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Direct Current Generation in Carbon Nanotubes by Terahertz Field

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Abstract

We report on a theoretical investigation of a direct current generation in carbon nanotubes (CNTs) that are stimulated axially by terahertz (THz) field. We consider the kinetic approach based on the semiclassical Boltzmann's transport equation with constant relaxation time approximation, together with the energy spectrum of an electron in the tight-binding approximation. Our results indicate that for strong THz-fields, there is simultaneous generation of DC current in the axial and circumferential directions of the CNTs, even at room temperature. We found that a THz-field can induce a negative conductivity in the CNTs that leads to the THz field induced DC current. For varying amplitude of the THz-field, the current density decreases rapidly and modulates around zero with interval of negative conductivity. The interval decreases with increasing the amplitude of the THz-field. We show that the THz-field can cause fast switching from a zero DC current to a finite DC current due to the quasi-ballistic transport, and that electron scattering is a necessary condition for switching.

1. Introduction

Investigation into the electronic properties of carbon nanotubes (CNTs) has attracted a great deal of interests ev-

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er since the discovery of these quasi-one-dimensional monomolecular structures by Iijima [1]. This may be due to their intriguing properties. The oscillatory response of the CNTs to moderate electric field strength makes CNTs inherently nonlinear, and as such, can exhibit plethora of transport phenomena. Under different conditions of an external electric field, an electron in CNT is predicted to reveal a variety of physical effects such as Bloch oscillations, self-induced transparency, negative differential conductivity, absolute negative conductance [2]-[9], and many more. Furthermore, CNTs have been shown to exhibit ballistic transport [10]-[12], Coulomb-blockade [13] [14], Luttinger Liquid [15] [16] and superconductivity [17] [18]. The unique architecture and physico-chemical properties have undoubtedly led to CNT which has been identified as a promising candidate for the fundamental building block of new generation of nanoelectronics [19]-[22], sensors [23] [24], electrochemical capacitors [25]-[27], Li-ion batteries [28]-[30] and terahertz (THz) generation and amplification [31]-[35], just to mention a few. There are several reports on CNTs for THz application [31]-[35]. Most of these reports focus on room temperature generation of THz radiation. Different proposals of CNTs for THz applications have been made. These ranges from multipliers [31] [32], amplifies [33], switches [34] to antennas [35] (see also [36]-[41]).

However, there are very limited reports on the effect of THz-fields on the transport properties of CNTs.

In this report, we present a theoretical investigation of the influence of THz-fields on the conductivity of CNTs that are stimulated axially, by considering the kinetic approach based on the semiclassical Boltzmann's transport equation with constant relaxation time approximation, together with the energy spectrum of electron in the tight-binding approximation, and predict the generation of DC current in both axial and circumferential directions of the CNTs.

2. Theory

We start with the Boltzmann equation and proceed as in refs [42]-[44],

$$\frac{\partial f}{\partial t} - \frac{e}{c}\frac{\partial A}{\partial t}\sum_i \frac{\partial f}{\partial p_i} = \frac{\left[F - f\left(p_i, t\right)\right]}{\tau} \tag{1}$$

In accordance with ref. [4]-[6] [11], we find that the distribution function is periodic in the quasimomentum and can be written in Fourier series as;

$$F\left(p_\gamma; p_\xi\right) = \frac{n_0 d_\gamma d_\xi}{2 I_0\left(\dfrac{\Delta_\gamma}{kT}\right) I_0\left(\dfrac{\Delta_\xi}{kT}\right)} \sum_{m=-\infty}^{\infty} I_m\left(\frac{\Delta_\gamma}{kT}\right) \sum_{n=-\infty}^{\infty} I_n\left(\frac{\Delta_\xi}{kT}\right) \mathrm{e}^{i\left(m\frac{p_\gamma d_\gamma}{\hbar} + n\frac{p_\xi d_\xi}{\hbar}\right)} \tag{2}$$

where e is electronic charge, the index $i = \gamma, \xi$; p_γ and p_ξ are components of the electron dynamical momentum along the axial and tubular axes respectively; $f \equiv f\left(p_\gamma; p_\xi; t\right)$ is the distribution function, and $F\left(p_\gamma; p_\xi\right)$ is the equilibrium distribution function; while τ is the electron relaxation time and assumed to be constant. The electric field is related to the vector potential A as $E = \frac{1}{c}\frac{\partial A}{\partial t}$. I_m is the modified Bessel function of the order m and $\hbar$ is Planck's constant, finally d_ξ and d_γ are the distances between along the axis and helix respectively.

The solution of Equation (1) by the method of characteristics is obtained in [5] [6] [11] as;

$$f\left(p_i, t\right) = F\left(p_\gamma; p_\xi + \frac{e}{c}A(t)\right)\mathrm{e}^{-\frac{t}{\tau}} + \frac{1}{\tau}\int_0^t \mathrm{e}^{-\frac{t}{\tau}}F\left(p_\gamma; p_\xi + \frac{e}{c}A(t)\right)\mathrm{d}t \tag{3}$$

Interesting to us is the situation that $vt \gg 1$ and Equation (2) reduces to the form

$$f\left(p_i, t\right) = \frac{1}{\tau}\int_0^t \mathrm{e}^{-\frac{t}{\tau}}F\left(p_\gamma; p_\xi + \frac{e}{c}A(t)\right)\mathrm{d}t \tag{4}$$

We proceed as in [5] [6] by considering an infinitely long chain of carbon atoms wrapped along a base helix as a model of a SWNT. This phenomenological model gives analytical tractability, which easily provides physically interpretable results. Also, the model gives a correct qualitative description of various electronic processes which are corroborated by the first principle numerical simulations. Thus, using the simple model of the tight-binding approximation, we describe the energy spectrum of the CNTs as ref [5] [6].

$$\varepsilon(p) = \varepsilon_o - \Delta_\gamma \cos\frac{p_\gamma d_\gamma}{\hbar} - \Delta_\xi \cos\frac{p_\xi d_\xi}{\hbar} \tag{5}$$

where ε_o is the energy of an outer-shell electron in an isolated carbon atom, Δ_γ and Δ_ξ are the real overlapping integrals for jumps along the respective coordinates.

The electron quasi classical velocity components for $v_\gamma(p_\gamma)$ and $v_\xi(p_\xi)$ are obtained as in refs [5] [13];

$$V_\gamma(p_\gamma) = \frac{\partial \varepsilon(p_\gamma)}{\partial p_\gamma} = \frac{\Delta_\gamma d_\gamma}{\hbar} \sin\left(\frac{p_\gamma d_\gamma}{\hbar}\right) \tag{6a}$$

$$V_\xi(p_\xi) = \frac{\partial \varepsilon(p_\xi)}{\partial p_\xi} = \frac{\Delta_\xi d_\xi}{\hbar} \sin\left(\frac{p_\xi d_\xi}{\hbar}\right) \tag{6b}$$

and the electron fluxes along the tubular axis and the base helix are given by after making the transformation $p \rightarrow p + \frac{e}{c}A(t)$ as ref [5] [6];

$$\xi = \frac{2e\tau^{-1}}{(2\pi\hbar)^2} \int_{-\frac{\pi\hbar}{d_\gamma}}^{\frac{\pi\hbar}{d_\gamma}} dp_\gamma \int_{-\frac{\pi\hbar}{d_\xi}}^{\frac{\pi\hbar}{d_\xi}} dp_\xi V_\xi\left(p_z + \frac{e}{c}A_\xi(t)\right) F(p_\xi) \tag{7a}$$

$$\gamma = \frac{2e\tau^{-1}}{(2\pi\hbar)^2} \int_{-\frac{\pi\hbar}{d_\xi}}^{\frac{\pi\hbar}{d_\xi}} dp_\xi \int_{\frac{\pi\hbar}{d_\gamma}}^{\frac{\pi\hbar}{dp_\gamma}} dp_\gamma V_\gamma\left(p_\gamma + \frac{e}{c}A_\gamma(t)\right) F(p_\gamma) \tag{7b}$$

where the integration is done over the first Brilloiun zone. The expressions for the axial and the circumferential components are as in [5];

$$j_\xi = \xi + \gamma \sin\theta_h \tag{8a}$$

$$j_\gamma = \gamma \cos\theta_h \tag{8b}$$

where θ_h is the chiral angle. We consider the CNTs stimulated by a uniform electric field E_o with a uniform sinusoidal THz radiation field of frequency ω_1 and amplitude E_1 *i.e.*, $E(t) = E_o + E_1 \cos\omega_1 t$. Substituting Equations (4) and (6) into Equation (7), we obtained the following direct current density expression from Equation (8) for circumferential and axial directions, respectively.

$$J_\xi = \frac{n_0 e \Delta_\xi d_\xi}{\hbar} \frac{I_1\left(\frac{\Delta_\xi}{kT}\right)}{I_0\left(\frac{\Delta_\xi}{kT}\right)} \sum_{v=-\infty}^{\infty} \frac{J_v^2(\beta_\xi)(\Omega_{o\xi} + v\omega)\tau}{1 + (\Omega_{o\xi}\tau + v\omega\tau)^2} + \frac{n_0 e \Delta_\gamma d_\gamma}{\hbar} \frac{I_1\left(\frac{\Delta_\gamma}{kT}\right)}{I_0\left(\frac{\Delta_\gamma}{kT}\right)} \sum_{v=-\infty}^{\infty} \frac{J_v^2(\beta_\gamma)(\Omega_{o\gamma} + v\omega)\tau}{1 + (\Omega_{o\gamma}\tau + v\omega\tau)^2} \sin(\theta_h) \tag{9a}$$

$$J_\gamma = \frac{n_0 e \Delta_\gamma d_\gamma}{\hbar} \frac{I_1\left(\frac{\Delta_\gamma}{kT}\right)}{I_0\left(\frac{\Delta_\gamma}{kT}\right)} \sum_{v=-\infty}^{\infty} \frac{J_v^2(\beta_\gamma)(\Omega_{o\gamma} + v\omega\tau)\tau}{1 + (\Omega_{o\gamma}\tau + v\omega\tau)^2} \cos(\theta_h) \tag{9b}$$

where $\Omega_{oi} = \frac{eE_{oi}d_i}{\hbar} (i = \xi, \gamma)$, $J_{0i} = \frac{n_0 e \Delta_i d_i}{\hbar} \frac{I_1\left(\frac{\Delta_i}{kT}\right)}{I_0\left(\frac{\Delta_i}{kT}\right)}$ and $\beta_i = \frac{eE_i d_i}{\hbar\omega}$.

If we re-write expressions (9) in the form of ref [44] and using the simplest case for [5] [6] that $\Delta_\xi = \Delta_\gamma$, $d_\xi = d_\gamma$, $\Omega_{o\xi} = \Omega_{o\gamma}$ and $\beta_\xi = \beta_\gamma$, we obtain the static current density as;

$$J_\xi = J_0 \sum_{v=-\infty}^{\infty} J_v^2(\beta_\xi) J_i^{dc}(\Omega_{o\xi} + v\omega)\tau \left[1 + \sin(\theta_h)\right] \tag{10a}$$

and

$$J_\gamma = J_0 \sum_{v=-\infty}^{\infty} J_v^2 (\beta_\gamma) J_i^{dc} (\Omega_{o\gamma} + v\omega) \tau \cos(\theta_h) \tag{10b}$$

respectively.

where $\xi = \gamma$ and $J_i^{dc} = J_{0i} \dfrac{(\Omega_{oi})\tau}{1+(\Omega_{oi}\tau)^2}$.

Equation (10) show the ac field can open up new transport channel for DC current as a result of multiphoton absorption or emission with probability of emission or absorption of photon given by $J_v^2(\beta_i)$ (see [44]).

For quasi static case *i.e.* $v\omega\tau \ll 1$, expression (9) reduces to;

$$\frac{J_\xi(\beta_\xi)}{J_\varepsilon} = \sum_{v=-\infty}^{\infty} \frac{J_v^2(\beta_\gamma)(\Omega_{o\gamma})\tau}{1+(v\omega\tau)^2 \left(\dfrac{\Omega_{o\gamma}\tau}{v\omega\tau}+1\right)^2} \tag{11a}$$

$$\frac{J_\gamma(\beta_\gamma)}{J_\delta} = \sum_{v=-\infty}^{\infty} \frac{J_v^2(\beta_\gamma)(\Omega_{o\gamma})\tau}{1+(v\omega\tau)^2 \left(\dfrac{\Omega_{o\gamma}\tau}{v\omega\tau}+1\right)^2} \tag{11b}$$

here $J_\varepsilon = J_{0i}[1+\sin(\theta_h)]$ and $J_\delta = J_{0i}\cos(\theta_h)$.

From Equation (11) we obtain the normalized differential conductivity as;

$$\frac{\sigma_i^{dc}}{\sigma_i^o} = \sum_{v=-\infty}^{\infty} J_v^2(\beta_i) \left[\frac{1-(v\omega\tau)^2 \left((\Omega_{oi}\tau/v\omega\tau)^2 - 1\right)}{\left(1+(v\omega\tau)^2 (\Omega_{oi}\tau/v\omega\tau+1)^2\right)^2} \right] \tag{12}$$

where $\sigma_i^o = \dfrac{n_0 e^2 \Delta_i d_i^2}{\hbar^2} \dfrac{I_1\left(\dfrac{\Delta_i}{kT}\right)}{I_0\left(\dfrac{\Delta_i}{kT}\right)}$.

3. Results and Discussion

We present the results of the kinetic equation approach of a CNT subjected to inhomogeneous THz field of the form $E(t) = E_o + E_1 \cos\omega_1 t$. The Boltzmann's equation is solved in the framework of constant relaxation time approximation. The expressions for the direct current densities along the axial and circumferential directions of the chiral CNT are given in Equation (9). The nonlinearity is analyzed using the dependence of the normalized direct current density J_i/j_{0i} as a function of the ac amplitude β_i for $\Omega\tau = 0.3$, 0.5, 0.9, 1 and 2.

In **Figure 1**, we show the dependence of the current density J_i/j_{0i} on the ac amplitude β_i, Equation (9), *i.e.*, when the CNTs are stimulated axially with a combination of a uniform electric field E_0 and a uniform sinusoidal THz radiation field of frequency ω_1 and amplitude $E_1 (E(t) = E_o + E_1 \cos\omega_1 t)$. The behavior is similar in the axial and circumferential directions. In the region of strong scattering ($\omega\tau < 1$) the DC conductivity J_i/j_{0i} remains positive, but decreases with increasing the strength of the ac amplitude. However, for ($\omega\tau > 1$), the current density decreases strongly with increasing β_i and then oscillates around $J_i/j_{0i} = 0$ with intervals of negative conductivity. The arrows in **Figure 1** indicate the regions of negative conductivity. We observed that the width of the intervals of the negative conductivity is largest at $\omega\tau \sim 2$ and decreases with decreasing scattering. The results indicate that negative conductance can be generated in chiral CNTs at room temperature by axial stimulation of the CNTs with THz frequencies ($\rightarrow 10^{12}$ Hz). On the other hand, the stable state with THz induced DC current is the region of dynamic localization for $\omega\tau \sim 2$ and is indicated by black boxes (see **Figure 2**). This suggests that stimulation of chiral CNTs with THz fields at room temperature can lead to switching from zero DC current to a finite DC current state, a process of quasi-ballistic electron transport where electron scattering is a critical component for the switching.
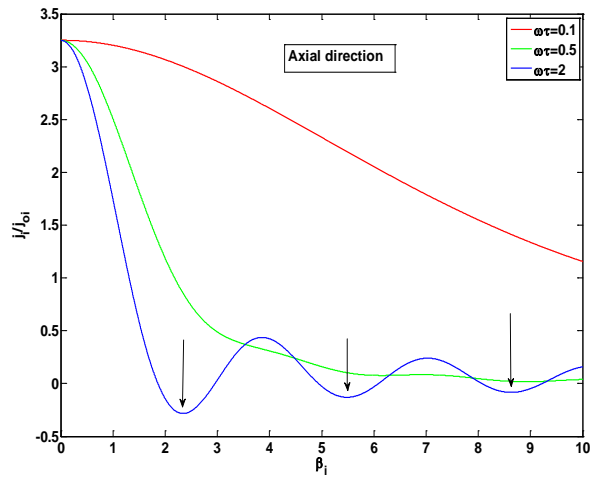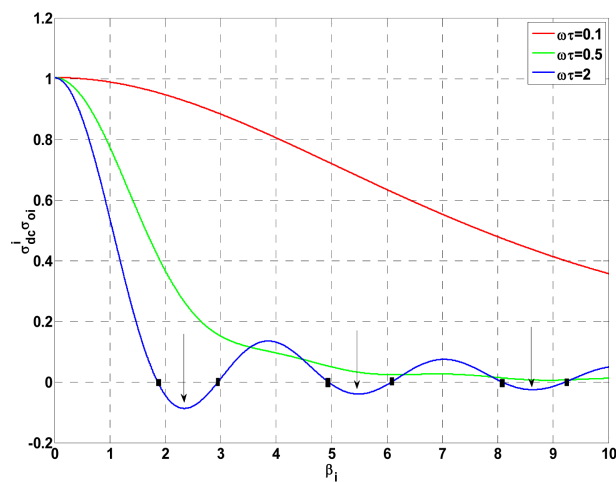
(a)
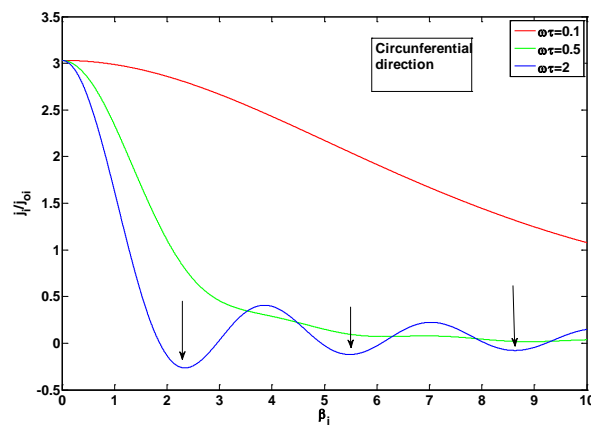
(b)

Figure 1. A plot of a normalized DC current density J_i/j_{0i} of CNTs obtained from expression (9) as a function of ac current amplitude β_i for (a) axial component (b) circumferential component when $\omega\tau = 0.1$, 0.5, and 2.

Figure 2. A plot of a DC conductivity $\sigma^i_{dc}/\sigma_o i$ of CNTs obtained from expression (12) as a function of ac current amplitude β_i. The arrows indicate regions of negative conductivity and the black shades show regions of dynamical location which is the stable state with THz induced DC current.

4. Conclusion

In conclusion, we considered the nonlinear electronic properties in CNTs stimulated by a high frequency THz field, *i.e.*, $E(t) = E_o + E_1 \cos \omega_1 t$ using the Boltzmann's kinetic equation in the constant relaxation time. The results indicate the creation of DC current densities along the axial and circumferential directions of the chiral CNTs.

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