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High frequency conductivity of hot electrons in carbon nanotubes

M. Amekpewu [a,*], S.Y. Mensah [b], R. Musah [a], N.G. Mensah [c], S.S. Abukari [b], K.A. Dompreh [b]

[a] Department of Applied Physics, University for Development Studies, Navrongo, Ghana
[b] Department of Physics, College of Agriculture and Natural Sciences, U.C.C., Ghana
[c] Department of Mathematics, College of Agriculture and Natural Sciences, U.C.C., Ghana

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ABSTRACT

High frequency conductivity of hot electrons in undoped single walled achiral Carbon Nanotubes (CNTs) under the influence of ac–dc driven fields was considered. We investigated semi-classically Boltzmann's transport equation with and without the presence of the hot electrons' source by deriving the current densities in CNTs. Plots of the normalized current density versus frequency of ac-field revealed an increase in both the minimum and maximum peaks of normalized current density at lower frequencies as a result of a strong injection of hot electrons. The applied ac-field plays a twofold role of suppressing the space-charge instability in CNTs and simultaneously pumping an energy for lower frequency generation and amplification of THz radiations. These have enormous promising applications in very different areas of science and technology.

1. Introduction

Carbon Nanotubes (CNTs) [1–3] have been the subject of intense research [4–18] since its discovery in 1991 by the Japanese scientist Sumio Iijima. Their unique structures, fascinating electronic, magnetic and transport properties have sparked the interest and imagination of researchers worldwide [19]. These quasi-one-dimensional nanostructural materials have a wide variety of possible applications [20–22]. Research in hot electrons, like any field in semiconductor research, has received a great deal of attention since the arrival of the transistor in 1947 [23]. Recently, it has become possible to fabricate semiconductor devices with submicron dimensions. The miniaturization of devices has led to the generation of high fields well outside the linear response region, where Ohm's law holds for any reasonable voltage signal [24]. The physical understanding of the microscopic processes which underlie the operations of such devices at high electric fields is provided by research into hot electron phenomena [25]. Whereas, there are several reports on hot electrons generation in CNTs [26–29], the reports on high frequency conductivity of hot electrons in CNTs are limited. Thus, in this paper, we present theoretical framework investigations of high frequency conductivity of hot electrons in (3,0) zigzag (*zz*) and (3,3) armchair (*ac*) CNTs. The Boltzmann transport equation is solved in the framework of momentum-independent relaxation time using the semi-classical approach to obtain current density for each achiral CNT. We probe the behaviour of the electric current density of the CNTs as a function of the frequency of ac field with and without the axial injection of the hot electrons.

2. Theory

When a d.c. field E_z is applied along a z-axis of an undoped single-wall carbon nanotube, electrons begin to move in accordance with the semiclassical Newton's law (neglecting scattering) [30] as

$$\frac{dP_z}{dt} = eE_z \tag{1}$$

where P_z and e are the axial component of the quasi-momentum and the electronic charge of the propagating electrons respectively. For CNTs, if energy level spacing $\Delta\varepsilon$ ($\Delta\varepsilon = \pi\hbar V_F/L$, $\hbar = h/2\pi$, h is Planck constant, V_F is Fermi velocity and L is the length of the nanotube) is large enough and the scattering rate ν is small such that $\Delta\varepsilon \gg aeE_z$ and $h\nu < aeE_z$ (*zz-CNT*), and $\Delta\varepsilon \gg \frac{a}{\sqrt{3}}aE_z$ $h\nu < \frac{a}{\sqrt{3}}aE_z$, (*ac-CNT*), then the electrons oscillate inside the lower level with the so-called Bloch frequency Ω given by [31]

$$\Omega_{zz} = \frac{aeE_z}{\hbar} \tag{2}$$

$$\Omega_{ac} = \frac{aeE_z}{\sqrt{3}\,\hbar} \tag{3}$$

for *zz*-CNT and *ac*-CNT respectively. Here, a is the lattice constant of the CNT. The investigation is done within the semi-classical

* Corresponding author.
E-mail address: mamek219@gmail.com (M. Amekpewu).

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approximation in which the motion of the π-electrons is considered as classical motion of free quasi-particles in the field of the crystalline lattice with dispersion law extracted from the quantum theory. Taking into account the hexagonal crystalline structure of a rolled graphene in a form of CNTs and using the tight binding approximation, the energies for *zz*-CNT and *ac*-CNT are expressed as in Eqs. (4) and (5), respectively [32]

$$\varepsilon(s\Delta p_\phi, p_z) \tag{4}$$

$$\equiv\varepsilon_s(p_z)= \tag{5}$$

$$\pm\gamma_0\sqrt{1+4\cos(ap_z)\cos\left(\frac{a}{\sqrt{3}}s\Delta p_\phi\right)+4\cos^2\left(\frac{a}{\sqrt{3}}s\Delta p_\phi\right)} \tag{6}$$

$$\varepsilon(s\Delta p_\phi, p_z) \tag{7}$$

$$\equiv\varepsilon_s(p_z)= \tag{8}$$

$$\pm\gamma_0\sqrt{1+4\cos(as\Delta p_\phi)\cos\left(\frac{a}{\sqrt{3}}p_z\right)+4\cos^2\left(\frac{a}{\sqrt{3}}p_z\right)} \tag{9}$$

where $\gamma_0 \approx 3.0$ eV is the overlapping integral, p_z is the axial component of quasi-momentum. Δp_ϕ is transverse quasi-momentum level spacing and s is an integer. The expression for lattice constant a in Eqs. (4) and (5) is given by

$$a=\frac{\sqrt{3}a_{c-c}}{2\hbar} \tag{10}$$

where $a_{(c-c)} = 0.142$ 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 P, its transverse component p_ϕ can take n discrete values,

$$p_\phi = s\Delta p_\phi = \frac{\pi\sqrt{3}s}{an}\quad (s=1,\ldots,n) \tag{11}$$

Unlike transverse quasi-momentum, p_ϕ, the axial quasi-momentum ϕ_z is assumed to vary continuously within the range $0 \le p_z \le 2\pi/a$, which corresponds to the model of infinitely long CNT ($L=\infty$). This model is applicable to the case under consideration because we are restricted to temperatures and voltages well above the level spacing [32], *i.e.* $k_\beta T > \varepsilon_c, \Delta\varepsilon$, where k_β is Boltzmann constant, T is the temperature, ε_c is the charging energy. The energy expression in Eqs. (4) and (5) can be expressed in the Fourier series as

$$\varepsilon(p_z, s\Delta p_\phi) = \varepsilon(p_z) = \gamma_0\sum_{r\neq 0}\exp(iarp_z) \tag{12}$$

where ε_{rs} is given as

$$\varepsilon_{r,s} = \frac{a}{2\pi\gamma_0}\int_0^{\frac{2\pi}{a}}\varepsilon_s(p_z)\exp(-irap_z)\,dp_z \tag{13}$$

The quasi-classical velocity of an electron moving along the CNTs axis is given by the expression $v_z(p_z, s\Delta p_\phi) = \partial\varepsilon_{rs}(p_z)/\partial p_z$. Substituting Eq. (9) into the velocity equation and expressing further give

$$v_z(p_z, s\Delta p_z) = \gamma_0\sum_{r\neq 0}\frac{\partial(\varepsilon_{rs}\exp(iarp_z))}{\partial p_z} = \gamma_0\sum_{r\neq 0}iar\varepsilon_{rs}\exp(iarp_z) \tag{14}$$

Considering the presence of hot electrons source, the motion of quasi-particles in an external axial electric field is described by the Boltzmann kinetic equation in the form as shown below [30,31]

$$\frac{\partial f(p)}{\partial t} + v_z\frac{\partial f(p)}{\partial x} + eE(t)\frac{\partial f(p)}{\partial p_z} = -\frac{f(p)-f_0(p)}{\tau} + S(p) \tag{15}$$

where $S(p)$ is the hot electron source function, $f_0(p)$ is equilibrium Fermi distribution function, $f(p,t)$ is the distribution function, v_z is the quasi-particle group velocity along the z-axis of CNTs and τ is the relaxation time. The relaxation term of Eq. (11) describes the electron–phonon scattering, electron–electron collisions [31,32] *etc*. Using the method originally developed in the theory of quantum semiconductor superlattices [31], an exact solution of Eq. (11) can be constructed without assuming a weak electric field. Expanding the distribution functions of interest in Fourier series we obtain for *ac*-CNTs

$$f(p,t) = \Delta p_\phi\sum_{s=1}^{n}\delta(p_\phi - s\Delta p_\phi)\sum_{r\neq 0}f_{rs}\exp(iarp_z)\psi_v(t) \tag{16}$$

$$f_0(p) = \Delta p_\phi\sum_{s=1}^{n}\delta(p_\phi - s\Delta p_\phi)\sum_{r\neq 0}f_{rs}\exp(iarp_z) \tag{17}$$

for *zz*-CNTs

$$f(p,t) = \Delta p_\phi\sum_{s=1}^{n}\delta(p_\phi - s\Delta p_\phi)\sum_{r\neq 0}f_{rs}\exp(ibrp_z)\psi_v(t) \tag{18}$$

$$f_0(p) = \Delta p_\phi\sum_{s=1}^{n}\delta(p_\phi - s\Delta p_\phi)\sum_{r\neq 0}f_{rs}\exp(ibrp_z) \tag{19}$$

for *ac*-CNTs where $b = a/\sqrt{3}$ or $a = b/\sqrt{3}$, $\delta(p_\phi - s\Delta p_\phi)$ is the Dirac-delta function, f_{rs} is the coefficients of the Fourier series and $\psi_v(t)$ is the factor by which the Fourier transform of the non-equilibrium distribution function differs from its equilibrium distribution counterpart. The expression for f_{rs} can be expanded in the analogous form as

$$f_{rs} = \frac{a}{2\pi}\int_0^{\frac{2\pi}{a}}\frac{\exp(-iarp_z)}{1+\exp(\varepsilon_s(p_z))/k_\beta T)}\,dp_z \tag{20}$$

The electron surface current density j_z along the CNTs axis is also given by the expression

$$j_z = \frac{2e}{(2\pi\hbar)^2}\iint f(p,t)v_z(p)\,d^2p \tag{21}$$

the integration is carried over the first Brillouin zone. For simplicity, we consider a hot electron source of the simplest form given by the expression,

$$S(p) = \frac{Qa}{\hbar}\delta(\phi-\phi') - \frac{aQ}{n_0}f_s(\phi) \tag{22}$$

where $f_s(p)$ is the stationary (static and homogeneous) solution of Eq. (23), Q is the injection rate of hot electron, n_0 is the equilibrium particle density, ϕ and ϕ' are the dimensionless momenta of electrons and hot electrons respectively which are expressed as $\phi_{zz} = ap_z/\hbar$ and $\phi'_{zz} = ap'_z/\hbar$ for *zz*-CNTs and $\phi_{ac} = ap_z/\sqrt{3}\hbar$ and $\phi'_{ac} = ap'_z/\sqrt{3}\hbar$ for *ac*-CNTs. We now find the high frequency conductivity of hot electrons in the non-equilibrium state for *zz*-CNT by considering perturbations with frequency ω and wave-vector k of the form

$$E(t) = E_z + E_{\omega,k}\exp(-i\omega t + ikx) \tag{23}$$