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Hot electrons injection in carbon nanotubes under the influence of quasi-static ac-field ☆

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

HIGHLIGHTS

- Hot electron injection.
- Carbon Nanotube (CNT).
- Quasi-static ac and dc field.
- Negative differential conductivity (NDC).
- Positive differential conductivity (PDC).

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ABSTRACT

The theory of hot electrons injection in carbon nanotubes (CNTs) where both dc electric field (E_z), and a quasi-static ac field exist simultaneously (i.e. when the frequency ω of ac field is much less than the scattering frequency ν ($\omega \ll \nu$ or $\omega\tau \ll 1$, $\nu = \tau^{-1}$) where τ is relaxation time) is studied. The investigation is done theoretically by solving semi-classical Boltzmann transport equation with and without the presence of the hot electrons source to derive the current densities. Plots of the normalized current density versus dc field (E_z) applied along the axis of the CNTs in the presence and absence of hot electrons reveal ohmic conductivity initially and finally negative differential conductivity (NDC) provided $\omega\tau \ll 1$ (i.e. quasi-static case). With strong enough axial injection of the hot electrons, there is a switch from NDC to positive differential conductivity (PDC) about $E_z \geq 75$ kV/cm and $E_z \geq 140$ kV/cm for a zigzag CNT and an armchair CNT respectively. Thus, the most important tough problem for NDC region which is the space charge instabilities can be suppressed due to the switch from the NDC behaviour to the PDC behaviour predicting a potential generation of terahertz radiations whose applications are relevance in current-day technology, industry, and research.

1. Introduction

Carbon nanotubes (CNTs) [1–3] are subject of many theoretical [4–9], and experimental [10–18] studies. Their properties include a thermal conductivity higher than diamond, greater mechanical strength than steel and better electrical conductivity than copper [19–21]. These novel properties make them potentially useful in a variety of applications in nanotechnology, optics, electronics, and other fields of materials science [22,23]. Rapid development of submicrometer semiconductor devices, which may be employed in high-speed computers and telecommunication systems, enhances the importance of hot electron phenomena [24,25]. Hot electron phenomena have become important for the understanding of all modern semiconductor devices [26,27].

There are several reports on hot electrons generation in CNTs [28–30], but the reports on hot electrons injection in CNTs under the influence of quasi-static ac field to the best of our knowledge are limited. Thus, in this paper, we analyzed theoretically hot electrons injection in (3, 0) zigzag (*zz*) CNT and (3, 3) armchair (ac) CNT where in addition to dc field, a quasi-static ac electric field is applied. Adopting semi-classical approach, we obtained current density for each achiral CNTs after solving the Boltzmann transport equation in the framework of momentum-independent relaxation time. We probe the behaviour of the electric current density of the CNTs as a function of the applied *dc* field E_z of

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

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$ac-dc$ driven fields when the frequency of ac field (ω) is much less than the scattering frequency (ν) $(\omega \ll \nu$ or $\omega\tau \ll 1$ i.e quasi-static case [31], where $\nu = \tau^{-1}$) with and without the axial injection of the hot electrons.

2. Theory

Suppose an undoped single walled achiral carbon nanotubes (CNTs) $(n, 0)$ or (n,n) of length L is exposed to a homogeneous axial dc field E_z given by $E_z = V/L$, where V is the voltage between the CNT ends. Under the influence of the applied dc field and assuming scattering is negligible, electrons with electronic charge (e) obey Newton's law of motion given by [32]

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

where P_z is a component of quasi-momentum along the axis of the tube. Adopting semi-classical approximation approach and considering the motion of π-electrons as a classical motion of free quasi-particles with dispersion law extracted from the quantum theory while taking into account to the hexagonal crystalline structure of CNTs and applying the tight-binding approximation gives the energies for zz-CNT and ac-CNT respectively

$$\varepsilon(s\Delta p_\vartheta, p_z) \equiv \varepsilon_s(p_z) = \pm\gamma_0\left[1 + 4\cos(ap_z)\cos\left(\frac{a}{\sqrt{3}}s\Delta p_\vartheta\right) + 4\cos^2\left(\frac{a}{\sqrt{3}}s\Delta p_\vartheta\right)\right]^{1/2} \tag{2}$$

$$\varepsilon(s\Delta p_\vartheta, p_z) \equiv \varepsilon_s(p_z) = \pm\gamma_0\left[1 + 4\cos(as\Delta p_\vartheta)\cos\left(\frac{a}{\sqrt{3}}p_z\right) + 4\cos^2\left(\frac{a}{\sqrt{3}}p_z\right)\right]^{1/2} \tag{3}$$

where $\gamma_0 \approx 3.0$ eV is the overlapping integral, Δp_ϑ is transverse quasi-momentum level spacing and s is an integer. The lattice constant a in Eqs. (2) and (3) is expressed as [33]

$$a = \frac{3b}{2\hbar} \tag{4}$$

where $b = 0.142$ nm is the C–C bond length. The $(-)$ and $(+)$ signs correspond to the valence and conduction bands respectively. Because of the transverse quantization of the quasi-momentum P, its transverse component p_ϑ can take n discrete values,

$$p_\vartheta = s\Delta p_\vartheta = \frac{\pi\sqrt{3}s}{an}(s = 1, \ldots, n) \tag{5}$$

As different from p_ϑ, we assume p_z continuously varying within the range $0 \le p_z \le 2\pi/a$ which corresponds to the model of infinitely long CNT ($L = \infty$). The model is applicable to the case under consideration because we are restricted to temperatures and/or voltages well above the level spacing [33], i.e. $k_BT > \varepsilon_c$, $\Delta\varepsilon$, where k_B is Boltzmann constant, T is the thermodynamic temperature, ε_c is the charging energy. In the presence of hot electrons source, the motion of quasi-particles in an external axial electric field is described by the Boltzmann kinetic equation as [32,33]

$$\frac{\partial f(p)}{\partial t} + v_z\frac{\partial f(p)}{\partial x} + eE(t)\frac{\partial f(p)}{\partial p} = -\frac{f(p) - f_0(p)}{\tau} + S(p) \tag{6}$$

where $f_0(p)$ is equilibrium Fermi distribution function, $f(p, t)$ is the distribution function, $S(p)$ is the hot electron source function, v_z is the quasi-particle group velocity along the axis of carbon nanotube and τ is the relaxation time. The relaxation term of Eq. (6) above describes the electron–phonon scattering, electron–electron collisions [34–36] etc.

The quasiparticle group velocity v_z along the axis of each type of carbon nanotube in Eq. (6) is calculated from the energy dispersion relation either in Eq. (2) or Eq. (3) depending on the form of CNT under consideration.

Applying the method originally developed in the theory of quantum semiconductor superlattices [38], an exact solution of Eq. (6) can be constructed without assuming a weak electric field. Considering the distribution functions in Eq. (6) by expanding these functions of interest in Fourier series, we have

$$f(p, t) = \Delta p_\vartheta \sum_{s=1}^{n} \delta(p_\vartheta - s\Delta p_\vartheta) \sum_{r\neq 0} f_{rs}\exp(iarp_z)\psi_v(t) \tag{7}$$

and

$$f_0(p) = \Delta p_\vartheta \sum_{s=1}^{n} \delta(p_\vartheta - s\Delta p_\vartheta) \sum_{r\neq 0} f_{rs}\exp(iarp_z) \tag{8}$$

for zz-CNT and

$$f(p, t) = \Delta p_\vartheta \sum_{s=1}^{n} \delta(p_\vartheta - s\Delta p_\vartheta) \sum_{r\neq 0} f_{rs}\exp(ira/\sqrt{3}p_z\psi_v(t)) \tag{9}$$

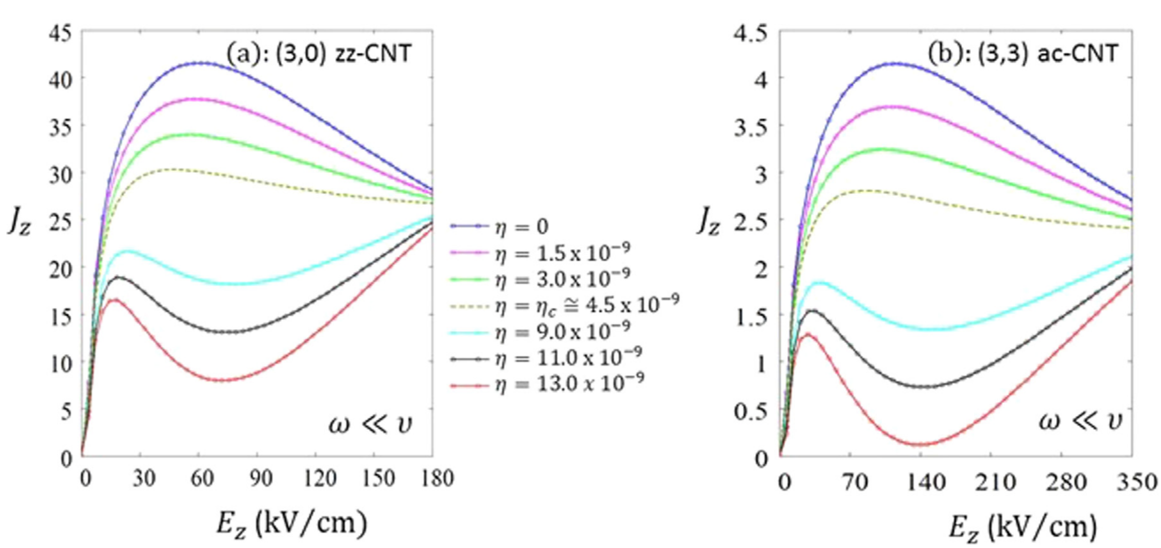

Fig. 1. A plot of normalized current density (J_z) versus applied dc field (E_z) as the on-equilibrium parameter η increases from 0 to 13.0×10^{-9} when $\omega \ll \nu$ or $\omega\tau \ll 1$ (i.e. quasi-static case), for (a) (3,0) zz-CNT and (b) (3,3) ac-CNT, $T = 287.5$ K, $\omega = 10^{-4}$ THz, $\nu = 1$ THz or $\tau = 1$ ps and $\omega\tau = 10^{-4}$.