Hot Phonons Contribution to scattering rates in Single-Walled Carbon Nanotubes

Pierre Gautreau*, Tarek Ragab**, Cemal Basaran***

*Electronic Packaging Laboratory, State University of New York at Buffalo, 102 Ketter Hall, Buffalo, NY, gautreau@buffalo.edu
** Alexandria University, Alexandria, Egypt and Nanotechnology Research Laboratory, University of Tabuk, Tabuk, KSA, tragab@ut.edu.sa
*** Electronic Packaging Laboratory, State University of New York at Buffalo, 102 Ketter Hall, Buffalo, NY, cjb@buffalo.edu

ABSTRACT

The influence of hot phonons on the electron-phonon scattering rates is studied via an Ensemble Monte Carlo(EMC) simulation with step by step update of the phonon occupation number to account for the generation of hot phonons in metallic armchair (10, 10) carbon nanotubes. EMC simulations are carried out at different temperatures ranging from 300 to 1800 K and at electric field forces ranging from 5KV/cm to 20 KV/cm. The energy dispersion relation is calculated using a tight binding formulation while the phonon dispersion relation is calculated using the Fourth nearest neighbor interactions between atoms. The hot phonon contribution to the scattering rates appears to be a function of applied electric force field at room temperature, while it becomes independent of the applied electric force field for higher temperatures.

Keywords: carbon nanotubes, Monte Carlo simulation, semi-classical transport, electron-phonon scattering rates, hot phonon effect

1 INTRODUCTION

Scaling down the size of electronic devices has been the principal approach of the electronic industry for the past 60 years. In an effort to further scale down the size of electronic devices, this industry is facing an increasing amount of challenges outlined in the ITRS 2011 roadmap. These challenges are primarily due to the nano-scale of these devices. As the size of these devices is reduced, the current density increases. Conventional metals used in metal-oxide electronics experience electro and thermo-migration under these high current densities, eventually resulting in failure. Carbon nanotubes (CNTs) and graphene are strong candidates to replace these metals as interconnects in integrated circuits [1].

SWCNTs have been reported to support current densities of up to 109 A/cm2 [2]. Their small dimension and ability to operate at high temperature well above 2000K [3], are well suited for interconnects applications. Before such applications can be implemented into electronic devices, much still needs to be understood about the electrical and thermal properties of SWCNTs.

Many electrical properties in SWCNTs has been study by various techniques. In ref. [4] non-equilibrium Green's functions were used within the Born approximation to calculate the joule heating and the phonon thermal conductance of (10,10) armchair SWCNTs and (10,0) zigzag SWCNTs. The authors of ref. [4] report a joule heating power ranging from 35 to 60 nW for biases between 0.3V and 1V (~1000 K and 1.5 nm long SWCNT). This result is one order of magnitude higher than the experimental data obtained in ref. [5], in which the authors report a joule heating of a 1-2 nW at a similar temperatures. This difference may be due to the theoretical approximations regarding the scattering potential used in ref. [4]. The authors of ref. [4] also report a decrease in the joule heating for increasing temperatures, whereas the results presented in ref. [5] and in ref. [6] show an increase in the Joule heating for increasing temperatures.

In addition to non-equilibrium Green's functions, Ensemble Monte Carlo (EMC) simulation is a very popular technique to study stochastic processes such as scattering occurring in SWCNTs. A recent study used EMC simulations to show the bias induced velocity oscillation in semiconducting zigzag SWCNTs [7]. The MC simulator used in ref. [7] requires the knowledge of the electron-phonon scattering rates. The scattering rates calculated in ref. [8] were used in that study. The same technique is used in ref. [9] to study the electrical characteristic of zigzag SWCNTs. In ref. [6], the EMC simulation model used in ref. [7] was applied to the calculation of joule heating in (10,10) armchair SWCNTs. The work presented in this paper is based on this model.

In this study, the goal is to underline the hot phonon contribution to electron-phonon scattering rates in single-walled carbon nanotubes. A quantum mechanical model of energy transfer between the charge carriers and the lattice was used. The non-equilibrium scattering rates calculations are carried out through an Ensemble Monte-Carlo (EMC)

simulation with a step by step update of the phonon occupation number. The continuous update of the phonon occupation number during the EMC simulation further improves the accuracy of the model and represents a novel and more inclusive way to calculate the scattering rates in carbon nanotubes.

2 DESCRIPTION OF THE MODEL

Under an electrical loading, electrons drift freely for a period time after which they scatter stochastically by the vibration of the lattice represented by phonons. During the scattering events, the charge carriers exchange energy with the lattice. In this study, only electron-LA phonon (Longitudinal Acoustic) and electron-LO phonon (Longitudinal Optical) scattering are considered. Although electron-electron scattering and electron-phonon scattering with vibrational modes other than LA and LO can take place in the lattice, it is not needed to include them in this model, because electron-electron scattering does not transfer energy to the lattice, and the scattering rate of other vibrational mode such as TA (Transverse Acoustic) and TO (Transverse Optical) is small compared to LA and LO in SWCNT [8, 10, 11].

$S_m((k,\nu),(k',\nu')_m)$ is the scattering rate between the final state $(k,\nu)_m$ and initial state $(k',\nu')_m$ for a given scattering mechanism m. k represents the longitudinal wavevector along the axis of the SWCNT, ν is the quantum number representing the wavevector along the circumference of the SWCNT. The calculation of the scattering rates is conducted over all the possible initial k values and over all the electronic sub-bands and scattering mechanisms [6, 8, 9]. Making use of the deformation potential approximation and Fermi's golden rule, the scattering rate S for LA and LO scattering mechanisms is given by [8],

$$S((k,\nu),(k',\nu')) = \frac{\hbar D_{LA}^2 (q^2 + (2\mu/d)^2)}{2\rho E_p^{LA}(q,\mu)} \times (N(E_p^{LA}(q,\mu)) + \frac{1}{2} \pm \frac{1}{2}) \left|\frac{dE}{dk}\right|^{-1}_{(k',\nu')} \quad (1)$$

and

$$S((k,\nu),(k',\nu')) = \frac{\hbar D_{LO}^2}{2\rho E_p^{LO}(q,\mu)} \times (N(E_p^{LO}(q,\mu)) + \frac{1}{2} \pm \frac{1}{2}) \left|\frac{dE}{dk}\right|^{-1}_{(k',\nu')} \quad (2)$$

DLA and DLO are deformation potential constants. EP(q,μ) is the energy of the phonon with wavevector q in sub-band μ. ρ is the linear mass density of the SWCNT. ħ is the modified Planck's constant. N is the phonon occupation number. (dE/dk)-1 is the density of states. The plus and minus signs respectively represent the emission and absorption of a phonon. In order to compute the scattering rates, the electron energy dispersion, the phonon dispersion relations must be calculated ahead of time.

In this study, the following electron (Fig. 1) and phonon (Fig.2) dispersion relations calculated in an earlier study [12] were used.

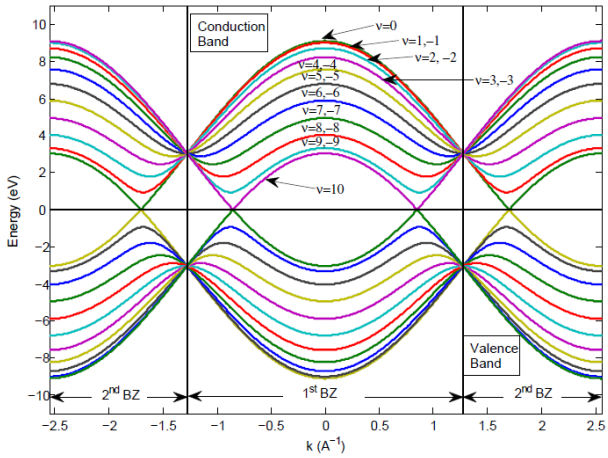


Fig. 1: (Color online) Energy dispersion relation of the valence and conduction bands for (10, 10) CNT in the first and second BZs.

In ref. [12], the electron dispersion relation was obtained using a tight binding formulation. A fourth nearest neighbor continuum mechanics interactions between atoms were used to obtain the phonon dispersion relation.

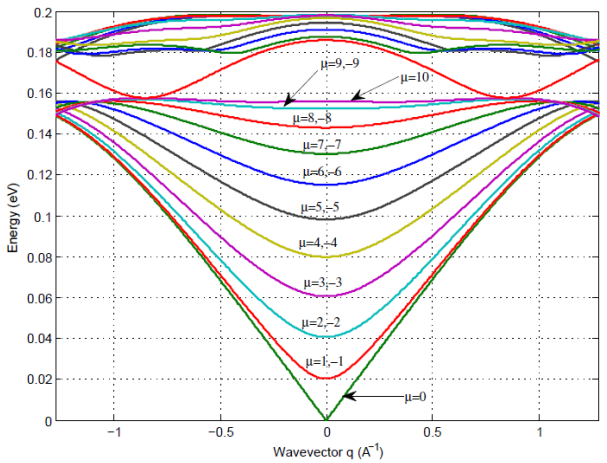


Fig. 2: (Color online) LA and LO phonon Dispersion relation for (10, 10) CNT in the first BZ. The lowered labeled sub-bands are for the LA mode, and the upper unlabeled sub-bands are the LO modes.

The heart of this model is in the calculation of the occupation probability of both the electrons and phonons that are changing continously with time. This calculation is calculate in this study using an Ensemble Monte Carlo (EMC) simulation.

Initially, all the simulated electrons are distributed in the lowest sub-band following a Fermi-Dirac distribution based

on the simulation temperature. At the beginning of the simulation, the phonon occupation number is set to a Bose-Einstein equilibrium distribution. At the beginning of each time step, each electron is classically drifted in the sub-band by the electric field force. The electrons are allowed to scatter stochastically with the phonons following the scattering rates calculated. If the electron scatters, the state of this electron is updated for the next time step according to the scattering mechanism selected. Every time an electron scatters, the specific phonon emitted or absorbed in the scattering mechanism is recorded, and the appropriate phonon occupation number is updated as well. From equations 1-2, it is clear that the scattering rate is directly proportional to the phonon occupation number. It is, therefore, important to update the scattering rate of all the electronic states that could interact with the phonon with which the electron had previously scattered. This process of continuously updating the non-equilibrium phonon occupation number and the related scattering rates in order to account for the generation of hot phonons is repeated throughout the simulation time.

In this study, the model described above is applied to a (10,10) armchair SWCNT under various electrical loading (2, 5, 10, 15, and 20 kV/cm) at five different temperatures (300K, 600K, 900K, 1200K, and 1800K). The simulation time is 100 pico-seconds, which is a thousand times larger than the minimum scattering time. This allows enough simulation time to capture the full behavior of hot phonons. The simulation is repeated a total of six times using different random number generation algorithms for each simulation to average out the EMC fluctuations.

3 RESULTS AND DISCUSSION

Figure 3 shows the phonon occupation number recorded at the end of the simulation time for sub-band 8 and 10 (see Fig. 1 for the sub-band numbering) at 1800K under an applied electric field of 2 kV/cm.

The solid curve represents the out of equilibrium distribution of phonons. The very large peaks are clear evidence of the presence of hot phonons in the SWCNT. The large increase in the phonon occupation number for very specific wavevectors results in localized increases in the scattering rates, as described by eq. 1 and 2.

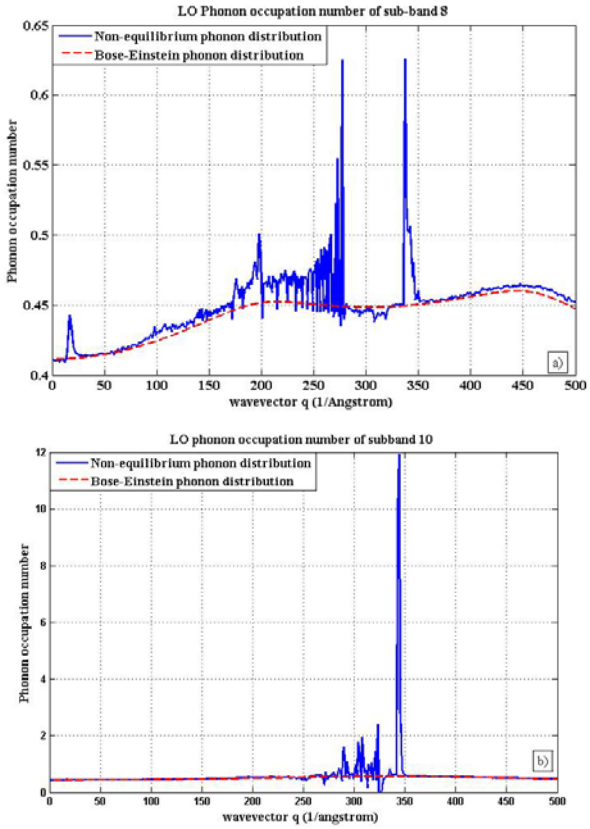
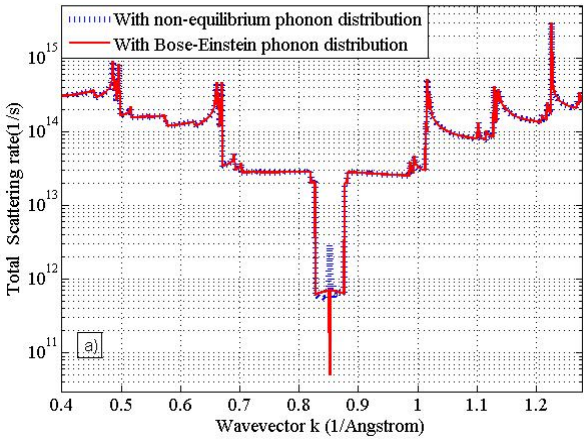


Fig. 3: Phonon occupation number of sub-band 8, a), and 10, b), at 1800K with an electric field of 2 kV/cm

Figure 4 shows the difference between the total scattering rate of sub-band 10 (the most populated sub-band) [6] calculated with a Bose-Einstein distribution and the total scattering rate updated with the non-equilibrium phonon distribution at the end of the simulation time. The figure shows that



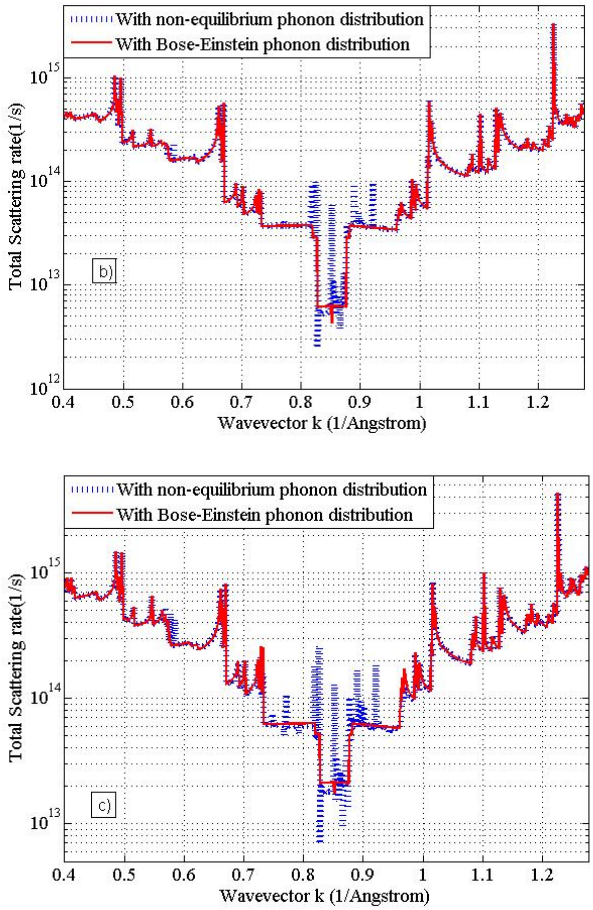


Fig. 4: (Color online) Total scattering rate of sub-band 10 at 300 K a), 900K b), and 1800 K c) with a 2 kV/cm electric field force

the presence of hot phonons creates an overall increase in the scattering rate. It is clear from Fig. 4 that as temperature increases the impact of hot phonons on the total scattering rate is more significant. At room temperature, the equilibrium scattering rate at the bottom of the sub-band (where most electron are originally located) is about ten times smaller than at 900K, which in comparison doesn't create a large population of hot phonons through phonon emission scattering mechanisms. As the temperature increases, the equilibrium scattering rate at the bottom of the sub-band increases as well; thus, creating a larger hot phonon population due to the increase in the number of scattering events.

It could be argued that the increase in the scattering rate at higher temperature is overestimated due to a lack of phonon-phonon interaction in the model. Phonon-phonon interactions, and more specifically hot phonon decay could lead to a reduced non- equilibrium phonon occupation, which would in turn reduce the scattering rate. It is, however, important to note that the hot phonon decay time is in the order of 1-10 pico-seconds [13-15], which is a much slower process than electron-phonon scattering (0.001-0.01 pico-seconds). It is fair to state that, at the end of the simulation time, the non-equilibrium phonon distribution is in steady state conditions. Furthermore, phonon-phonon interactions can also generate additional hot phonons from scattering with equilibrium phonons, which would further increase the hot phonon population.

4 CONCLUSIONS

Using a quantum mechanical model and an EMC simulation, the influence of hot phonons on the scattering rate of electron-phonon mechanisms in SWCNTs has been studied.

Further research studying the effects of hot phonon scattering rates presented in this paper on Joule heating and Electron wind forces is underway in our group.

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