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РЕЛЯТИВИСТСКИЙ ЭЛЕКТРИЧЕСКИЙ ПОТЕНЦИАЛ ВБЛИЗИ НЕПОДВИЖНОЙ ПРЯМОЙ УГЛЕРОДНОЙ НАНОТРУБКИ КОНЕЧНОЙ ДЛИНЫ СО СТАЦИОНАРНЫМ ТОКОМ[1]

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Исходя из потенциалов Лиенара – Вихерта для равномерно и прямолинейно движущегося электрона, исследуется релятивистское электрическое поле вблизи плотно заполненной атомами калия однослойной углеродной нанотрубки (K@CNT) со стационарным электрическим током внутри нее. Релятивистское электрическое поле в лабораторной системе координат возникает (вследствие преобразований Лоренца) только для нанотрубки конечной длины. Это есть результат суммирования кулоновских полей неподвижных положительно заряженных ионных остовов калия и равного им числа создающих ток баллистически движущихся валентных электронов калия. Показано, что величина отрицательного релятивистского электрического потенциала K@CNT в перпендикулярном нанотрубке направлении не зависит от направления плотности тока. Установлена взаимосвязь между радиусом K@CNT и числом открытых каналов баллистического переноса электронов по атомам калия. Используется формула Ландауэра, связывающая число открытых квазиодномерных каналов и электрическую проводимость на постоянном токе. Впервые получены аналитические формулы для зависимости релятивистского потенциала вблизи K@CNT от электрического напряжения между концами нанотрубки и ее радиуса в пределе нулевой абсолютной температуры. Рассмотрен случай, когда расстояние от точки регистрации релятивистского потенциала над центром

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нанотрубки много меньше ее длины. Для нанотрубки диаметром 2 нм и длиной 100 мкм при напряженности внешнего электрического поля 5 мВ/мкм величина релятивистского потенциала составляет примерно 2 мкВ. Современные методы измерений позволяют зарегистрировать предсказываемый релятивистский потенциал.

Ключевые слова: углеродная нанотрубка; щелочной металл; постоянный ток; электронная проводимость; релятивистский электрический потенциал; низкие температуры.

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RELATIVISTIC ELECTRIC POTENTIAL NEAR A RESTING STRAIGHT CARBON NANOTUBE OF A FINITE-LENGTH WITH STATIONARY CURRENT

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Based on the Lienard – Wiechert potentials for a uniformly and rectilinearly moving electron, a relativistic electric field is studied near a densely filled with potassium atoms single-walled carbon nanotube (K@CNT) with a stationary electric current inside it. The relativistic electric field in the laboratory coordinate system arises (due to the Lorentz transformations) only for a nanotube of a finite length. This field is a result of summation of the Coulomb fields of stationary positively charged ionic cores of potassium and an equal number of ballistically moving valence electrons of potassium that create a current. It is shown that the magnitude of the negative relativistic electric potential of K@CNT in the direction perpendicular to the nanotube does not depend on the direction of the current density. The relationship is obtained between the K@CNT radius and the number of open channels of ballistic electron transfer over potassium atoms. The Landauer formula is used, which relates the number of open quasi-one-dimensional channels and the direct current electrical conduction. For the first time, analytical formulas are obtained for the dependence of the relativistic potential near K@CNT on the electric voltage between the ends of the nanotube and on its radius in the limit of zero absolute temperature. The case is considered when the distance from the point of registration of the relativistic potential above the center of the nanotube is much less than its length. For nanotube with diameter of 2 nm and length of 100 μm, under an external electric field strength of 5 mV/μm, the magnitude of the potential of the relativistic electric field is of about 2 μV. Modern measurement techniques make it possible to register the predicted relativistic potential.

Keywords: carbon nanotube; alkali metal; steady current; electronic conduction; relativistic electric potential; low temperatures.

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Introduction

One-dimensional metallic and semiconducting nanowires have a number of unique properties (see, e. g., [1; 2]) and wide areas for real and possible applications [3–5]. However, nanowires are susceptible to oxidation, which leads to degradation of their operating parameters over time. At the same time, nanowires formed by filling carbon nanotubes (CNT) with metal atoms [6] are protected from oxidation, since the carbon frame of a nanotube is chemically inert. It is also worth saying, that it is possible to produce proton conducting nanowire made of molecular complexes of HF (hydrogen fluoride) inside CNT [7].

The aim of the work is to calculate the relativistic electrostatic potential near a straight resting carbon nanotube filled with potassium atoms (K@CNT) with a stationary electric current in it in order to evaluate parameters of its conductive potassium channel.

Basic equations

Let us consider a straight wire in the form of K@CNT with length L and cross section area S. Let the steady ballistic electric current be excited in it, then

$$I = -envS, \tag{1}$$

where e is the elementary charge; n is volume concentration of conduction electron; v is the ballistic velocity of electron; the value and direction of the electron velocity are constant along the carbon nanotube.

The current is led into the wire through two electrodes (ohmic contacts). Further, we assume, that the transfer of electrons in the wire is ballistic, and in the electrodes it is drift-diffusion [8]. The cross section area of electrodes is much larger than S. That is why when electron concentrations are approximately equal in the contacts and in the wire, the drift-diffusion velocity of electrons in the contacts much less than v. We neglect the manifestation of the acceleration of electrons on one contact of electrode to the wire and deceleration on the other contact of the wire to the electrode, since these regions are significantly less than the wire length. We also do not take into account the possibility of a configuration electromotive force [9] appearing on the contacts to the wire with steady current. Note that the electric field strengths associated with contacts to the wire with a stationary current are directed along the wire. In addition, equation (1) does not take into account the action of the magnetic field of the current on the electrons creating this current [10; 11]. Specifically, in the pinch effect, under the action of an intrinsic magnetic field, the electrons drifting with a velocity v goes to the axis of the conductor until the action of the magnetic field is balanced by their repulsion. Under the pinch effect the stream of electrons becomes compressed (pinched) and surface of the conductor acquires a positive charge, the surface density of which does not depend on the conductor length [10].

In the wire with current there are nSL mobile (free) electrons and their velocity is v. The amount of immobile atomic (ion) cores in the wire equals to the amount of mobile electrons, i. e., nSL. In the laboratory coordinate system the electric fields produced by electrons $\mathbf{E}_-$ and ions $\mathbf{E}_+$ of wire are different. Indeed, the strength of electrostatic field of uniformly (ballistically) moving electron with the velocity v at a distance r from the electron [12; 13] is

$$\mathbf{E}_- = -\frac{e\mathbf{r}}{4\pi\varepsilon_r\varepsilon_0 r^3}\frac{1-\beta^2}{\left(1-\beta^2\sin^2\theta\right)^{3/2}}, \tag{2}$$

where $\varepsilon_r \approx 1$ is the isotropic relative permittivity of the medium around the wire; ε_0 is the electric constant; $\beta = \frac{v}{c}$ is the ratio of electron velocity v in wire to the speed of light c in vacuum; θ is the angle between the electron velocity $\mathbf{v}$ and radius vector $\mathbf{r}$. The strength of electric field created by immobile ions $\mathbf{E}_+$ is equal in magnitude and opposite in sign of the strength of electric field created by electrons $\mathbf{E}_-$ with zero velocity (equation (2) at $\beta = 0$; see discussion of Lorentz transformations for moving objects in [14; 15]).

After summing up the fields from ion cores $\mathbf{E}_+$ (it is equal $-\mathbf{E}_-$ at $\beta = 0$) and conduction electrons $\mathbf{E}_-$ over the entire wire one can obtain the relativistic electric field in perpendicular direction to the ballistic flow of electrons at a distance r from the middle of the wire [16]:

$$E_\perp(r) = \frac{enSL}{2\pi\varepsilon_0 r}\left[\left(L^2+4r^2\right)^{-1/2} - \left(L^2+4r^2\left(1-\beta^2\right)\right)^{-1/2}\right] < 0. \tag{3}$$

It follows from equation (3) that for $L \to \infty$ the field $E_\perp \to 0$ at $r = \text{const}$ (see also [17; 18]). (In the frame of classical electrodinamics, it was shown [19] that the relativistic electric field around the superconducting ring with steady current is zero.)

The field $E_\perp(r)$ by equation (3) corresponds to the following electrostatic potential at a distance d from the center of the wire (approximation is given for $\beta = \frac{v}{c} \ll 1$ and $d \ll L$):

$$\varphi_\perp = \int_d^\infty E_\perp(r)\,dr = -\frac{enS}{2\pi\varepsilon_0}\ln\left(\frac{L+\sqrt{L^2+4d^2\left(1-\beta^2\right)}}{\sqrt{1-\beta^2}\left[L+\sqrt{L^2+4d^2}\right]}\right) \approx -\beta^2\frac{enS}{4\pi\varepsilon_0}\left(1-\frac{2d^2}{L^2}\right) < 0. \tag{4}$$

Here it is taken into account that at the point infinitely far from the wire the potential $\varphi_\perp = 0$.

Thus, from equation (4) taking into account equation (1) it follows that

$$\varphi_\perp \approx -\frac{\mu_0 I^2}{4\pi enS}\left(1-\frac{2d^2}{L^2}\right) < 0, \tag{5}$$

where $\mu_0 = \frac{1}{\varepsilon_0 c^2}$ is the vacuum permeability. From equation (5) it can be understood, that the value of the potential $|\varphi_\perp|$ is higher, when the concentration n maintaining the current I in the wire is lower. That is why the potential $|\varphi_\perp|$ is higher, when the ballistic velocity v of electrons is higher, i. e., $|\varphi_\perp| \propto \frac{I^2}{enS} = Iv$.

The calculations of number of subbands $N(R) = N \geq 1$ for electrons inside K@CNT were presented in [20]. It is shown that the number of subbands N and the Fermi momentum p_F of electrons moving along the CNT as functions of CNT radius R are determined by a system of two equations:

$$p_F = \frac{\pi^2 \hbar n R^2}{N(N+1)} + \frac{2\sqrt{2m\hbar\omega}}{N(N+1)} \sum_{j=0}^{N-1} (j+1)\sqrt{j}, \quad \frac{p_F^2}{2m} = N\hbar\omega, \tag{6}$$

where m is the electron mass (further it is assumed to be equal to the electron mass in vacuum); $\hbar = \frac{h}{2\pi}$ is the Planck constant; $\omega^2 = \frac{2U_0}{mR^2} = \frac{0.967e^2}{4\pi\varepsilon_0 m a_0^2 R}$ is the square of the angular frequency of zero-point oscillations of electron in parabolic potential well with depth $U_0 = \frac{e^2 R}{15\sqrt{3}\varepsilon_0 a_0^2}$; a_0 = 0.142 nm is the distance between two nearest carbon atoms in carbon nanotube. The potential well for electrons, which move in a chain of potassium atoms, is caused by the positively charged potassium ions adjacent to the negatively charged carbon frame of CNT. (The CNT frame is an acceptor: every 10 carbon atoms capture about one valence electron from potassium atoms. Subbands are due to the discreteness of the energy spectrum for the «transverse» electron motion inside K@CNT.)

Eliminating the unknown quantity p_F from the system of equations (6), we obtain

$$\left(\frac{\pi^2 \hbar n R^2}{N(N+1)} + \frac{2\sqrt{2m\hbar\omega(R)}}{N(N+1)} \sum_{j=0}^{N-1} (j+1)\sqrt{j} \right)^2 - 2mN\hbar\omega(R) = 0. \tag{7}$$

From equation (7) the relationship between the radius R and the number of open channels (subbands) $N = N(R) \geq 1$ for K@CNT can be found in the form

$$R = \left(N(N+1)\sqrt{N} - 2\sum_{j=0}^{N-1} (j+1)\sqrt{j} \right)^{4/9} \left(\frac{8e^2 m}{15\sqrt{3}\pi^8 \varepsilon_0 \hbar^2 a_0^2 n^4} \right)^{1/9}. \tag{8}$$

Results and discussion

According to Landauer's theory (see, e. g., [21; 22]), the direct current electrical conductivity G of quasi-one-dimensional conductor (inner part of K@CNT) in the limit of zero absolute temperature is equal to the number of open nondissipative channels of ballistic electron transfer multiplied by the conductivity quantum $\frac{2e^2}{h}$. The number of channels of ballistic electron transfer in K@CNT is equal to $\frac{N(R)[N(R)+1]}{2}$, i. e., to the number of subbands in which electrons are located, taking into account degeneracy multiplicity of the subband, which is equal to its number $N(R)$. Thus, the conductivity G has the form [20]

$$G(R) = \frac{2e^2}{h} \frac{N(R)[N(R)+1]}{2}, \tag{9}$$

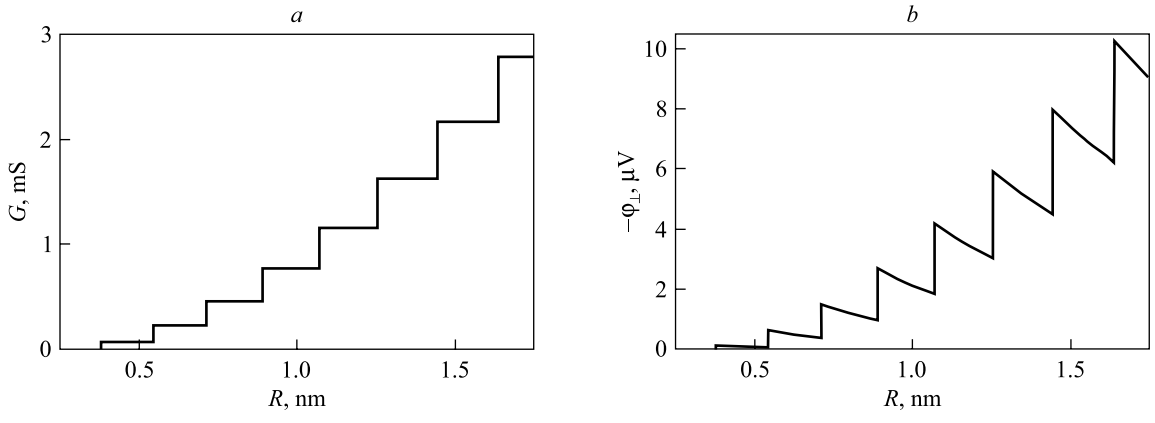
where $N(R)$ could be found from equation (8). Results of calculation of electrical conductivity $G(R)$ using equation (9) are shown (figure *a*).

Let a direct current voltage U be applied to the ends of K@CNT with radius R and length L. So that there is the electric ballistic current $I(R) = G(R)U$. (We assume that the electrical conductivity of the carbon frame of CNT is much less, than the conductivity via potassium atoms.) According to equation (5), neglecting $\frac{2d^2}{L^2} \ll 1$, the relativistic electrostatic potential $\varphi_\perp(R)$ does not depend on the potential registration distance d from the center of K@CNT and has the form

$$\varphi_{\perp}(R) \approx -\frac{\mu_0}{4\pi^2 e}\frac{G^2(R)}{nR^2}U^2, \tag{10}$$

where $n = 14$ nm^{-3} is the concentration of conduction electrons inside K@CNT (here it equals to the electron concentration in metallic potassium [23] and it does not depend on the radius R of nanotube); $S = \pi R^2$. The results of calculations of relativistic electrostatic potential $\varphi_{\perp}(R)$ using equation (10) are shown in figure *b*.

It follows from equation (10), that the magnitude of the electrical conductivity $G(R)$ can be determined from the magnitude of the measured relativistic potential $\varphi_{\perp}(R)$ for the known nanotube radius R and voltage U (voltage generator mode). With known electric current $I(R) = G(R)U$ (current generator mode) and nanotube radius R, according to equation (10), it is possible to determine the concentration n of ballistically moving electrons inside K@CNT.



Dependence of the direct current electrical conductivity G,
according to equation (9), on the radius of K@CNT (*a*). Relativistic electrostatic potential $\varphi_{\perp}$,
according to equation (10), at the distance $d \ll L$ from the center of K@CNT to the registration point
of the potential, as a function of the radius R for $L = 100$ μm at the electric field strength $\frac{U}{L} = 5$ mV/μm (*b*)

Conclusion

The dependence of relativistic potential $\varphi_{\perp}$ near a potassium-filled straight resting carbon nanotube with a stationary electric current on nanotube radius R in the limit of zero absolute temperature was studied analytically and numerically. The potential is calculated at a distance d, from the center of K@CNT, that is much less than the nanotube length L. At a fixed distance from the center of the nanotube the value of $\varphi_{\perp}$ increases in a sawtooth manner with the nanotube radius R. The appearance of «teeth» in the dependence of $\varphi_{\perp}$ on R is a consequence of two competing factors: i) the electrical conductivity $G(R)$ changes in a stepwise manner (increases with the radius R), i. e., it increases with the number of subbands filled with electrons in the discrete energy spectrum of the «transverse» motion of electrons inside K@CNT; ii) when the nanotube radius R increases until the next jump of conductivity G, the value of the potential $\varphi_{\perp}(R)$ decreases (since, for fixed K@CNT conductivity, the potential is inversely proportional to the square of CNT radius). For nanotube with diameter $2R \approx 2$ nm and length $L = 100$ μm, under an external electric field of strength $\frac{U}{L} = 5$ mV/μm, the magnitude of the potential of the relativistic electric field is of about $\varphi_{\perp} \approx 2$ μV.

It is shown that the value of the electrical conductivity $G(R)$ can be determined from the measured magnitude of relativistic potential $\varphi_{\perp}(R)$ for known nanotube radius R and applied voltage U. While for known electric current $I(R) = G(R)U$ and radius R the concentration n of electrons ballistically moving inside K@CNT can be determined.

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