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# High frequency conductivity in carbon nanotubes

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We report on theoretical analysis of high frequency conductivity in carbon nanotubes. Using the kinetic equation with constant relaxation time, an analytical expression for the complex conductivity is obtained. The real part of the complex conductivity is initially negative at zero frequency and become more negative with increasing frequency, until it reaches a resonance minimum at $\omega \sim \omega_B$ for metallic zigzag CNs and $\omega < \omega_B$ for armchair CNs. This resonance enhancement is indicative for terahertz gain without the formation of current instabilities induced by negative dc conductivity. We noted that due to the high density of states of conduction electrons in metallic zigzag carbon nanotubes and the specific dispersion law inherent in hexagonal crystalline structure result in a uniquely high frequency conductivity than the corresponding values for metallic armchair carbon nanotubes. We suggest that this phenomenon can be used to suppress current instabilities that are normally associated with a negative dc differential conductivity. *Copyright 2012 Author(s). This article is distributed under a Creative Commons Attribution 3.0 Unported License.* [http://dx.doi.org/10.1063/1.4771677]

## I. INTRODUCTION

The nonlinear dynamics of electrons in carbon nanotubes (CNs) under the action of an external electric field has been the subject of intense research.[1–5] Tans *et. al.*[1] and Bezryadin *et. al.*[2] have measured the current-voltage characteristics for single-wall CNs at low temperatures, i.e when $k_B T < \mathcal{E}_C, \Delta \mathcal{E}$, where $k_B$ is Boltzmann constant, $T$ is the temperature, $\epsilon_C$ is the charging energy. The energy level spacing $\Delta \mathcal{E}$ is given by $\Delta \mathcal{E} = \pi \hbar v_F / L$ where $v_F$ is the Fermi velocity and $L$ is the carbon nanotube length.[4] At this low temperatures the current is produced by the electrons tunneling through the CNs in the presence of the Coulomb blockade induced by long-range Coulomb interactions.[4] Nonlinear coherent transport through doped nanotube junctions was considered in Ref. 3 and it also showed the possibility of negative differential conductivity (NDC) for tunneling electrons. Using semiclassical Boltzmanns equation, Maksimenko *et. al.*[4] found that the dc current-voltage characteristics of CNs biased by a constant electric field along the axis of undoped CNTs at room temperatures ($k_B T > \mathcal{E}_C, \Delta \mathcal{E}$) showed NDC up to frequencies on the order of the Bloch frequency. Here the current density is produced by conduction electrons with energies below the energy of the interband transitions and move in the crystalline field like free quasiparticles, with a modified dispersion law allowing the use of quasiclassical approach to describe the electron motion. However, existing theories on Bloch oscillations have been observed in semiconductor

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superlattices.[6,7] These Bloch oscillations are caused by Bragg reflection of electrons at the edges of the Brillouin regions and the occurrence of Bloch oscillations are concluded from the observation of NDC. Also see.[8–12]

Like Maksimenko *et. al.*,[4] quantum phenomena like interband transitions, quantum mechanical corrections to intraband motion as well as Coulomb interactions will be excluded from this report. Our report will be quasiclassical with an extension to the high-frequency electric field in CNs by following the approach of Ktitorov *et. al.*[8]

## II. THEORETICAL MODEL

Following,[8] the high-frequency differential conductivity is derived starting with the Boltzmann kinetic equation. For simplicity, we shall ignore the difference between the energy - momentum relaxation rates and assume a common relaxation time $\tau$ for both processes. The equations of the symmetric $f_s$ and antisymmetric $f_a$ parts of the distribution functions are

$$\frac{\partial f_s}{\partial t} + eE(t)\frac{\partial f_a}{\partial k_x} = -\frac{[f_s - f_0(p)]}{\tau}. \tag{1}$$

$$\frac{\partial f_a}{\partial t} + eE(t)\frac{\partial f_a}{\partial k_x} = -\frac{f_a}{\tau}. \tag{2}$$

Writing the distribution functions in Fourier series as

$$f_a^1 = \Delta p_\varphi \sum_{s=1}^{n} \delta(p_\varphi - s\Delta p_\varphi) \sum_{r \neq 0} f_{rs} e^{ibrp_z} \Phi_a^1, \tag{3}$$

$$f_s^1 = \Delta p_\varphi \sum_{s=1}^{n} \delta(p_\varphi - s\Delta p_\varphi) \sum_{r \neq 0} f_{rs} e^{ibrp_z} \Phi_s^1, \tag{4}$$

$$f_0(p) = \Delta p_\varphi \sum_{s=1}^{n} \delta(p_\varphi - s\Delta p_\varphi) \sum_{r \neq 0} f_{rs} e^{ibrp_z}, \tag{5}$$

where $e$ is the electron charge, $f_0(p)$ is the equilibrium distribution function, $\delta(x)$ is the Dirac delta function, $r$ is summation over the stark component, $f_{rs}$ is the coefficient of the Fourier series and $\Phi_s^1$ and $\Phi_a^1$ are the factors by which the Fourier transform of the symmetric $f_s^1$ and antisymmetric $f_a^1$ parts of the distribution functions are different from the equilibrium distribution function $f_0(p, t)$ and $\tau_e = \tau_p = \tau$ is the relaxation time. The electric field $E$ is applied along CNs axis and the equilibrium distribution function can be expanded in the analogous series with the coefficients $f_{rs}$ expressed as

$$f_{rs} = \frac{a}{2\pi} \int_0^{\frac{2\pi}{a}} \frac{e^{-ibrp_z}}{1 + exp(\mathcal{E}_s(p_z)/k_B T)} dp_z. \tag{6}$$

Similarly, expanding $\mathcal{E}_s(p_z)/\gamma_0$ in Fourier series with coefficients $\mathcal{E}_{rs}$ defined as

$$\mathcal{E}_{rs} = \frac{a}{2\pi} \int_0^{\frac{2\pi}{a}} \mathcal{E}_s(p_z) e^{-iarp_z} dp_z$$

The investigation is done within the semiclassical approximation in which conduction electrons with energy below the energy of the interband transitions move in the crystalline lattice like free quasi-particles with dispersion law extracted from quantum theory.[4] Taking into account the hexagonal crystalline structure of a rolled graphene in a form of CNT and using the tight binding approximation, the energy dispersion for zigzag and armchair CNTs for which the Fermi energy $E_F = 0$, are expressed

as in Eqs. (7) and (8), respectively[4, 14, 15]

$$\mathcal{E}_s(s\Delta p_\varphi, p_z) \equiv \mathcal{E}_s(p_z)$$

$$= \pm\gamma_0\Big[1 + 4cos(ap_z)cos\left(\frac{a}{\sqrt{3}}s\Delta p_\varphi\right)$$

$$+ 4cos^2\left(\frac{a}{\sqrt{3}}s\Delta p_\varphi\right)\Big]^{1/2} \tag{7}$$

and

$$\mathcal{E}_s(s\Delta p_\varphi, p_z) \equiv \mathcal{E}_s(p_z)$$

$$= \pm\gamma_0\Big[1 + 4cos(as\Delta p_\varphi)cos\left(\frac{a}{\sqrt{3}}p_z\right)$$

$$+ 4cos^2\left(\frac{a}{\sqrt{3}}p_z\right)\Big]^{1/2} \tag{8}$$

where $\gamma_0 \sim 3.0$ eV is the overlapping integral, $p_z$ is the axial component of quasi-momentum, $\Delta p_\varphi$ is transverse quasi-momentum level spacing and $s$ is an integer. The expression for a in Eqns (7) and (8) is given as $a = 3b/2\hbar$, $b = 0.142$ nm is the C-C bond length. The "−" and "+" signs correspond to the valence and conduction bands respectively. Due to the transverse quantization of the quasi-momentum, its transverse component can take n discrete values, $p_\varphi = s\Delta p_\varphi = (\pi\sqrt{3}s)an$ ($s = 1, \ldots, n$). Unlike transverse quasi-momentum $p_\varphi$, the axial quasi momentum is assumed to vary continuously within the range $0 \le p_z \le 2\pi/a$, which corresponds to the model of infinitely long of CNT ($L = \infty$).

The quasiclassical velocity $v_z(p_z, s\Delta p_\varphi)$ of an electron moving along the CNT axis is given by the expression

$$v_z(p_z, s\Delta, p_\varphi) = \frac{\partial\mathcal{E}_s(p_z)}{\partial p_z} = \gamma_0 \sum_{r \ne 0} iar\mathcal{E}_{rs}e^{ibrp_z}. \tag{9}$$

The surface current density is also defined by the integral over the first Brillouin zone as:

$$j_z = \frac{2e}{(2\pi\hbar)^2} \int\int f(p)v_z(p)d^2p.$$

or

$$j_z = \frac{2e}{(2\pi\hbar)^2} \sum_{s=1}^{n} \int_0^{\frac{2\pi}{a}} f(p_z, s\Delta p_\varphi, \Phi_v(t))v_z(p_z, s\Delta p_\varphi)dp_z. \tag{10}$$

By linearizing Eqs. (3)–(5) with the perturbations $f_s = f_s^0 + f_s^1 exp(-i\omega t)$, $f_a = f_a^0 + f_a^1 exp(-i\omega t)$ and $E = E_0 + E_1 exp(-i\omega t)$ and substituting into Eqn (1) and (2) we obtain the high-frequency conductivity as:

$$\sigma_z(\omega) = \sigma_0 \sum_{r=1} r^2 \left[\frac{1 - i\omega\tau - (r\omega_B\tau)^2}{(r^2\omega_B^2 - \omega^2)\tau^2 + 1 - 2i\omega\tau}\right]$$

$$\times \sum_{s=1}^{n} f_{rs}\epsilon_{rs}. \tag{11}$$

This is similar to Ref. 13. Where

$$\sigma_0 = \frac{4e^2\gamma_0\sqrt{3}}{n\hbar^2} \frac{\sigma_0(0)}{(r\omega_B\tau)^2 + 1} \tag{12}$$

is the low-filed dc conductivity. We take $\hbar = 1$ and $\omega_B = eaE_0/\sqrt{3}$ for armchair and $\omega_B = eaE_0$ for zigzag CNs.
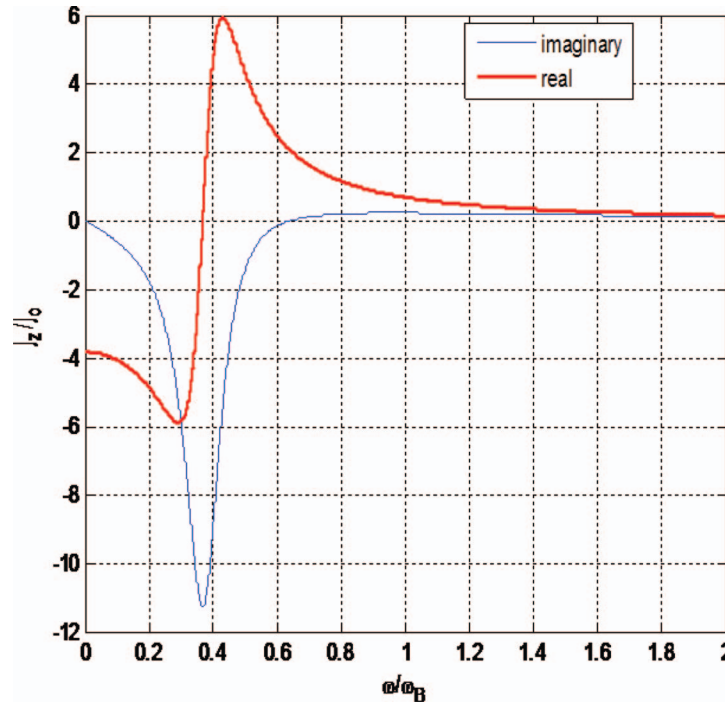
FIG. 1.  Real (red) and imaginary (blue) parts of conductivity for armchair CNTs for $\omega_B\tau = 5$.

## III.  RESULTS, DISCUSSION AND CONCLUSION

Using quasiclassical approach, we consider the dynamics of an electron transport in a CNs simultaneously exposed to both constant (dc) and ac electric fields. An analytical expression for the complex conductivity is obtained. The nonlinearity is analyzed basically on the dependence of the complex high frequency conductivity $\sigma(\omega)/\sigma(0)$ on the dimensionless frequency $\omega/\omega_B$.

The high-frequency conductivity obtained via the calculation of Eq. (11) is presented in Figures 1 and 2 for metallic zigzag CNT (9, 0) and metallic armchair CNT (6, 6) respectively. We noted that when $\omega \to 0$, Eq. (11) reduces to

$$\sigma_z(\omega) \to \sigma_d \equiv \frac{d}{E_0}(\sigma_0 E_0)$$

$$= \sigma_0(0) \sum_{r=1} r^2 \left[\frac{(r\omega_B\tau)^2 - 1}{[r^2\omega_B^2 + 1]^2}\right] \sum_{s=1}^{n} f_{rs}\epsilon_{rs}.$$

where $\sigma_d$ is the differential conductivity; for $(\omega_B)^2 > 1$, $\sigma_d < 0$. We observed that the real part of the complex conductivity is negative in the frequency interval from $\omega = 0$ to $\omega \sim \omega_B$ for metallic zigzag CNs and then turning positive (resonance enhancement) at $\omega \sim \omega_B$, whereas for the metallic armchair CNs resonance enhancement occurs at $\omega < \omega_B$. This resonance enhancement is indicative for terahertz gain without the formation of current instabilities induced by negative dc conductivity. For small values of n the magnitudes of $\omega/\omega_B$ and $\sigma_z(\omega)/\sigma(0)$ for the metallic armchair CNs turn out to be less than for metallic zigzag CNs with similar radius by a factor of approximately 2. See Figures 1 and 2. We noted that because of the high density of states of conduction electrons in metallic zigzag CNTs (9,0) and the specific dispersion law inherent in hexagonal crystalline structure result in a uniquely high frequency conductivity than the corresponding values for metallic armchair CNTs (6,6).

In conclusion, we have studied electron transport properties in carbon nanotubes. Using the kinetic equation with constant relaxation time, an analytical expression for the complex conductivity is obtained. The real part of the complex conductivity is initially negative at zero frequency
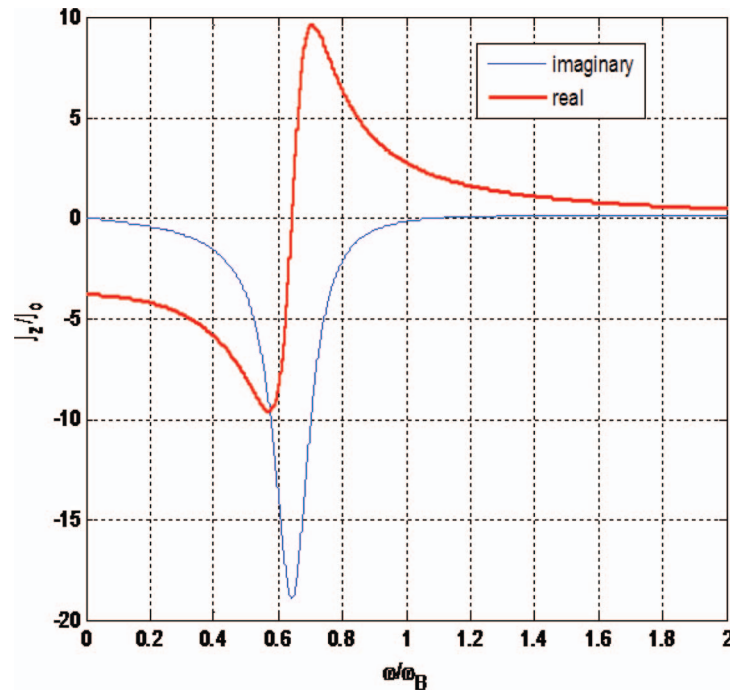
FIG. 2.  Real (red) and imaginary (blue) parts of conductivity for zigzag CNTs for $\omega_B \tau = 5$.

and become more negative with increasing frequency, until it reaches a resonance minimum at $\omega \sim \omega_B$ for metallic zigzag CNs and $\omega < \omega_B$ for armchair CNs. This negative-conductivity resonance close to the Bloch frequency makes a metallic zigzag CNs operating in this range an attractive gain medium for an active Bloch oscillator than the metallic armchair CNs.

[1] S. J. Tans *et al.*, Nature **386**, 474 (1997).
[2] A. Bezryadin *et al.*, Phys. Rev. Lett. **80**, 4036 (1998).
[3] A. A. Farajian, K. Estarjani, and Y. Kawazoe, Phys. Rev. Left. **82**, 5084 (1999).
[4] A. S. Maksimenko and G. Ya. Slepyan, Phys. Rev. Left. **84**, 362 (2000).
[5] S. S. Abukari, S. Y. Mensah, N. G. Mensah, K. W. Adu, K. A. Dompreh, and A. K. Twum, arXiv:1101.5498 (to be published).
[6] L. Esaki and R. Tsu, IBM J. Res. Develop. **14**, 61 (1970).
[7] A. Sibille, J. F. Palmier, H. Wang, and F. Mollot, Phys. Rev. Lett **64**, 52 (1990).
[8] H. Kroemer, cond-mat/0007482 (to be published).
[9] Kroemer, cond-mat/0009311 (to be published).
[10] Y. Romanov, V. Bovin, and L. Orlov, Sov. Phys. Semicond. **12**(9), 987 (1978) [Fiz. Tekh. Poluprovodn. **12**, 1665 (1978)].
[11] A. Ignatov, K. Renk, and E. Dodin, Phys. Rev. Lett. **70**, 1996 (1993).
[12] E. Schomburg, T. Blomeier, K. Hofbeck, J. Grenzer, S. Brandl, I. Lingott, A. Ignatov, K. Renk, D. Pavelev, and Y. Koschurinov, *et al.*, Phys. Rev. B **58**(7), 4035 (1998).
[13] S. A. Ktitorov, *et al.*, Soviet Physics - Solid State **13**, 1872 (1972).
[14] G. Ya. Slepyan, *et al.*, Phy. Rev. **81**, 205423 (2000).
[15] G. Ya. Slepyan, *et al.*, Phy. Rev. B **60**, 777 (1999).