Modeling Carbon Nanotube Electron-Phonon Resonances Shows Terahertz Current Oscillations

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Abstract

We report on Terahertz (THz) current oscillations in single-walled semiconducting zig-zag carbon nanotubes (CNTs) upon application of a step DC bias, as shown in Fig. 1. To investigate the electron transport on a tube with fundamental indices of n = 13 and m = 0, we developed a transient ensemble CNT Monte Carlo (MC) simulator. In the simulator, electron transport in time and space is resolved with the effects of charge distribution on the potential profile along the tube. The solution shows that electron-phonon resonances give rise to current, velocity and concentration oscillations upon application of a DC bias.

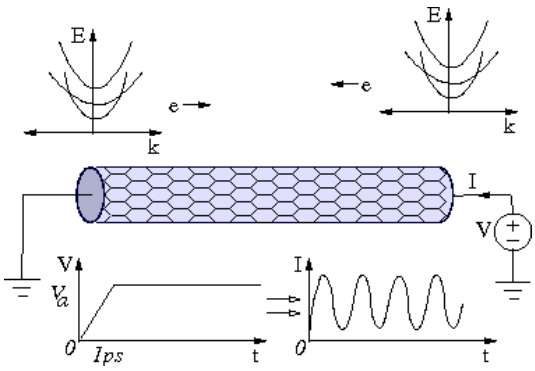

Figure 1: Simulated CNT. Left side is grounded. Voltage on the right side changes from 0 to V_a in 1 ps, and then stays at this level. Electrons, chosen using the Fermi-Dirac distribution, are injected from both ends. Electron transport in the tube is solved self-consistently with the Poisson equation.

1 Introduction

In our previous work [1], we reported MC simulation results that showed position-dependent velocity and electron concentration oscillations due to intra-subband electron-phonon scatterings. (This was a steady-state case, where the applied field

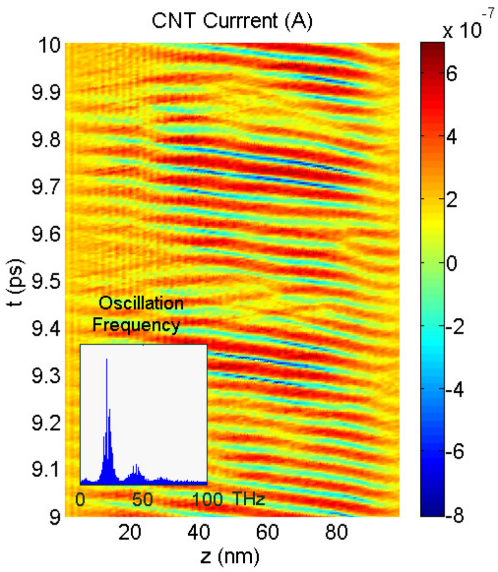

Figure 2: Calculated CNT electron current as a function of time and space. CNT current has a strong self-sustained oscillation at approximately 23 THz, as shown by frequency domain representations of time signals at different tube locations plotted in the inset.

was equal to the local electric fields.) This encouraged us to extend our work into the self-consistent transient regime to investigate whether these velocity oscillations [1-3] do indeed give rise to current oscillations. Here, we show self-consistent transient ensemble CNT MC results that are obtained using the transport equations and the Poisson equation. The MC results indicate that we do indeed have Terahertz current oscillations in time upon the application of a DC bias [4]. We associate these temporal and spatial oscillations to intra-subband and inter-subband electron-phonon resonant scatterings, and the effects of the CNT electron energy dispersion curves. Specifically, optical intra-subband phonon emissions that enable electron transfers to subbands' energy minima are high due to the peaking of the electron density-of-states at the subbands' minima. At subband minima, electron velocities are low, giving rise to electron bunching at locations where these intra-subband phonon emissions occur. Furthermore, for electrons that successfully gain energy, there is also another energy range that is associated with high scattering rates due to inter-subband electron-phonon scatterings. This is again due to high density-of-states associated with the subbands' minima. When this happens, electrons scatter from the first subband to the energy minimum of the second subband, where the average velocity is low. This creates additional electron bunching where it happens. In summary, due to low and high density electron regions on the tube caused by different velocity dispersion phenomena, a charge dipole forms. This dipole, due to the applied field, travels along the tube giving rise to self-sustained velocity, concentration, potential and current oscillations.

2 Transient Monte Carlo (MC) Results

We use Fermi's Golden Rule and deformation potential approximation to calculate electron-phonon scatterings in a CNT [1-5] from $\vec{k}$ (k in subband β) to $\vec{k}'$ (k' in subband β') via a phonon q (q in subband η):

$$\Gamma(\vec{k},\vec{k}') = \frac{\pi\hbar D^2 Q^2}{L\rho E_p(\vec{q})}\left[\frac{1}{\exp\left(\frac{E_p(\vec{q})}{E_{th}}\right)-1}+\frac{1}{2}\pm\frac{1}{2}\right]\delta(E(\vec{k}')-E(\vec{k})\pm E_p(\vec{q})) . \quad (1)$$

Here, D is the deformation potential (9 eV); Q is a wavevector [1,4,5]; L is the tube's length; E_{th} is the room temperature thermal energy (25.8 meV); ρ is the CNT linear mass density; and $E_p(\vec{q})$ is the phonon energy that enables possible emission or absorption (plus or minus above, respectively) from initial electron state $E(\vec{k})$. Above, δ-Delta function explicitly refers to the energy conservation before and after the electron-phonon interaction. To find possible final electron states, momentum conservation is also simultaneously checked.

To obtain the spatial and temporal profile of local electric fields in conjunction with local net charge densities (electron concentration N minus doping N^+), we solve the Poisson equation written below in addition to the electron transport :

$$\nabla^2\phi(z,t) = \frac{e}{\varepsilon_{CNT}}[N(z,t)-N^+(z)] , \quad (2)$$

where ϕ, e and ε_{CNT} are the CNT electrostatic potential, electronic charge and the CNT dielectric constant [5], respectively.

We simulated a 100 nm long single-walled n = 13 zig-zag CNT. We grounded the left side of the tube, and raised the potential on the right side from 0 to V_a (= 0.9 V) in 1 ps, as shown in Fig. 1. Figure 2 shows our calculated self-consistent CNT current in amperes as a function of time and position on the tube. There is a pronounced current oscillation at approximately 23 THz. We associate this with intra-subband and inter-subband electron-phonon scatterings, and the electron subband structure. Specifically, due to intra- and inter- subband scatterings and the peaking of the electron density-of-states, electrons scatter to the subbands' minima with high rates, whenever there is an allowed phonon for this transition. Since average electron velocities are low at

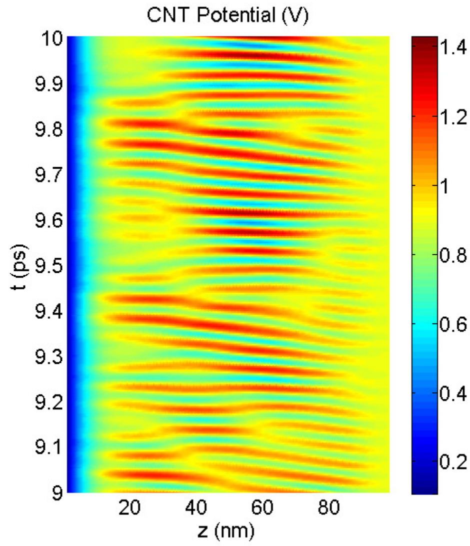

Figure 3: Calculated CNT potential profile as a function of time and space. Dipole formed due to electron velocity dispersion travels along the tube, and causes oscillations in potential.

subbands' minima, electrons bunch together where it happens. This creates a propagating charge dipole, which modifies the potential as shown in Fig. 3.

3 Conclusion

Terahertz CNT current and potential oscillations due to charge dipole formations are reported. We associate these charge dipoles and subsequent current oscillations with strong CNT velocity dispersions, mainly due to the peaking of the one-dimensional density of states at subbands' minima. Furthermore, these intrinsic oscillations might be utilized to build Terahertz sources for future RF applications.

References

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