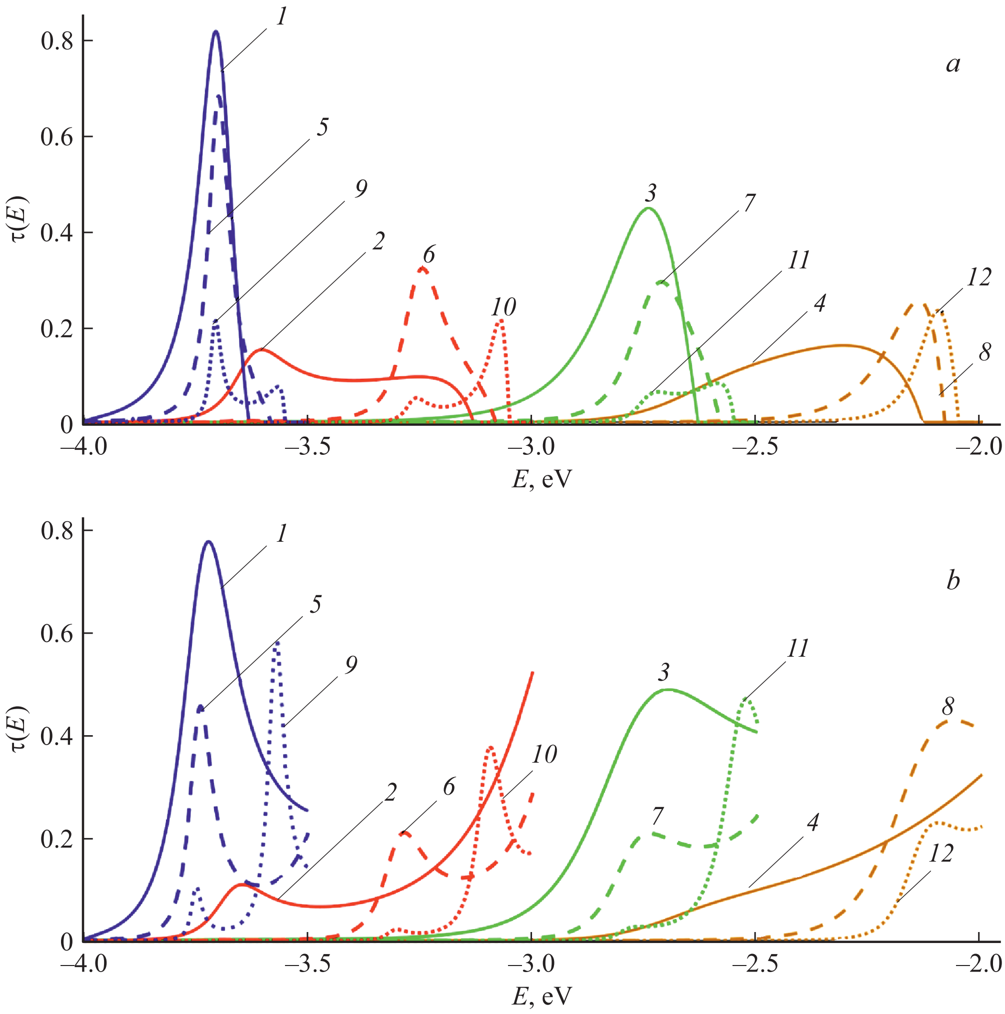

Figure 1. Transmission function vs. electron energy E.

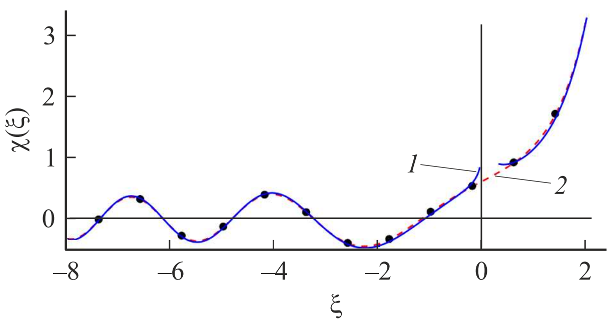

Figure 2. Airy function χ vs. variable ξ.

where $k_1 = \sqrt{2m|E - U_1|}/\hbar$, $k_2 = \sqrt{2m|E - U_{2a}|}/\hbar$. The Airy function $\chi(z)$ is a solution to the equation $\partial^2\psi/\partial\xi^2 - \xi\psi = 0$, where $\xi = (2m|e|W/\hbar^2)^{1/3}(L_2 - z)$, $L_2 = -E/(|e|W)$, E — particle energy.

The transmission function shown in Fig. 1, *a* was calculated when the Airy function (curve *1* in Fig. 2) was obtained analytically (by the saddle-point method [15], the condition $|\xi| \gg 1$ must be satisfied)

$$\chi_1(\xi) = \begin{cases} \dfrac{-i}{2\sqrt{\pi}|\xi|^{1/4}} \exp\left[i\left(\dfrac{2}{3}|\xi|^{3/2} + \dfrac{\pi}{4}\right)\right], & \xi < 0, \\ \dfrac{-i}{2\sqrt{\pi}\xi^{1/4}} \exp\left(\dfrac{2}{3}\xi^{3/2}\right), & \xi > 0. \end{cases} \quad (3)$$

Taking into account the Airy function (3), we obtain the expression for the transmission function depending on the energy of the particle, and from the continuity condition for the function $\psi(z)$, and the derivative of the function $\partial\psi/\partial z$ from (2) (continuity condition for current density $j = i\hbar(\psi\partial\psi^*/\partial z - \psi^*\partial\psi/\partial z)/(2m)$) at the discontinuity points $z = 0$, $z = L_1$ (for more details see [14])

$$\tau = \left|\frac{C}{A_1}\right|^2 \frac{1}{k_1}\left(|\chi|^2 \frac{d\eta}{dz}\right)\bigg|_{z > L_2}$$

$$= \frac{2\kappa k_2}{k^2 + k_2^2} \frac{2k_1 k_2}{k_1^2 + (k_2^2 - k_1^2)\sin^2(k_2 L_1 - \varphi_0)} D(y),$$

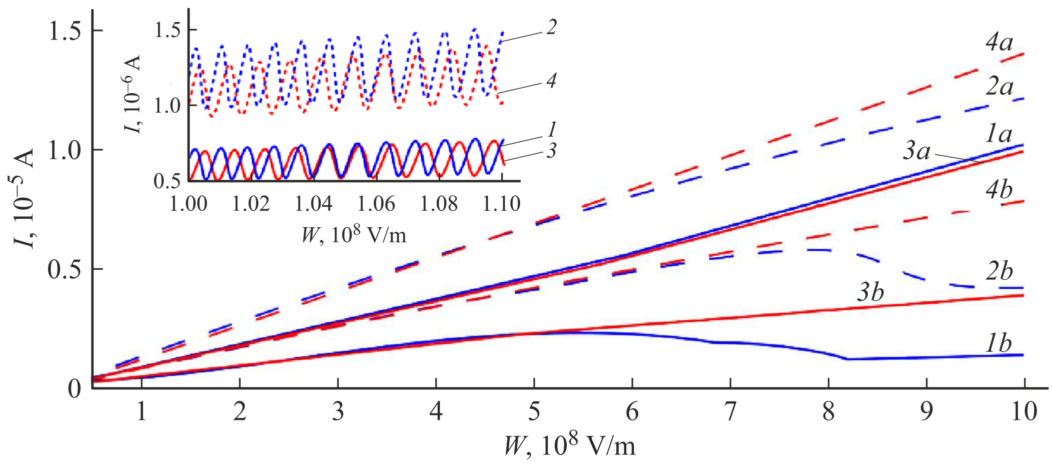

Figure 3. Currents through CNTs at different voltages U at the ends of nanotubes.

$$D = \exp\left[-\frac{4\sqrt{2m|E|^3}}{3\hbar}\frac{1}{|e|W}\Theta(y)\right],$$

$$\Theta(y) = (1-y)^{3/2}, \quad y = \frac{L_1}{L_2},$$

$$\eta = \frac{2}{3}|\xi|^{2/3}, \quad \varphi_0 = \arctan(\kappa/k_2),$$

$$\kappa = \frac{\sqrt{2m|e|W(L_2 - L_1)}}{\hbar}\left|1 - \frac{1}{4\xi^{3/2}|_{z=L_1}}\right|. \qquad (4)$$

In the paper [14] when obtaining the expression for the transmission function, the value κ, in contrast to (4), was equal to $\kappa = \sqrt{2m|e|W(L_2 - L_1)}/\hbar$, which led to the fact that in the paper [14] the transmission coefficient was greater than one. The presence of the term $1/4\xi^{3/2}|_{z=L_1}$ in the variable κ from (4) is explained by the fact that in the system of equations when calculating the variable $(\partial\chi/\partial z)|_{z=L_1}$ the influence of the pre-exponential part of the variable χ from (3) was not taken into account. The quantities k_1, k_2, ξ are defined after expression (2). In (4) the quantity C/A_1 is calculated according to Cramer's method [15] for a system of linear equations from unknowns B_1, A_2, B_2, C

$$A_1 + B_1 = A_2 + B_2,$$

$$A_1k_1 - B_1k_1 = A_2k_2 - B_2k_2,$$

$$A_2e^{ik_2L_1} + B_2e^{-ik_2L_1} = C\chi(L_1),$$

$$iA_2k_2e^{ik_2L_1} - iB_2k_2e^{-ik_2L_1} = C\left(\frac{\partial\chi}{\partial z}\right)\bigg|_{z=L_1}, \qquad (5)$$

where, when obtaining the transmission function from equality (4), it was taken into account that $|\chi|^2\,|_{z>L_2} = 4\pi|\xi|^{1/2}$.

The transmission function shown in Fig. 1, b was calculated when as solution of Schredinger equation $\partial^2\psi/\partial\xi^2 - \xi\psi = 0$ we used a linear combination of Airy functions of the first $Ai(\xi)$ and second $Bi(\xi)$ kind ([15], p. 116) (curve *2* in Fig. 2), obtained numerically using the MATLAB software package.

In this paper, the current during field emission from the tip of nanoparticles was calculated by the Landauer formula [16,17] (for details, see [14]) using the function of particle passage from the anode to the cathode (Fig. 1). Fig. 3 shows the dependence of the envelopes of the current I in a single CNT on the field strength W at a constant voltage U at the ends of the CNT, where $5 \cdot 10^7 \leqslant W \leqslant 10^9$ V/m, $U = WL_1$, L_1 — nanotube length. In Fig. 3, the solid curves correspond to the case when the transmission function was approximated by the asymptotic solution (3), and the dashed curves correspond to the case when the solution of the Airy function corresponds to the curve *2* in Fig. 1. Curves *1a*, *1b*, *2a*, *2b* in Fig. 3 correspond to the voltage $U = 3.5$ V at the ends of the nanotubes, and the curves *3a*, *3b*, *4a*, *4b* — voltage $U = 3.0$ V. The insert shows a similar dependence of the current on the field strength in the interval $10^8 \leqslant W \leqslant 1.1 \cdot 10^8$ V/m, curves *1–4* correspond to the envelopes (*1a*, *1b*)–(*4a*, *4b*). The range of field strength $5 \cdot 10^7 \leqslant W \leqslant 10^9$ V/m means that at voltage $U = 3.5$ V at the ends of the nanotubes, their length changed in the range $3.5 \leqslant L \leqslant 70$ nm, and at $U = 3.0$ V the nanotube length changed in the range $2.0 \leqslant L \leqslant 40$ nm.

It can be seen from Fig. 3 that the currents corresponding to the dashed curves are larger than the currents corresponding to the solid curves. This is explained by the fact that in the case of solid curves, when calculating the current value using the Landauer formula [16,17], integration is not carried out over ξ in the interval $|\xi| < 1$ (in this interval in Fig. 2 the curve *1*of the Airy function $\chi(\xi)$ from (3) is not defined), i. e. the region of integration decreases.

The Table shows the dependence of the Nordheim function $\theta(y)$ [11] and the function $\Theta(y)$, where the argument y for the function $\Theta(y)$ is calculated according to formula (4). The function $\Theta(y)$, which enters the expression (4) for the transparency function D, performs

Dependence on y of the Nordheim function $\theta(y)$ and the function $\Theta(y)$

Function	y										
	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
$\theta(y)$	1	0.98	0.94	0.87	0.79	0.68	0.58	0.45	0.31	0.16	0
$\Theta(y)$	1	0.85	0.72	0.59	0.46	0.35	0.25	0.16	0.09	0.03	0

a role similar to the Nordheim function $\theta(y)$, and for $\Theta(y)$ the function argument $y = L_1/L_2 = |e|WL_1/|E|$ depends both on the energy of the charged particle and on the nanotube length and field strength. It follows from the Table that the value of the $\Theta(y)$ function in the interval $0 < y < 1$ is much less than that of the Nordheim function. This pattern partially compensates for the low aspect number of nanotubes considered in this paper. The dependence of the transparency function D on the function $\Theta(y)$ should lead to a significant increase in the current during field emission compared to the case of field emission from the metal surface under other things being equal. The results on field emission can be obtained using a more accurate model of two-point and four-point elementary cells (kp-type continuum model [18–20], where for „zigzag" type CNTs and nanoribbons with „armchair" edges the electron wave functions can be expressed in terms of Hermite functions [18,19].

It follows from the calculation results that in the case of field emission in nanotubes with a length ranging from several nanometers to one hundred nanometers, there is a linear dependence of the current envelopes on the field strength W in the range $0.5 \cdot 10^8 \leqslant W \leqslant 0.5 \cdot 10^9$ V/m, which corresponds to the functional dependence $I = AW[1 + f(W)]$, where $W = U_1/L_1$. A linear dependence also exists in the case of the current dependence on the field strength in the Fowler–Nordheim coordinates and in the case of I/W^2 dependence on the value $1/W$ in the interval $10^{-9} \leqslant 1/W \leqslant 10^{-8}$ m/V, where $U_1 = \text{const}$ was used in the calculations for the voltage at the ends of the CNT. This regularity is explained by the fact that the CNT length is $L_1 < 1\,\mu$m, when the ballistic mechanism is not fulfilled during electron transport in nanomaterials.

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Conflict of interest

The authors declare that they have no conflict of interest.

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