Diamond & Related Materials 49 (2014) 72–76

Contents lists available at ScienceDirect

Diamond & Related Materials

journal homepage: www.elsevier.com/locate/diamond

Electron–phonon mechanism of conduction in magnetized nanotubes ☆

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ARTICLE INFO

Available online 7 August 2014

Keywords:
Nanotube
Conductivity
Electron–phonon scattering
Magnetic field
Aharonov–Bohm parameter

ABSTRACT

Analysis of the contribution of electron scattering on phonons, longitudinal and flexural resistance in the nanotube in a longitudinal magnetic field has been carried out quantitatively. The dependence of the conductance of the nanostructure on the nanotube radius, surface electron density, temperature, and Aharonov–Bohm parameter in the case of an isotropic phonon spectrum and taking into account the effects of phonons confinement has been studied.

1. Introduction

The electron scattering process in carbon nanotubes (CNT) attracts big research attention [1–5]. Among the most important mechanisms contributing to electron momentum relaxation in CNT are electron–phonon scattering, electron–electron scattering and scattering by static impurities. Balents and Fisher have previously shown that for dominant electron–electron interactions the resistivity behavior is linear on temperature [2]. On the other hand the electron–phonon scattering time increases also linearly with temperature [1,3,4], while impurity scattering in practice has no temperature dependence. As the result, the resistivity R vs. temperature T curves for single wall CNT is expected to be linear for both electron–electron and electron–phonon backscattering. Therefore, these two principal scattering mechanisms can hardly be discriminated on the basis of the R vs. T plots only. In this work we show the possibility to discriminate between them using a careful analysis of R vs. T curves.

Another possibility to distinguish between them can be revealed from the analysis of magnetic field dependences [6,7]. For the ballistic case, it was already shown [5–7] that a metal nanotube under application of a magnetic field is becoming an insulator. This is caused by the band gap increase with the Aharonov–Bohm parameter to a maximum value when $\Phi/\Phi_0 = 1/2$. Further increase in the magnetic flux reduces gap width to zero at $\Phi/\Phi_0 = 1$ [5–7]. Therefore, it will be important to carry out further theoretical and experimental work to explore the nanotube resistivity dependence from Aharonov–Bohm parameter for non-ballistic case with different mechanisms of electron–phonon interaction.

According to the results discussed in [3,4] ballistic approximation is valid for metallic carbon nanotubes with a length not exceeding the order of a few micrometers. For nanotubes with larger length [8] one of the most important scattering mechanisms should originate from acoustic phonons. In the reference [9] for the different mechanisms of electron scattering by acoustic phonons analytical formulas for the conductivity of a quantum cylinder in a longitudinal magnetic field were obtained, taking into account effects of phonon confinement. However, quantitative analysis of the results obtained in this work has not been completed. The purpose of this article is to quantify the contribution of the electron–phonon scattering to conductivity of nanostructure in dependence on the parameters of nanotubes, temperature and magnetic field.

2. The electron–phonon scattering and conductivity of the nanotube in a longitudinal magnetic field

The motion of an electron in an unperturbed electric field of the problem is described by the stationary solution of the Schrödinger equation on a cylindrical surface, with a dc magnetic field applied along the axis. The wave functions of the steady states and the energy spectrum are given by the formulas (Ref. [9]):

$$\psi(n, p_3) = \frac{1}{\sqrt{S}} \exp\left[in\phi + i\frac{zp_3}{\hbar}\right], \tag{1}$$

$$E(n, p_3) = \varepsilon\left(n + \frac{\Phi}{\Phi_0}\right)^2 + \frac{p_3^2}{2m}, \tag{2}$$

where m is the electron effective mass, p_3 is the electron longitudinal momentum, $S = 2\pi RL$ is the surface area of a nanotube of length L and radius R, $n \in Z$ is the azimuthal quantum number, $\varepsilon = \hbar^2/(2mR^2)$ is the dimensional confinement energy, $\Phi = \pi R^2 H$ is the magnetic flux through the cylinder cross-section, $\Phi_0 = 2\pi\hbar c/|e|$ is the magnetic flux quantum, and Φ/Φ_0 is the Aharonov–Bohm parameter.

☆ Presented at the International Conference on Diamond and Carbon Materials (DCM 2013), September 2–5, 2013, Riva del Garda, Italy.

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http://dx.doi.org/10.1016/j.diamond.2014.07.012
0925-9635/

Because we are interested in the linear response of the quantum cylinder to an external electric field, we express the Boltzmann kinetic equation in the relaxation time approximation as [10]

$$\frac{\partial f_1}{\partial t} + \left(\frac{p_3}{m}\right)\left(\frac{\partial f_o}{\partial E}\right)(eE_3) = -\frac{f_1}{\tau}. \tag{3}$$

Here, $f_0 = f_0(n,p_3)$ is the equilibrium electron distribution function in the original quantum state $p = (n,p_3)$; i.e.,

$$f_o(n,p_3) = \left\{ \exp\left[\frac{E(n,p_3)-\mu}{T}\right] + 1\right\}^{-1} \tag{4}$$

where f_1 is a correction to the equilibrium distribution function f_0, E_3 is the electric field along the cylinder axis, and μ is the chemical potential of the electron gas in the quantum cylinder. For the relaxation mechanism, we assume electron scattering by acoustic phonons.

Thus, the correction f_1 to the equilibrium distribution function is described by the formula

$$f_1(n,p_3) = (-e)\tau(n,p_3)\left(-\frac{\partial f_o}{\partial E(n,p_3)}\right)\left(\frac{p_3}{m}\right)E_3. \tag{5}$$

By summing the contributions of all transverse motion energy bands, for the longitudinal conductivity of the nanotube in the magnetic field we obtain the formula

$$\sigma = e^2 \sum_n \int_{-\infty}^{\infty} \left(\frac{1}{2\pi^2 R}\right)\left(\frac{p_3}{m}\right)^2 \tau(n,p_3)\left[-\frac{\partial f_0}{\partial E}\right] dp_3, \tag{6}$$

where $\rho = \sigma^{-1}$ indicates nanotube resistance per unit length.

First, consider electron scattering in the nanotube by acoustic phonons with an isotropic linear dispersion relation for the case in which the deformation scattering mechanism [9,11,12] prevails. In this case, the nanotube conductivity can be expressed as [9,12]

$$\sigma = \sum_{n,n'} \sigma_{n,n'}, \tag{7}$$

where

$$\sigma_{n,n'} = e^2 \frac{N_S^n}{m} \tau(n,n'), \tag{8}$$

and the inverse relaxation time is determined by the formula

$$\tau^{-1} = \frac{B_D m}{\pi}\frac{1}{p_F(n')}\int_0^{\infty} q_\perp J_{n-n'}^2(q_\perp R)\left[\left(1-\frac{p_F(n')}{p_F(n)}\right)\frac{\sqrt{q_\perp^2+(p_F-p_F{}')^2}}{\exp\left(\frac{v}{T}\sqrt{q_\perp^2+(p_F-p_F{}')^2}\right)-1} + \right.$$
$$\left. + \left(1+\frac{p_F(n')}{p_F(n)}\right)\frac{\sqrt{q_\perp^2+(p_F+p_F{}')^2}}{\exp\left(\frac{v}{T}\sqrt{q_\perp^2+(p_F+p_F{}')^2}\right)-1}\right] dq_\perp. \tag{9}$$

Here, $p_F(n)$ is the longitudinal Fermi momentum of the n-th energy band of the electron transverse motion, which is given by

$$p_F(n) = \frac{1}{R}\sqrt{(p_F R)^2 - \left(n+\frac{\Phi}{\Phi_0}\right)^2} = \pi^2 R N_S^n, \tag{10}$$

$p_F = \sqrt{2mE_F}$, E_F is the Fermi energy, N_S^n is the number of electrons in the n-th band per unit surface area of the quantum cylinder, T is temperature, and $J_n(x)$ is the Bessel function of the real argument.

Thus, formulas (7)–(10) solve the problem regarding the contribution of the electron–phonon scattering to the nanotube resistance in the presence of a longitudinal magnetic field in the relaxation time approximation for the case of an isotropic phonon spectrum. The dependence of the nanotube conductivity on the Aharonov–Bohm parameter and temperature is shown in Fig. 1a and b, respectively. A change in the fractional part of the Aharonov–Bohm parameter is accompanied by a change of approximately 10–20% in the conductivity, the reference value being the nanotube conductivity in the magnetic-field-free case. For the case of an isotropic phonon spectrum, the contribution of the electron–phonon scattering to the nanotube resistivity depends linearly on temperature at high temperatures and cubically at moderately low temperatures.

Next, consider electron scattering by longitudinal and flexural acoustic phonons. Let an acoustic wave with quasi-momentum q_3 along the nanotube axis and azimuthal quantum number l be excited in the nanotube. The explicit form of the polarization vector for various modes and of the corresponding dispersion laws for the acoustic vibrations in the long-wave approximation was obtained in Refs. [5,13]. It was shown that:

1. For an axisymmetric phonon ($l = 0$) in the long-wave limit, electrons interact via the deformation potential only with the longitudinal wave, which obeys a linear dispersion law, and the interaction amplitude is described by the formula

$$\Gamma(q_3,0) = iq_3\sqrt{\frac{E_d^2}{2S\rho E_{ph}(q_3,0)}}, \tag{11}$$

$$E_{ph}(q_3,0) = v|q_3|. \tag{12}$$

Here, E_d is the deformation potential constant, ρ is the surface density of the nanotube material, and $v \approx 10^4$ m/s is the longitudinal acoustic wave velocity.

2. In the long-wave approximation, where $|q_3|R \ll 1$, electrons interact via the deformation potential nearly only with the flexural wave, which obeys a quadratic dispersion law,

$$E_{ph}(q_3, l=\pm1) = vRq_3^2, \tag{13}$$

$$\Gamma(q_3, l=\pm1) = \frac{i}{R\sqrt{2}}\sqrt{\frac{E_d^2}{2S\rho E_{ph}(q_3, l=\pm1)}}. \tag{14}$$

The latter result corresponds to the dispersion relation for flexural waves in elastic rods, and the parameter v in Eq. (13) coincides with the longitudinal acoustic wave velocity. Thus, the electron–phonon interaction Hamiltonians with $l = 0$ and $l = \pm1$ on the cylindrical surface are given by

$$H_{\text{int}}(l=0) = \sum_{q_3}(iq_3)\sqrt{\frac{E_d^2}{2S\rho v|q_3|}}a(q_3)\cdot \quad \cdot \exp(iq_3 z - iv|q_3|t) + s.a. \tag{15}$$

$$H_{\text{int}}(l=\pm1) = \cdot \exp\left(iq_3 z \pm i\phi - ivRq_3^2 t\right) + s.a. \tag{16}$$

If only the longitudinal acoustic mode contributes to the scattering rate, then the conductivity of the quantum cylinder can be expressed as [9]

$$\sigma = \sum_n \sigma_n. \tag{17}$$

where

$$\sigma_n = \frac{e^2}{2m}N_S^n[\tau(p_F(n)) + \tau(-p_F(n))], \tag{18}$$