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Laser induced resistivity of chiral single wall carbon nanotubes

Anthony Twum , Samuel Yeboah Mensah, Raymond Edziah and Augustine Arthur
Department of Physics, University of Cape Coast, Cape Coast, Ghana
E-mail: atwum@ucc.edu.gh

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Abstract

Using the Boltzmann transport equation within the semi-classical approximation with constant relaxation time, we theoretically studied the dynamics of electrons in chiral single wall nanotubes (SWNTs) subjected to a temperature gradient (∇T) in the presence of a combined direct current and high frequency alternating fields. We obtained an expression for the resistivity (ρ_c) of the SWNTs which varies with temperature and depends among others on material's chiral angle (θ_h), dc field strength (E_o) and ac field amplitude (E_s). Our results show that chiral SWNTs exhibit metallic behavior with resistivity increasing approximately linearly with temperature over a wide temperature range well above 100 K. Based on the low chiral resistivity obtained for the SWNTs at room temperatures, we propose these materials as good candidates for possible optoelectronic applications.

1. Introduction

Carbon nanotubes (CNTs) are a class of nanomaterials that consist of two-dimensional hexagonal lattice of carbon atoms, bent and joined seamlessly in one direction so as to form a hollow cylinder [1, 2]. For the past few decades, interest in the study of CNTs has increased due to their unique electrical, electronic and mechanical properties caused by their small diameters and lattice orientation [3]; they can either be single-walled or multi-walled [3]. Single wall nanotubes (SWNTs) are produced in the outflow of a carbon arc and in much higher yield by laser vaporization of a graphite rod in an oven at 1200 °C [4]. SWNTs can either be semiconducting or metallic, depending on their diameter and chirality [5]. Authors in [6] studied the temperature dependent resistivity of single wall carbon nanotubes and compared their results with the predictions of the twiston theory [7]. The outcome of their study predicted that intrinsic resistivity of twistons is proportional to the absolute temperature. In this study, we investigate theoretically temperature dependent electrical resistivity of chiral SWNTs along the base helix in the presence of a laser using the Boltzmann's transport equation (BTE) with constant relaxation time. To the best of our knowledge, no such study has been reported.

2. Theory

We consider a chiral SWNT under a temperature gradient ∇T placed in an electric field applied along the nanotube axis. The carrier current density and resistivity in the SWNT are studied using the BTE following the approach of [8] together with the phenomenological model of a SWNT developed in references [9, 10]. The BTE which is based on the principle of conservation of charge, is a semi-classical formulation of transport and is capable of including self-consistently the transport of both electrons and phonons, as well as externally applied electric fields, electron-phonon interaction, anharmonic phonon decay, and many other types of scattering to a desired level of accuracy and detail [11]. Within the classical domain of the BTE, each particle is assumed to occupy a spatial and momentum coordinate and is described by a distribution function $f(r, p, t)$ which counts the number of particles occupying each set of coordinate in space and momentum. To express the conservation of particles in both space and time, the total rate of change in time is equated to the total rate of change in the distribution function due to various scattering mechanisms. In the semi-classical formulation of the BTE, position and momentum are both independent and functions of time only and can be expressed as [12]:

$$\frac{\partial f(r,p,t)}{\partial t}+v(p)\frac{\partial f(r,p,t)}{\partial r}+eE\frac{\partial f(r,p,t)}{\partial p}=-\frac{f(r,p,t)-f_0(p)}{\tau} \tag{1}$$

where $f(r, p, t)$ is the distribution function, $f_0(p)$ is the equilibrium distribution function, $v(p)$ is the electron velocity, r is the electron position, p is the electron dynamical momentum, t is the elapsed time , τ is the electron relaxation time which is assumed to be constant and e is the electronic charge. The applied dc-ac field, $E(t) = E_o + E_S \cos wt$, where E_o is the constant electric field. E_s and w are the amplitude and frequency of the ac field, respectively.

Using the perturbation approach, equation (1) is solved in which the second term on the left-hand side is treated as a weak perturbation. In the linear approximation of ∇T and quasi-fermi level $\nabla\mu$, the solution to equation (1) is expressed as

$$\begin{aligned} f(p)=\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)f_0\left(p-e\int_{t-t'}^{t}[E_0+E_s\cos wt']dt'\right)dt \\ +\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\left\{\left[\varepsilon\left(p-e\int_{t-t'}^{t}[E_0+E_s\cos wt']dt'\right)-\mu\right]\frac{\nabla T}{T}+\nabla\mu\right\} \\ \times v\left(p-e\int_{t-t'}^{t}[E_0+E_s\cos wt']dt'\right)\frac{\partial f_0}{\partial\varepsilon}\left(p-e\int_{t-t'}^{t}[E_0+E_s\cos wt']dt'\right) \end{aligned} \tag{2}$$

where μ is the electrochemical potential which ensures conservation of electrons and $\varepsilon(p)$ is the tight-binding energy of the electron.

The current density is defined as

$$j=e\sum_p v(p)f(p) \tag{3}$$

Substituting equation (2) into equation (3) gives

$$\begin{aligned} j=e\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p v(p)f_0\left(p-e\int_{t-t'}^{t}[E_0+E_s\cos wt']dt'\right) \\ +e\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p v(p)\left\{\left[\varepsilon\left(p-e\int_{t-t'}^{t}[E_0+E_s\cos wt']dt'\right)-\mu\right]\frac{\nabla T}{T}+\nabla\mu\right\} \\ \times v\left(p-e\int_{t-t'}^{t}[E_0+E_s\cos wt']dt'\right)\frac{\partial f_0}{\partial\varepsilon}\left(p-e\int_{t-t'}^{t}[E_0+E_s\cos wt']dt'\right) \end{aligned} \tag{4}$$

Making the transformation

$$p-e\int_{t-t'}^{t}[E_0+E_s\cos wt']dt'\to p$$

Equation (4) becomes

$$\begin{aligned} j=e\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p v\left(p-e\int_{t-t'}^{t}[E_0+E_s\cos wt']dt'\right)f_0(p) \\ +e\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p\left\{[\varepsilon(p)-\mu]\frac{\nabla T}{T}+\nabla\mu\right\} \\ \times\left\{v(p)\frac{\partial f_0(p)}{\partial\varepsilon}\right\}v\left(p-e\int_{t-t'}^{t}[E_0+E_s\cos wt']dt'\right) \end{aligned} \tag{5}$$

Using the phenomenological model [9, 10], a SWNT is considered as an infinitely long periodic chain of carbon atoms wrapped along a base helix. Based on this model, the circumferential and axial current densities can be expressed respectively in the form

$$j_c=S'\cos\theta_h \tag{6}$$

$$j_z=Z'+S'\sin\theta_h \tag{7}$$

where Z' and S' are respectively the components of the current density along the nanotube axis and the base helix, and θ_h is the chiral angle.

Neglecting the interference between the axial and helical paths connecting a pair of atoms, transverse motion quantization is ignored [9, 10]. This approximation best describes doped chiral carbon nanotubes and was experimentally confirmed in [13]. In our study, the analysis is restricted to the properties of the current density along the circumferential direction. Therefore, we resolve the current density along the base helix and obtain

$$S' = e\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p v_s\left(p - e\int_{t-t'}^{t}[E_0 + E_s\cos wt']dt'\right)f_0(p)$$
$$+ e\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p \left\{[\varepsilon(p) - \mu]\frac{\nabla_s T}{T} + \nabla_s\mu\right\}$$
$$\times \left\{v_s(p)\frac{\partial f_0(p)}{\partial\varepsilon}\right\}v_s\left(p - e\int_{t-t'}^{t}[E_0 + E_s\cos wt']dt'\right) \quad (8)$$

Using the transformation

$$\sum_p \rightarrow \frac{2}{(2\pi\hbar)^2}\int_{-\pi/d_s}^{\pi/d_s} dp_s\int_{-\pi/d_z}^{\pi/d_z} dp_z$$

in equation (8) where d_z and d_s are the inter-atomic distance along the nanotube axis and the base helix respectively, the flux along the base helix can further be expressed as

$$S' = \frac{2e\tau^{-1}}{(2\pi\hbar)^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\int_{-\pi/d_s}^{\pi/d_s} dp_s\int_{-\pi/d_z}^{\pi/d_z} dp_z v_s\left(p - e\int_{t-t'}^{t}[E_0 + E_s\cos wt']dt'\right)f_0(p)$$
$$+ \frac{2e\tau^{-1}}{(2\pi\hbar)^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\int_{-\pi/d_s}^{\pi/d_s} dp_s\int_{-\pi/d_z}^{\pi/d_z} dp_z\left\{[\varepsilon(p) - \mu]\frac{\nabla_s T}{T} + \nabla_s\mu\right\}$$
$$\times \left\{v_s(p)\frac{\partial f_0(p)}{\partial\varepsilon}\right\}v_s\left(p - e\int_{t-t'}^{t}[E_0 + E_s\cos wt']dt'\right) \quad (9)$$

where the integrations are carried out over the first Brillouin zone. The parameters v_s, p_s, E_s, ∇_sT, and $\nabla_s\mu$ represent the respective components of v, p, E, ∇T and $\nabla\mu$ along the base helix.

The energy dispersion relation for a chiral nanotube obtained in the tight-binding approximation is expressed as

$$\varepsilon(p) = \varepsilon_0 - \Delta_s\cos\frac{p_s d_s}{\hbar} - \Delta_z\cos\frac{p_z d_z}{\hbar} \quad (10)$$

where ε_o is the energy of an outer-shell electron in an isolated carbon atom, Δ_z and Δ_s are the real overlapping integrals for jumps along the respective coordinates, p_s and p_z are the components of momentum tangential to the base helix and along the nanotube axis, respectively. The components v_s and v_z of the electron velocity v are respectively

$$v_s(p) = \frac{\partial\varepsilon(p)}{\partial p_s} = \frac{\Delta_s d_s}{\hbar}\sin\frac{p_s d_s}{\hbar} \quad (11)$$

$$v_z(p) = \frac{\partial\varepsilon(p)}{\partial p_z} = \frac{\Delta_z d_z}{\hbar}\sin\frac{p_z d_z}{\hbar} \quad (12)$$

Also

$$v_s\left(p - e\int_{t-t'}^{t}[E_0 + E_s\cos wt']dt'\right) = \frac{\partial\varepsilon}{\partial p_s}\left(p - e\int_{t-t'}^{t}[E_0 + E_s\cos wt']dt'\right)$$
$$= \frac{\Delta_s d_s}{\hbar}\left\{\sin\frac{p_s d_s}{\hbar}\cos\left(p - e\int_{t-t'}^{t}[E_0 + E_s\cos wt']dt'\right)\right.$$
$$\left. - \cos\frac{p_s d_s}{\hbar}\sin\left(p - e\int_{t-t'}^{t}[E_0 + E_s\cos wt']d'\right)\right. \quad (13)$$

Similarly

$$v_z\left(p - e\int_{t-t'}^{t}[E_0 + E_s\cos wt']dt'\right) = \frac{\Delta_z d_z}{\hbar}\left\{\sin\frac{p_s d_s}{\hbar}\cos\left(p - e\int_{t-t'}^{t}[E_0 + E_s\cos wt']dt'\right)\right.$$
$$\left. - \cos\frac{p_z d_z}{\hbar}\sin\left(p - e\int_{t-t'}^{t}[E_0 + E_s\cos wt']dt'\right)\right. \quad (14)$$

To calculate the carrier current density for the non-degenerate electron gas of the SWNT, the Boltzmann equilibrium distribution function $f_0(p)$ is expressed in the form

$$f_0(p) = C\exp\left(\frac{\Delta_s\cos\frac{p_s d_s}{\hbar} + \Delta_z\cos\frac{p_z d_z}{\hbar} + \mu - \varepsilon_0}{kT}\right) \quad (15)$$

where C is a normalization constant and is defined as

$$C = \frac{d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)}\exp\left(-\frac{\mu - \varepsilon_0}{kT}\right)$$

and n_0 is the surface charge density, $I_n(x)$ is the modified Bessel function of the nth order, $\Delta_s^* = \frac{\Delta_s}{kT}$, $\Delta_z^* = \frac{\Delta_z}{kT}$ and k is the Boltzmann's constant.

Substituting equations (10)–(15) into equation (9) and evaluating the integrals, the following expression is obtained for S'.

$$S' = -\sigma_s(E)E_{sn}^* - \sigma_s(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0 - \mu}{kT}\right) - \Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)} + 2 - \Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s T \tag{16}$$

where we have defined

$$E_{sn}^* = E_n + \nabla_s\frac{\mu}{e}$$

Also, the electrical conductivity of the chiral SWNT is expressed as

$$\sigma_i(E) = \frac{e^2\tau\Delta_i d_i^2 n_0}{\hbar^2}\frac{I_1(\Delta_i^*)}{I_0(\Delta_i^*)}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{1}{1 + (ed_iE_0/\hbar + nw)^2\tau^2}\right],\ i = s,\ z \tag{17}$$

Substituting equation (16) into equation (6), the circumferential component of the current density is obtained as

$$j_c = -\sigma_s(E)\sin\theta_h\cos\theta_h E_{zn}^* - \sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\left\{\left(\frac{\varepsilon_0 - \mu}{kT}\right) - \Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)} + 2 - \Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_z T \tag{18}$$

Defining

$$\xi = \frac{\varepsilon_0 - \mu}{kT},\quad A_i = \frac{I_1(\Delta_i^*)}{I_0(\Delta_i^*)},\quad B_i = \frac{I_0(\Delta_i^*)}{I_1(\Delta_i^*)} - \frac{2}{\Delta_i^*},\quad i = s,\ z \tag{19}$$

the current density becomes

$$j_c = -\sigma_s(E)\sin\theta_h\cos\theta_h E_{zn}^* - \sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\{\xi - \Delta_s^*B_s - \Delta_z^*A_z\}\nabla_z T \tag{20}$$

The circumferential component of the electrical conductivity is the coefficient of the electric field E_{zn}^* and is given as

$$\sigma_c = \sigma_s(E)\sin\theta_h\cos\theta_h \tag{21}$$

The resistivity of the SWNT along its circumferential direction is defined as

$$\rho_c = \frac{1}{\sigma_s(E)\sin\theta_h\cos\theta_h} \tag{22}$$

3. Results and discussion

In this paper, we analytically studied the electrical resistivity of a chiral SWNT using the Boltzmann transport equation. An expression was derived for the circumferential component of the electrical conductivity in the presence of applied field E and is shown in equation (22). To analyze this expression numerically, a chiral SWNT having the following parameters was chosen: $d_s = 1$Å, $d_z = 2$Å, $\tau = 0.3 \times 10^{-12}$ s and $\theta_h = 4.0°$.

The ac source has a frequency, $w = 10^{12}\ s^{-1}$ and amplitude $E_s = 5 \times 10^7\ V\ m^{-1}$. The d. c. electric field, $E_o = 6.9063 \times 10^7 V\ m^{-1}$, chosen such that $\Omega\tau = 1$, where $\Omega\tau = ed_zE_o/\hbar$. Figure 1(a) shows the dependence of the circumferential electrical resistivity, ρ_c on temperature, T, for various fixed values of the dc field E_o.

It is observed that ρ_c changes slowly with temperature at low temperatures up to about 200 K and then increases linearly with increasing temperature. This trend is attributed to electron-phonon interactions which cause scattering of charge carriers along the circumferential direction of the chiral SWNT as temperature increases. The low values of resistivity observed clearly suggest that chiral SWNTs do exhibit metallic properties. Also noted is a significant increase in the circumferential resistivity as the electric field strength E_o increases. As E_o is increased, the electrons in the SWNT become more energetic, leading to increased collision with carbon atoms within the walls of the SWNT which sets these carbon atoms into large amplitude oscillations which enhance the scattering of the electrons. Experimentally, it has been observed that the resistivity of carbon

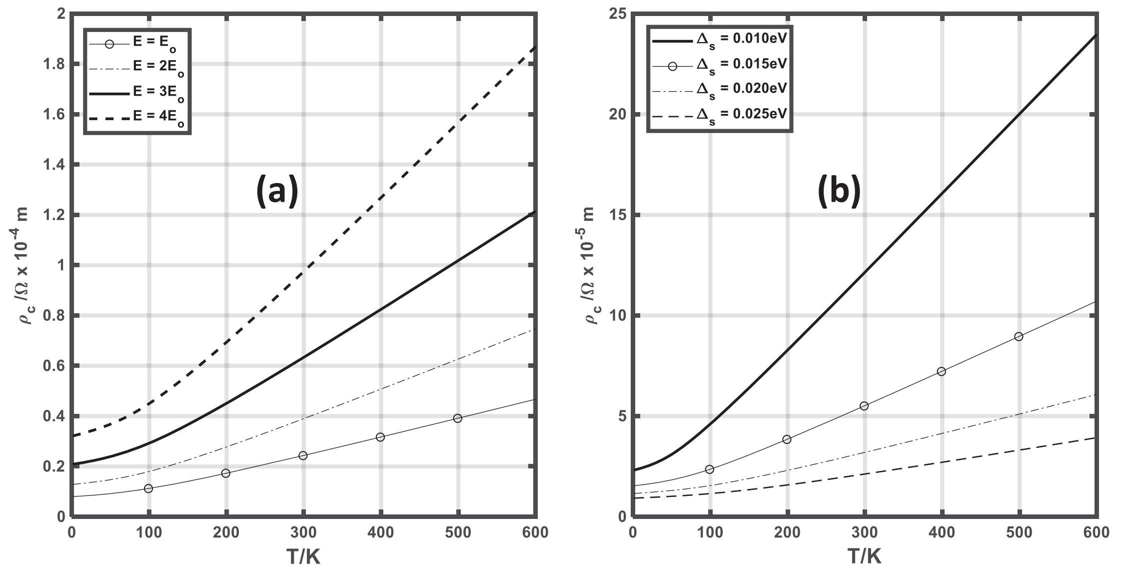

Figure 1. Dependence of circumferential current density (ρ_c) on temperature (T) for (a) fixed values of the d.c. field E_o, $2E_o$, $3E_o$ and $4E_o$, where $E_o = 6.9063 \times 10^7$ V m^{-1}. $E_s = 5.0 \times 10^7$ V m^{-1}, $\Delta_s = 0.018$ eV and $\Delta_z = 0.024$ eV (b) fixed values of Δ_s, $\Delta_z = 0.024$ eV, $E_s = 5.0 \times 10^7$ V m^{-1}, $E = 2E_o$, where $E_o = 6.9063 \times 10^7$ V m^{-1}.

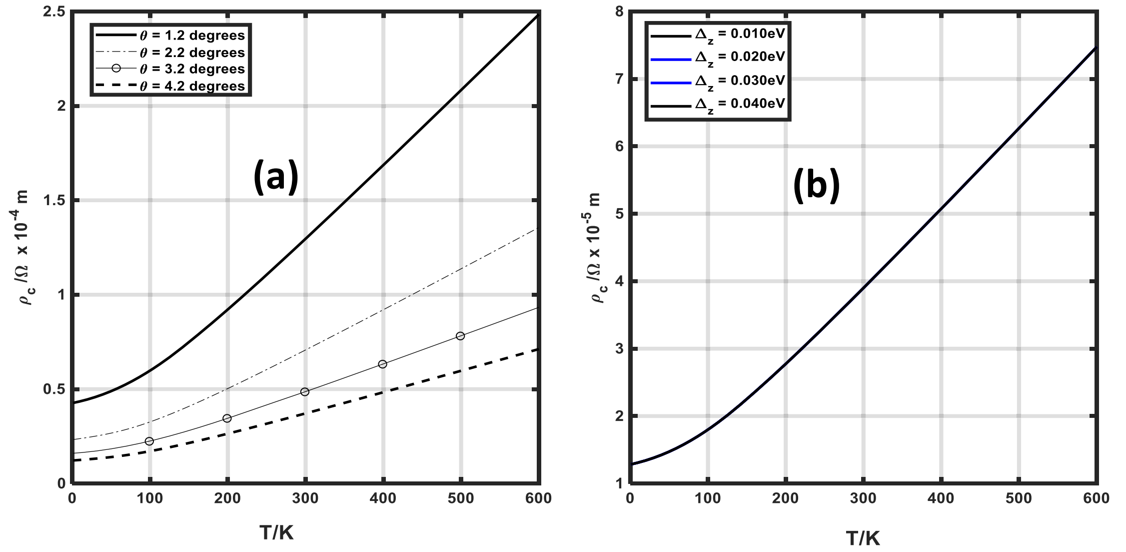

Figure 2. The variation of ρ_c with temperature for (a) various fixed values of chiral angle, θ_h. $\Delta_z = 0.024$ eV, $\Delta_s = 0.018$ eV, $E_s = 5.0 \times 10^7$ V m^{-1}, $E = 2E_o$, where $E_o = 6.9063 \times 10^7$ (b) The dependence of ρ_c on temperature for various fixed values of Δ_z, $\Delta_s = 0.018$ eV, $E_s = 5.0 \times 10^7$V m^{-1}, $E = 2E_o$, where $E_o = 6.9063 \times 10^7$V m^{-1}.

nanotubes varies with temperature [14–16]. The resistance generally decreases with decreasing temperature (as shown theoretically in our study) up to a threshold temperature which is determined by the type and purity of the carbon nanotube. Based on available experimental results, interesting electrical models have been developed as a function of temperature range and carbon nanotube fabrication technique [17, 18]. For chiral SWNTs however, our results are the first of such low temperature resitivity dependence study; to the best of knowledge. On the other hand, figure 1(b) shows that the resistivity decreases markedly with increasing Δ_s.

The dependence of the circumferential resistivity on temperature for given values of the chiral angle θ_h is depicted in figure 2(a). The figure shows that increasing θ_h results in a decrease in the resistivity ρ_c of the chiral SWNT.

Interestingly, figure 2(b) indicates that keeping Δ_s constant and altering Δ_z reduces ρ_c by an order of magnitude.

When the ac source is switched off, $E_s = 0, a = 0, w = 0$ and $J_n^2(a)$ becomes unity and equation (17) reduces to

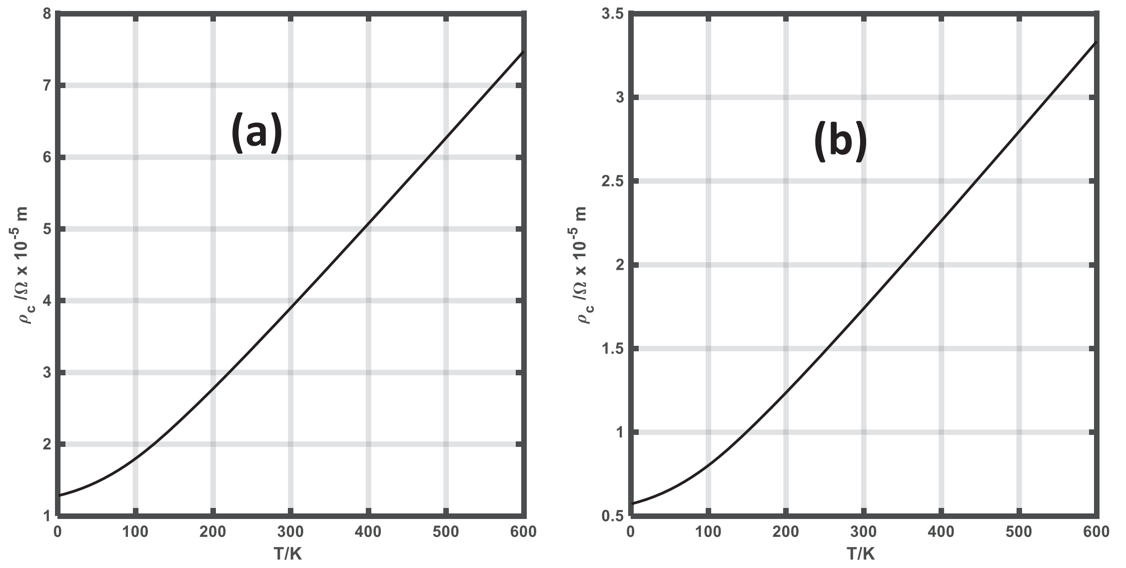

Figure 3. The dependence of ρ_c on temperature T for $\Delta_s = 0.018$ eV, $\Delta_z = 0.024$ eV, E = 2 E_o. $E_s = 5 \times 10^7$V m^{-1} and chiral angle, $\theta_h = 4.0°$ for the case in which (a) laser is turned and (b) laser is turned off.

$$\sigma_i(E) = \frac{e^2\tau\Delta_i d_i^2 n_0}{\hbar^2}\frac{I_1\Delta_i^*}{I_0\Delta_i^*}\left[\frac{1}{1+(ed_iE_0/\hbar)^2\tau^2}\right],\ i = s,\ z.$$

Figure 3 shows the circumferential current density dependence on temperature in the presence of a laser (laser on) and absence of a laser (laser off).

It is noted that when the laser source is off, ρ_c reduces by a factor of two which indicates that within the temeperature range under consideration, the laser field modulates the dc field and enhances the momentum and kinetic energy of those electrons which are deficient in energy.

4. Conclusion

The circumferential resistivity, ρ_c of a chiral SWNT induced with a laser field has been investigated using the semi-classical approach. Our results indicate that the nanotube parameters (Δ_s, Δ_z, θ_h) and the d.c. field E_o and laser source strength E_s have significant influence on the resistivity with ρ_c increasing with increasing E_o. The results reveal that increases in both Δ_s and θ_h decrease ρ_c. The observed low resistivity exhibited by the chiral SWNT at increasing temperatures indicate that this unique material is a good conductor of electricity and could serve as a good candidate for optoelectronic applications.

ORCID iDs

Anthony Twum https://orcid.org/0000-0002-5358-1115

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