Available online at www.sciencedirect.com
SCIENCE DIRECT
Physica E 33 (2006) 336–342
PHYSICA E
www.elsevier.com/locate/physe

Electron transport in armchair single-wall carbon nanotubes

D.V. Pozdnyakov*, V.O. Galenchik, F.F. Komarov, V.M. Borzdov

Radiophysics and Electronics Department, Belarus State University, Nezavisimosty av. 4, 220050 Minsk, Belarus

Received 15 February 2006; accepted 27 March 2006
Available online 30 May 2006

Abstract

The rates of electron scattering via phonons in the armchair single-wall carbon nanotubes were calculated by using the improved scattering theory within the tight-binding approximation. Therefore, the problem connected with the discrepancy of the scattering rates calculated in the framework of the classical scattering theory and ones predicted by experimental data was clarified. Then these results were used for the solving of the kinetic Boltzmann equation to describe electron transport properties of the nanotubes. The equation was solved numerically by using both the finite difference approach and the Monte Carlo simulation procedure.

PACS: 71.10.Ca; 72.10.Di; 73.50.Bk; 73.63.Fg

Keywords: Carbon nanotube; Electron transport; Phonon scattering

1. Introduction

At present the interest to the study of carbon nanotubes increases dramatically [1–23]. First of all it is caused by prompt development of nanoelectronics technologies. Due to these achievements it is possible to fabricate the pure carbon nanotubes with high-quality structure [18,19]. The prospect of their future application as active and passive elements of nanoelectronics is out of doubts today [6,8,11–17]. Moreover, it is necessary to note that the theoretical study of carbon nanotubes presently has much to be desired. It concerns both the descriptions of the physical properties of nanotubes, and the descriptions of the charge carrier transport in such structures. In our opinion, this problem is connected on the one hand by that the nanotubes are specific objects of quantum nature. That is why the study of them is a rather complicated task. And on the other hand these structures have been investigated intensively in only one decade.

One of the important areas in investigations of the nanotubes is the study of their electrophysical properties, especially the properties of the armchair single-wall nanotubes. It is known that such nanotubes can be reproduced in the best way, and their electrophysical properties are practically independent on their diameter [14,15,21]. This cannot be said about the nanotubes with another chiralities. So, for example, zigzag type nanotubes can have either metallic or semi-conducting properties depending on their diameter [1]. That is why we will consider armchair nanotubes only. Therefore, to avoid the account of the edge effects let us consider rather long structures ($L > 20$ nm), i.e. we will consider the armchair nanotubes with the length greater than electron mean free path [6,14,21].

To describe the electron transport in such carbon nanotubes the semiclassical approach and the kinetic Boltzmann equation for one-dimensional electron gas can be used [6,24]. Both the finite difference method [6,24] and the Monte Carlo imitative simulation [25–28] can be used for solving this equation. Nevertheless, the correct use of these approaches is possible only when all the dominating charge carrier scattering processes are described in the most precision way. In single-wall nanotubes these scattering processes are the phonon ones [3–6,10,14,20–23]. At the same time, as far as we know, this problem is very poorly studied yet. Hitherto, in particular, the reason of a huge difference in theoretical calculations and experimental

*Corresponding author.
E-mail address: pozdnyakov@bsu.by (D.V. Pozdnyakov).

1386-9477/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.physe.2006.03.158

definition of electron–phonon scattering rates as well as the independence of the latter from the diameter of nanotubes [14,21] are not cleared up. That is why the purposes of the present paper are to calculate the rate of electron scattering via phonons in the armchair single-wall nanotubes and to develop a model of electron transport in such nanotubes based on the solution of the Boltzmann transport equation.

2. Theory

Let us consider the phonon scattering in nanotubes at the electric quantum limit, i.e. when the angular momentum of all electrons is equal to zero [10]. To meet this condition the nanotubes with small diameter $d<3$ nm are considered. Such nanotubes correspond to (n,n) armchair nanotubes with the chirality index $n\leqslant 20$ [1]. In this case the scattering rates can be calculated by using the perturbation theory [29]. Then, taking into account the one-dimensional nature of the electron gas in nanotubes, the following equations are valid [20,24,27,30–33]:

$$W_v^{e/a}(k)=\frac{\omega_v^{e/a}}{2}\left(N(\omega_v^{e/a},T_v)+\frac{1}{2}\pm\frac{1}{2}\right)\times|g_v(k,k_v^{e/a})|^2\left|\frac{\partial E}{\partial k}\right|^{-1}_{k=k_v^{e/a}},\quad(1)$$

$$N(\omega_v^{e/a},T_v)=\left(\exp\left(\frac{\hbar\omega_v^{e/a}}{k_B T_v}\right)-1\right)^{-1},\quad(2)$$

$$k_v^{e/a}=k+q,\quad(3)$$

$$E(k_v^{e/a})=E(k)\mp\hbar\omega_v^{e/a}(q),\quad(4)$$

where k is the electron wave vector; q is the phonon wave vector; $\hbar$ is the Plank constant; E is the electron energy relative to Fermi level E_F which is taken as zero ($E_F=0$); g is the matrix element of electron–phonon coupling; k_B is the Boltzmann constant; $\omega_v^{e/a}$ is the cyclic phonon frequency; T_v is the phonon gas temperature; v is the index signing the phonon branch; e/a are the indexes signing phonon emission or absorption. Furthermore, it should be noted that in Eq. (1) the Pauli principle is not taken into account [29]. The latter can be taken into consideration while the Boltzmann equation is being solved or while the Monte Carlo simulation of the electron ensemble drift checking whether the final state is free [25–27]. Moreover, the formula for the angular momentums of electrons and phonons have not appeared in the system of Eqs. (3) and (4). This formula is not considered by us because in the electric quantum limit the electrons will be scattered by only the phonons with zero angular momentum due to the angular momentum conservation. Therefore we will be taking into account only such phonons.

The relation between the electron wave vector and the electron energy is given by the known formula [2,37]

$$E_{1,2}(k)=\mp J_0\left(1-2\cos\left(\frac{ak}{2}\right)\right),\quad(5)$$

where $E_{1,2}$ is the electron energy in the band 1 and 2, respectively [2,4,15]; $a=0.246$ nm is the lattice constant [1,5]; $J_0=2.7$ eV is the overlap integral [7,9]. The matrix element of electron–phonon coupling can be calculated by using the classical scattering theory within the tight-binding model [2,34,35], but only with some improvements which we are dwelling on below. In this case the basic equations for the calculation of the matrix element can be taken from [2,35]

$$|g_l|^2=\frac{12q_l^2J_0^2}{\mu_l(\omega_l^{e/a})^2}\cos^2\left(\frac{(k+k_l^{e/a})a}{4}\right)\sin^2\left(\frac{(k-k_l^{e/a})a}{4}\right),\quad(6)$$

$$|g_t|^2=\frac{4q_t^2J_0^2}{\mu_t(\omega_t^{e/a})^2}\sin^2\left(\frac{(k+k_t^{e/a})a}{4}\right)\sin^2\left(\frac{(k-k_t^{e/a})a}{4}\right),\quad(7)$$

where l and t are the indexes signing the longitudinal and transverse phonon modes, respectively [2].

Having calculated the scattering rates of all possible phonon scattering processes in the armchair nanotubes we have concluded that the dominant scattering mechanisms are the longitudinal optical (LO) and acoustic (LA) phonon backscattering processes as well as the transverse acoustic (TA) phonon (twiston) backscattering. The longitudinal phonon scattering is intraband with the transition from one Dirac point to another [2–4,10,15], whereas the TA scattering causes interband transition in the vicinity of Dirac points. The other phonon scattering processes can be neglected because their rates are very little in comparison with the TA, LA and LO backscattering rates of active electrons, the electrons, which are in a vicinity of the Dirac points K and K′ close to the Fermi level. It should be noted that in other studies only these dominant scattering mechanisms are taken into account [4,6,14,20–23]. Thus, the scattering rates in the armchair single-wall nanotubes can be calculated according to Eqs. (1)–(7) and the following formulae describing the dispersion relations between the phonon wave vector q and the phonon energy $\hbar\omega$ for the phonons with zero angular momentum

$$\hbar\omega_{LA}(y)=\begin{cases}C_{4-}^{LA}y^4-C_{3-}^{LA}y^3+C_{2-}^{LA}y^2+C_{1-}^{LA}y, & y\leqslant 2/3,\\ C_{4+}^{LA}y^4-C_{3+}^{LA}y^3+C_{2+}^{LA}y^2-C_{1+}^{LA}y+C_{0+}^{LA}, & y>2/3,\end{cases}\quad(8)$$

$$\hbar\omega_{LO}(y)=\begin{cases}C_{4-}^{LO}y^4-C_{3-}^{LO}y^3+C_{2-}^{LO}y^2+C_{1-}^{LO}y+C_{0-}^{LO}, & y\leqslant 2/3,\\ -C_{3+}^{LO}y^3+C_{2+}^{LO}y^2+C_{1+}^{LO}y+C_{0+}^{LO}, & y>2/3,\end{cases}\quad(9)$$

$$\hbar\omega_{\mathrm{TA}}(y)=\begin{cases} C_{1-}^{\mathrm{TA}}\sin(1.880y+2.411y^5), & y\leqslant 2/3,\\ C_{1+}^{\mathrm{TA}}(1-0.140\sin^2(3\pi y))\cos(3\pi y)+C_{0+}^{\mathrm{TA}}, & y>2/3,\end{cases} \tag{10}$$

$$y=|ak|(2\pi)^{-1}. \tag{11}$$

There are $C_{4-}^{\mathrm{LA}}=0.459\,\mathrm{eV}$, $C_{3-}^{\mathrm{LA}}=0.645\,\mathrm{eV}$, $C_{2-}^{\mathrm{LA}}=0.029\,\mathrm{eV}$, $C_{1-}^{\mathrm{LA}}=0.359\,\mathrm{eV}$, $C_{4+}^{\mathrm{LA}}=4.740\,\mathrm{eV}$, $C_{3+}^{\mathrm{LA}}=17.28\,\mathrm{eV}$, $C_{2+}^{\mathrm{LA}}=23.33\,\mathrm{eV}$, $C_{1+}^{\mathrm{LA}}=13.77\,\mathrm{eV}$, $C_{0+}^{\mathrm{LA}}=3.146\,\mathrm{eV}$, $C_{4-}^{\mathrm{LO}}=0.918\,\mathrm{eV}$, $C_{3-}^{\mathrm{LO}}=1.100\,\mathrm{eV}$, $C_{2-}^{\mathrm{LO}}=0.195\,\mathrm{eV}$, $C_{1-}^{\mathrm{LO}}=0.020\,\mathrm{eV}$, $C_{0-}^{\mathrm{LO}}=0.196\,\mathrm{eV}$, $C_{3+}^{\mathrm{LO}}=0.069\,\mathrm{eV}$, $C_{2+}^{\mathrm{LO}}=0.059\,\mathrm{eV}$, $C_{1+}^{\mathrm{LO}}=0.094\,\mathrm{eV}$, $C_{0+}^{\mathrm{LO}}=0.083\,\mathrm{eV}$, $C_{1-}^{\mathrm{TA}}=0.124\,\mathrm{eV}$, $C_{1+}^{\mathrm{TA}}=0.023\,\mathrm{eV}$ and $C_{0+}^{\mathrm{TA}}=0.101\,\mathrm{eV}$ in Eqs. (8)–(10). These equalities have been found by using the analytical approximation with high precision for the phonon-zone structure of the armchair single-wall nanotubes. This zone structure is determined by means of the zone folding method [37] conformably to phonon-zone structure of graphene [36]. The validity of such an approach is discussed in Ref. [23].

Now let us consider the values μ_{l}, μ_{t}, q_{l} and q_{t}. Due to our investigations it is found out that there are values $\mu_{\mathrm{l}}=2m_{\mathrm{C}}/a$ and $\mu_{\mathrm{t}}=4m_{\mathrm{C}}/a$ ($m_{\mathrm{C}}=2\times10^{-26}\,\mathrm{kg}$—the mass of carbon atom) in $|g_{\mathrm{l}}|^2$ and $|g_{\mathrm{t}}|^2$, respectively, instead of the value of the armchair single-wall nanotube linear mass density $\mu=4nm_{\mathrm{C}}/a$ [2] (the first improvement of the classical scattering theory). It is caused by equality of the carbon atom oscillation phases on the whole circumference of the cross-section perpendicular to the nanotube axis for the phonon modes with zero angular momentum, i.e. by the synchronism of oscillations of all the carbon atoms in a half of the primitive cell. In that case it is possible to consider all the atoms in the primitive cell like two, for the longitudinal modes, or four, for the transverse ones, massive particles bounded with each other $2n$ or n times, respectively, as strong as two carbon atoms. The discussed phenomenon clarifies the fact that the electron–phonon scattering rates in the armchair single-wall nanotubes do not depend on their diameters [14,21] as the values μ_{l} and μ_{t} do not, too, in contrast to the value μ.

As for the values q_{l} and q_{t}, which are the deformation constants in the directions along axis and circumference of the nanotube, respectively, they can be calculated by using the plane-wave approach. In contrast to the well-known Slater local-orbital one giving the wrong results (see Ref. [4]), where the values $q_{\mathrm{l}}=q_{\mathrm{t}}=q_0$ are determined by means of analysis of alteration of the overlap integral J_{ov} due to the distance alteration between two carbon atoms in graphene [34,35], in the plane-wave approach the values q_{l} and q_{t} can be defined by the same way, but at some different assumptions. The difference is that the Slater local-orbital model assumes that the electrons are individual particles belonging to individual atoms, whereas the plane-wave model assumes that the electrons are de Broglie waves filling the whole space in the crystal lattice of graphene. Moreover, it is supposed that the phonon displaces only the ion but it does not displace the electron orbit in crystal lattice within the Slater local-orbital approach [34,35], whereas within the plane-wave one it is supposed that the phonon displaces the whole carbon atom. In an approach like that, in fact, it is taken into consideration the "orbital relaxation" (see Ref. [4]) when the relaxation time is assumed to be equal to zero.

Then, using the results of Refs. [2,34,35,37], the following formulae can be written for the unfolded graphite sheet obtained from the armchair single-wall nanotube within the plane-wave approach at the tight-binding approximation

$$q_{\mathrm{l}}=\frac{1}{J_0}\frac{\partial J_{\mathrm{ov}}}{\partial|\mathbf{R}_x|}\bigg|_{R=a}=\frac{1}{3}\left(0+\frac{\sqrt{3}}{2}+\frac{\sqrt{3}}{2}\right)\frac{1}{J_0}\frac{\partial J_{\mathrm{ov}}}{\partial R}\bigg|_{R=a}, \tag{12}$$

$$q_{\mathrm{t}}=\frac{1}{J_0}\frac{\partial J_{\mathrm{ov}}}{\partial|\mathbf{R}_y|}\bigg|_{R=a}=\frac{1}{3}\left(1+\frac{1}{2}+\frac{1}{2}\right)\frac{1}{J_0}\frac{\partial J_{\mathrm{ov}}}{\partial R}\bigg|_{R=a}, \tag{13}$$

$$\frac{\partial J_{\mathrm{ov}}}{\partial R}\bigg|_{R=a}=2\frac{\partial}{\partial R}\left[\int_{(\text{primitive cell})}V_{\mathrm{ov}}(R)\,\mathrm{d}\mathbf{r}\right]\bigg|_{R=a}, \tag{14}$$

$$V_{\mathrm{ov}}(R)=\frac{1}{(2\pi)^2}\int_{(\text{Brillouin zone})}E_{\mathrm{ov}}(R,\mathbf{k})\,\mathrm{d}\mathbf{k}, \tag{15}$$

$$E_{\mathrm{ov}}(R,\mathbf{k})=-J_0\sqrt{1+4\cos^2(Rk_x/2)+4\cos(Rk_x/2)\cos(\sqrt{3}Rk_y/2)}. \tag{16}$$

Here $\mathbf{r}$ is the two-dimensional radius-vector; $\mathbf{k}$ is the two-dimensional wave vector; x is the coordinate along the nanotube axis $0x$; y is the coordinate along the nanotube circumference $0y$. In Eq. (14) the coefficient equal to 2 appeared because there are two carbon atoms in the primitive cell of graphene. According to Eqs. (12)–(16) the value of q_{l} is equal to $8.643\,\mathrm{nm}^{-1}$, and the value of q_{t} is equal to $9.980\,\mathrm{nm}^{-1}$. Let us note that the values of q_{l} and q_{t} calculated in the framework of the plane-wave approach (the second improvement of the classical scattering theory) are less than the value of $q_0=25\,\mathrm{nm}^{-1}$ calculated within the Slater local-orbital approach [35]. Our results are in a good agreement with the assumption of Ref. [4] in which the values of $q_{\mathrm{l}}=8\,\mathrm{nm}^{-1}$ and $q_{\mathrm{t}}=10\,\mathrm{nm}^{-1}$ were considered so as to secure the accordance of the theoretical results with the experimental data.

For example, in Fig. 1 the functions of the electron–phonon scattering rates versus the electron wave vector for the armchair nanotubes calculated by using Eqs. (1)–(11) at temperature $T_v=290\,\mathrm{K}$ are presented. It can be noted that the LA and LO phonon scattering rates are of the same order whereas the TA phonon scattering rate is about ten times less than those at $T_v=290\,\mathrm{K}$.

Let us write down the equations describing the state of the electron gas in the armchair nanotube. In general, these

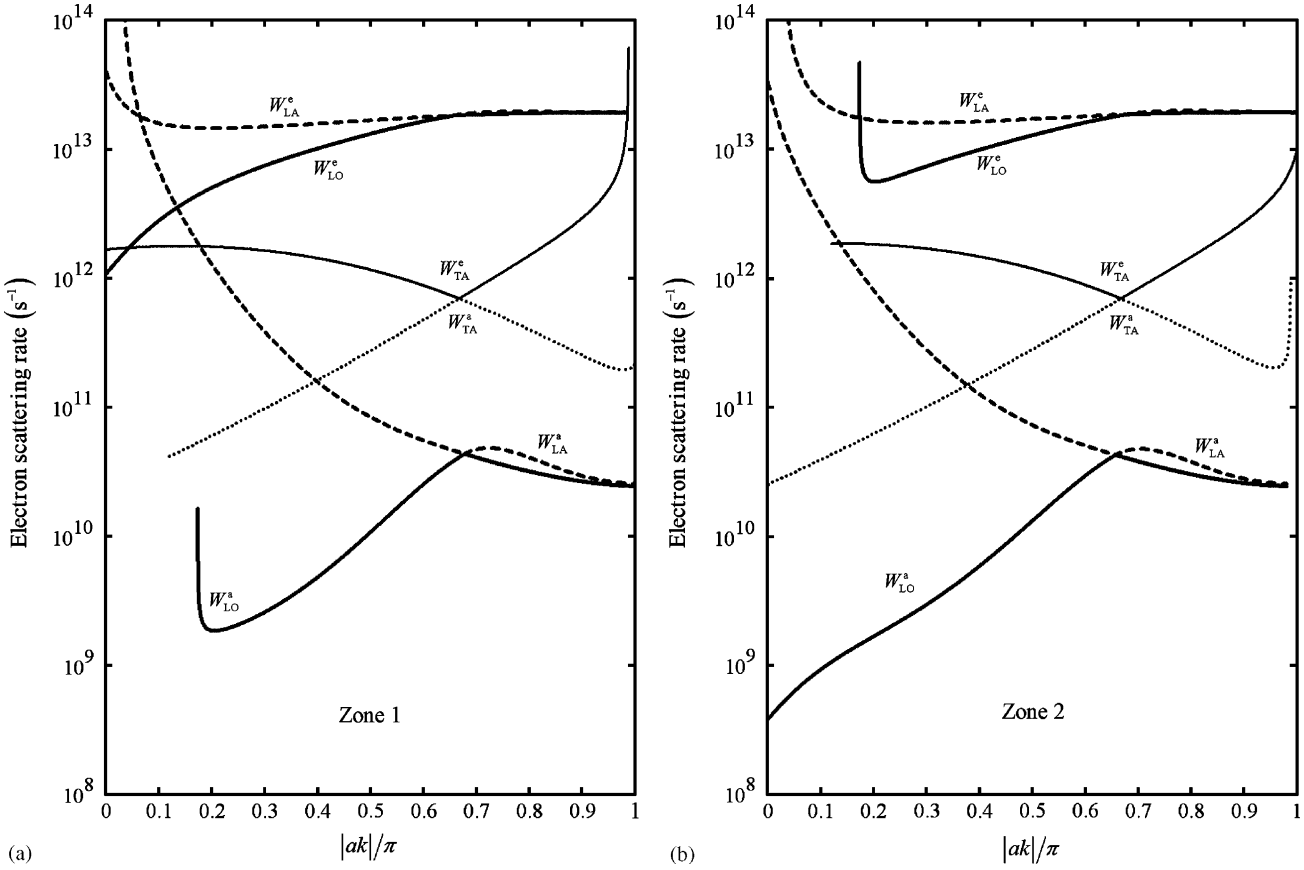

Fig. 1. LA, LO and TA phonon scattering rates in the band 1 (a) and 2 (b) of the armchair single-wall carbon nanotubes.

equations can be presented as [6,20,24–28]

$$\frac{\partial f_{1,2}}{\partial t}+\frac{\partial f_{1,2}}{\partial k}\frac{\mathrm{d}k}{\mathrm{d}t}+\frac{\partial f_{1,2}}{\partial x}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)_{1,2}+\hat{I}f_{1,2}=0, \tag{17}$$

$$\frac{\mathrm{d}k}{\mathrm{d}t}=-\frac{e}{\hbar}F, \tag{18}$$

$$\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)_{1,2}=u_{1,2}=\frac{1}{\hbar}\frac{\partial E_{1,2}}{\partial k}, \tag{19}$$

$$n_{\mathrm{L}}=\frac{1}{\pi}\int_{-\pi/a}^{+\pi/a}(f_1+f_2)\,\mathrm{d}k, \tag{20}$$

$$u_{\mathrm{dr}}=\frac{1}{\pi n_{\mathrm{L}}}\int_{-\pi/a}^{+\pi/a}(u_1f_1+u_2f_2)\,\mathrm{d}k, \tag{21}$$

$$J=-en_{\mathrm{L}}u_{\mathrm{dr}}. \tag{22}$$

Here t is the time; $f_{1,2}=f_{1,2}(k,x,t)$ is the electron distribution function in the band 1 and 2, respectively; $\hat{I}$ is the operator of the electron–phonon interaction with account of the Pauli principle; $F=F(x,t)$ is the electric field strength in the nanotube along $0x$; $u_{1,2}=u_{1,2}(k)$ is the electron group velocity in the band 1 and 2, respectively; $n_{\mathrm{L}}=n_{\mathrm{L}}(x,t)$ is the electron linear concentration; $u_{\mathrm{dr}}=u_{\mathrm{dr}}(x,t)$ is the electron drift velocity; $J=J(x,t)$ is the electric current in the nanotube; e is the value of elementary charge. According to Ref. [27] the operator $\hat{I}$ effects on the electron distribution function as follows:

$$\hat{I}f=\sum(Wf(1-f')-W'f'(1-f)). \tag{23}$$

Here the sum is over all possible final states; f' is the electron distribution function in a final state; W' is the rate of scattering causing the return of electrons to the initial state.

At the tight-binding approximation Eq. (19) can be written as (see Eq. (5))

$$u_{1,2}=\mp\frac{aJ_0}{\hbar}\sin\left(\frac{ak}{2}\right). \tag{24}$$

So, to study the kinetic processes in the armchair single-wall carbon nanotubes it is necessary to solve the kinetic Boltzmann equation (17) using the equations of motion (18) and (24). Then the kinetic parameters n_{L}, u_{dr} and J can be calculated according to Eqs. (20)–(22).

3. Results and discussion

Let us consider electron transport in the infinite length armchair nanotubes in uniform constant electric field. Such a transport is practically equivalent to electron transport in rather a long nanotube placed on the ideal metal contacts [6,14,21]. Meanwhile, the nanotube can be considered as long if its length is greater or at least the same order as the

TA phonon limited mean free path of active electrons. In this case Eqs. (17) and (20) are reduced to

$$\frac{eF}{\hbar}\frac{\partial f_{1,2}}{\partial k} - \hat{I} f_{1,2} = 0, \tag{25}$$

$$n_{\mathrm{L}} = \frac{2}{a}. \tag{26}$$

The solving of Eq. (25) allows the kinetic parameters to be calculated. Specifically it may be the electric current in the nanotube.

In Figs. 2 and 3 some results of calculations of the electric current in the armchair nanotubes at $T_{\mathrm{TA}} = T = 290\,\mathrm{K}$ are presented. Here T is the temperature of the nanotube surroundings. These results are obtained by using both the numerical solution of Eq. (25) by the finite difference approximation and the imitative Monte Carlo simulation of the electron ensemble drift [38–40]. The results coincide and are not resolved in the figure scale.

Moreover, the experimental data are presented in Figs. 2 and 3 along with the theoretical results obtained by Javey et al. [14], who applied the Monte Carlo simulation procedure with use of fitting parameters. These figures evidently demonstrate a very good agreement between the theory and experiment. Especially it concerns those results where the non-equilibrium LA and LO phonons ($T_{\mathrm{LA,LO}} > T = 290\,\mathrm{K}$) [23] are taken into account. Some discrepancy of the results in Fig. 3 at low fields is explained by the TA phonon pinning effect at some conditions when the TA phonon mode is partly suppressed due to an influence of the substrate on oscillations of carbon atoms in the nanotube [6].

We did not consider the pinning effect, which is probably difficult to describe theoretically, but we considered a most important effect like heating of the LA and LO phonon

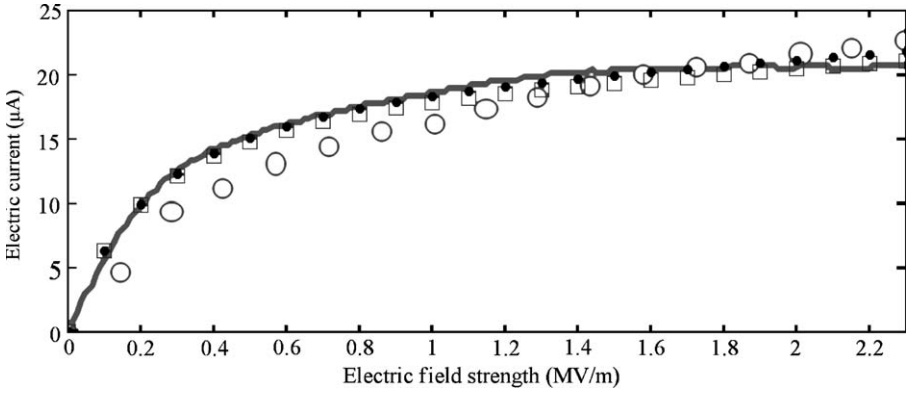

Fig. 2. The function of the electric current versus the electric field strength in armchair single-wall carbon nanotubes ($\eta = 1.063 \times 10^{-4}\,\mathrm{W^{-1}\,m}$). The solid curve is the experimental data from Ref. [14] ($L = 700\,\mathrm{nm}$). The circles are the theoretical results from Ref. [14] ($L = 700\,\mathrm{nm}$). The points are our theoretical results at $T_{\mathrm{LA,LO}} = 290\,\mathrm{K}$ ($L = \infty$). The squares are our theoretical results in which it is taken into account the non-equilibrium LA and LO phonons ($L = \infty$).

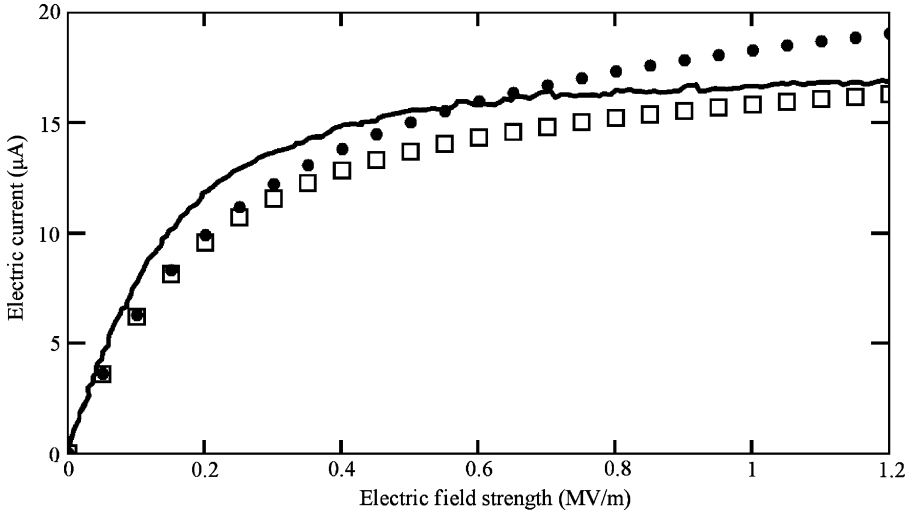

Fig. 3. The function of the electric current versus the electric field strength in armchair single-wall carbon nanotubes ($\eta = 6.737 \times 10^{-4}\,\mathrm{W^{-1}\,m}$). The solid curve is the experimental data from Ref. [21] ($L = 1000\,\mathrm{nm}$). The points are our theoretical results at $T_{\mathrm{LA,LO}} = 290\,\mathrm{K}$ ($L = \infty$). The squares are our theoretical results in which it is taken into account the non-equilibrium LA and LO phonons ($L = \infty$).

gas, i.e. the non-equilibrium LA and LO phonons [23]. As a first order approximation this effect can be described by the following obvious formula found from the energy conversation law

$$N(\omega_K, T_{LA,LO}) - N(\omega_K, T) = \eta F J(F, T_{LA,LO}), \quad (27)$$

where ω_K is the cyclic frequency of the LA and LO phonons at K point ($\hbar\omega_K = 0.151$ eV) [36]; η is the parameter which is determined by the quality of the thermal contact between the nanotube and its surroundings. The value of this parameter obviously depends on the type of matter of the surroundings and the area of the contact as well as another factors.

In our opinion, it is a very difficult task to calculate the value of η theoretically, but it is easy to find it from the experimental data by using the fitting procedure to theoretical results. So, we did like this. And the results presented in Figs. 2 and 3 have been obtained at such values of η which give rise to the best agreement between the theoretical results and experimental data. In Fig. 4, in addition, the functions of the LA and LO phonon gas temperature versus the electric field strength are given. These functions have been calculated by means of Eq. (27) at the best fitted parameter η. It is clear from this figure that the non-equilibrium phonons cause the superheating of the LA and LO phonon gas (see Ref. [23]).

We would like to add that the TA phonon pinning effect can be described, in principle, by the same way like the superheating effect of the LA and LO phonon gas in nanotubes. In other words it is possible to consider the pinning effect as if the supercooling of the TA phonon gas takes place ($T_{TA} < T$). Then to achieve the agreement between theory and experiment in Fig. 3, like it is in Fig. 2, it must be guessed that the temperature of the TA phonon gas T_{TA} is equal to 200 K ($T = 290$ K).

So, the validity of the improved scattering theory is verified by the things discussed above and the results presented in Figs. 2 and 3. Moreover, it is confirmed by the following reasons. The TA phonon limited mean free path of active electrons l_t as well as the LA and LO phonon limited one l_l calculated theoretically are in a good accordance with the same values, respectively, found from the experiments. For instance, the experiments, which the pining effect is not observed in, predict that the value of l_t is equal to 500 ± 200 nm at $T = 290$ K [14,22]. The improved scattering theory predicts that the value of $l_t = u_F(W^e_{TA}(k_F) + W^a_{TA}(k_F))^{-1}$ [21] is equal to 632 nm. Here u_F and k_F are the absolute value of the group velocity and electron wave vector, respectively, at the Fermi level in the armchair single-wall nanotube. It also follows from the experiments that l_l is equal to 10–15 nm at very high electric fields ($\sim 10^7$ V/m) [6,14,21]. The theory gives that the quantity of $l_l = u_F(W^e_{LA}(k_F) + W^a_{LA}(k_F) + W^e_{LO}(k_F) + W^a_{LO}(k_F))^{-1}$ possesses the following values: $l_l(T_{LA,LO} = 290\,K) = 23.8$ nm, $l_l(T_{LA,LO} = 1200\,K) = 15.0$ nm and $l_l(T_{LA,LO} = 1970\,K) = 10.0$ nm. According to the results discussed above and taking into consideration the superheating of the LA and LO phonon gas, one can draw a conclusion that the improved scattering theory appropriately describes the real scattering processes in the armchair single-wall carbon nanotubes. Besides, it predicts that the temperature of the LA and LO phonon gas is between 1000 and 2000 K at very high electric fields. These temperatures are much less and more reliable than those which were guessed in Ref. [23] (>6000 K).

Thus, in the present paper the rates of the electron scattering via phonons in the armchair single-wall carbon nanotubes are calculated by using the improved scattering theory. The model of charge carrier transport in such nanotubes based on the solving of the Boltzmann transport equation is developed. It is found out that the discrepancy

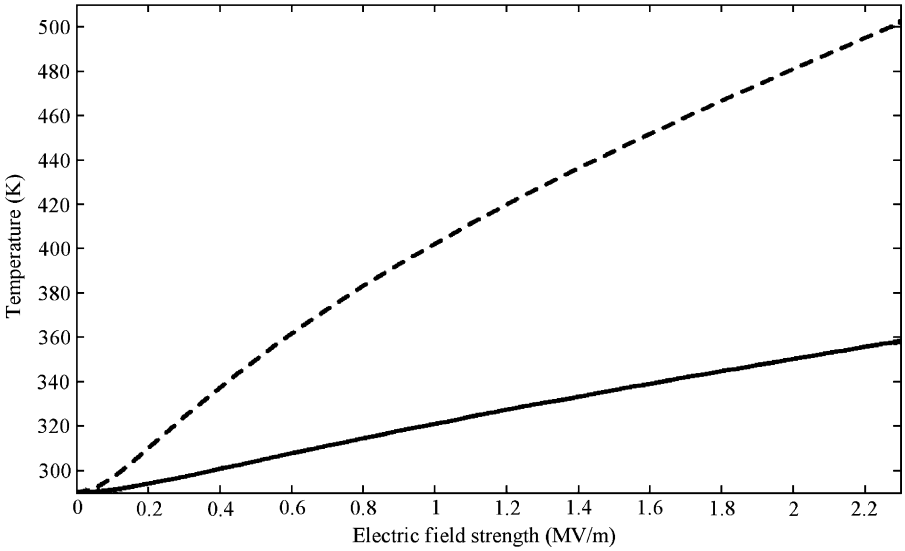

Fig. 4. The function of the temperature of the LA and LO phonon gas versus the electric field strength in the infinite length armchair single-wall carbon nanotubes at $\eta = 1.063 \times 10^{-4}\,W^{-1}$ m (solid curve) and $\eta = 6.737 \times 10^{-4}\,W^{-1}$ m (dashed curve).

of theoretical calculations in the framework of the classical scattering theory and experimental estimations of the values of l_l and l_t has the following reasons: (i) the features of carbon atom oscillations for the one-dimensional phonon modes with zero angular momentum are not taken into account; (ii) the excessive values of q_l and q_t, obtained by Pietronero et al. for graphene [35] by using the Slater local-orbital approximation [34], are used; (iii) the superheating of the phonon gas is not taken into consideration. Everything noted above sets conditions for that there is a discrepancy between the value of l_l (l_t) calculated in the framework of the classical scattering theory and the value of l_l (l_t) obtained experimentally. As an example, this discrepancy is more than two times for (10, 10) nanotube. Therefore, to provide the agreement of theory with experiment it is necessary to use the values μ_l and μ_t instead of the value μ (the first improvement of the classical scattering theory) as well as the value of $q_l = 8.643\,\mathrm{nm}^{-1}$ and $q_t = 9.980\ \mathrm{nm}^{-1}$ instead of the value of $q_0 = 25\,\mathrm{nm}^{-1}$ (the second improvement of the classical scattering theory) while calculating the phonon scattering rates of electrons in armchair single-wall carbon nanotubes. Moreover, it is also necessary to take into account the non-equilibrium LA and LO phonons at high electric fields.

We think that we would succeed much more in the agreement of the theoretical results with the experimental ones if we considered the finite length nanotubes instead of the infinite ones. But in that case the computational complexity would increase much more, too. So, in conclusion we would like to say that our subsequent purpose is the calculation of the electrical characteristics of the armchair single-wall carbon nanotubes at various electric fields $F = F(t)$ in the framework of the developed scattering theory.

Acknowledgments

The authors gratefully wish to acknowledge Dr. D. Weiss for his careful examination of the paper.

References

[1] M.S. Dresselhaus, G. Dresselhaus, R. Saito, Solid State Commun. 84 (1992) 201.
[2] R.A. Jishi, M.S. Dresselhaus, G. Dresselhaus, Phys. Rev. B 48 (1993) 11385.
[3] T. Ando, T. Nakanishi, J. Phys. Soc. Japan 67 (1998) 1704.
[4] T. Hertel, G. Moos, Phys. Rev. Lett. 84 (2000) 5002.
[5] A. Sedeki, L.G. Caron, C. Bourbonnais, Phys. Rev. B 62 (2000) 6975.
[6] Zh. Yao, Ch.L. Kane, C. Dekker, Phys. Rev. Lett. 84 (2000) 2941.
[7] G. Dresselhaus, et al., in: D. Tomanek, R. Enbody (Eds.), Science and Application of Nanotubes, Kluwer Academic, Plenum, New York, 2000, p. 275.
[8] J. Taylor, H. Guo, J. Wang, Phys. Rev. B 63 (2001) 245407.
[9] S.G. Lemay, et al., Nature 412 (2001) 617.
[10] R. Klesse, Phys. Rev. B 66 (2002) 085409.
[11] K. Xiao, et al., Appl. Phys. Lett. 83 (2003) 150.
[12] S.J. Wind, J. Appenzeller, Ph. Avouris, Phys. Rev. Lett. 91 (2003) 058301.
[13] S. Heinze, J. Tersoff, Ph. Avouris, Appl. Phys. Lett. 83 (2003) 5038.
[14] A. Javey, et al., Phys. Rev. Lett. 92 (2004) 106804.
[15] S.V. Rotkin, K. Hess, Appl. Phys. Lett. 84 (2004) 3139.
[16] M.S. Dresselhaus, G. Dresselhaus, Ph. Avouris, Topics Appl. Phys. 80 (2001) 391.
[17] M. Dresselhaus, G. Dresselhaus, Ph. Avouris (Eds.), Carbon Nanotubes, Springer, Berlin, 2001.
[18] T.W. Odom, et al., J. Phys. Chem. B 104 (2000) 2794.
[19] T.W. Odom, et al., Nature 391 (1998) 62.
[20] D.V. Pozdnyakov, et al., in: P. Wegierek, T. Koltunowicz (Eds.), IV International Conference NEET'2005: New electrical and electronic technologies and their industrial implementation, PRINT-6, Lublin, 2005, p. 270.
[21] J.-Y. Park, et al., Nano Lett. 4 (2004) 517.
[22] D. Mann, et al., Nano Lett. 3 (2003) 1541.
[23] M. Lazzeri, et al., Phys. Rev. Lett. 95 (2005) 236802.
[24] T. Yamada, J. Sone, Phys. Rev. B 40 (1989) 6265.
[25] C. Jacoboni, P. Lugly, in: S. Selberherr (Ed.), The Monte Carlo Method for Semiconductor Device Simulation, Springer, Wien, New York, 1989.
[26] K. Hess (Ed.), Monte Carlo Device Simulation: Full Band and Beyond, Kluwer Academic Publishers, Boston, Dordrecht, London, 1991.
[27] V.M. Ivaschenko, V.V. Mitin, Monte Carlo Simulation of Kinetic Effects in Semiconductors, Naukova dumka, Kiev, 1990 (in Russian).
[28] V.M. Borzdov, F.F. Komarov, Simulation of Electrophysical Properties of Solid State Layer Structures of Integrated Electronics, BSU, Minsk, 1999 (in Russian).
[29] A.S. Davydov, Quantum Mechanics, Nauka, Moscow, 1973 (in Russian).
[30] D. Calecki, J. Phys. C: Solid State Phys. 19 (1986) 4315.
[31] V.M. Borzdov, et al., Phys. Low-Dim. Struct. 11/12 (2002) 21.
[32] V.M. Borzdov, et al., Phys. Lett. A 319 (2003) 379.
[33] D.V. Pozdnyakov, V.M. Borzdov, Phys. Solid State 45 (2003) 2348.
[34] S. Barisic, J. Labbe, J. Friedel, Phys. Rev. Lett. 25 (1970) 919.
[35] L. Pietronero, et al., Phys. Rev. B 22 (1980) 904.
[36] L. Wirtz, A. Rubio, Solid State Commun. 131 (2004) 141.
[37] R. Satio, et al., Appl. Phys. Lett. 60 (1992) 2204.
[38] V.M. Borzdov, et al., Phys. Low-Dim. Struct. 10 (1997) 63.
[39] V.M. Borzdov, et al., Proc. SPIE: Nanotubes and Nanowires 5219 (2003) 159.
[40] V. Borzdov, et al., Proc. SPIE: Nanomodeling 5509 (2004) 206.