CARBON 57 (2013) 59–64

Available at www.sciencedirect.com

SciVerse ScienceDirect

journal homepage: www.elsevier.com/locate/carbon

Influence of hot phonons on wind forces in metallic single walled carbon nanotubes

Pierre Gautreau [a], *Tarek Ragab* [b], *Cemal Basaran* [a,*]

[a] *Electronic Packaging Laboratory, State University of New York at Buffalo, 102 Ketter Hall, Buffalo, NY 14260, United States*
[b] *Nanotechnology Research Laboratory, University of Tabuk, Saudi Arabia 71491b- Faculty of Engineering, Alexandria University, Egypt 21526*

ARTICLE INFO

Article history:
Received 24 September 2012
Accepted 13 January 2013
Available online 24 January 2013

ABSTRACT

The wind force exerted on the lattice by the flux of electrons under electric loading in single walled carbon nanotubes is studied using an ensemble Monte-Carlo simulation. The momentum transfer between electrons and the lattice is treated using Quantum Mechanics. The phonon distribution and the electron distribution of the carbon nanotubes are allowed to be populated away from thermal equilibrium to study the influence of hot phonons on the wind forces. While the presence of hot phonons creates a net increase in the phonon–electron scattering rates, it appears to have a very small influence on the amount of force exerted on the lattice.

1. Introduction

Carbon nanostructures have received a lot of attention in the past decade, due to their extraordinary mechanical [1] and electrical properties. These properties combined with the nano-scale of carbon nanotubes (CNTs) have inspired novel designs for nano-electronic devices [2–4]. The nano-scale of these devices is both an advantage and a source of new challenges as outlined by the ITRS-2011 roadmap. One of these challenges is the calculation of the forces applied on the lattice of nanostructures, which may cause problems such as electro-migration [5] and breakdown of devices [6] in conventional metal-oxide electronics. In this study, we focus our attention on the wind force effect and its behavior with non-equilibrium (hot) phonons.

CNTs can be made to be metallic depending on which direction a graphene sheet is rolled up. The lattice structure of graphene is shown in Fig. 1.

The direction upon which the CNT is rolled up is defined by the chiral vector,

$$C_h = m\overrightarrow{a_1} + n\overrightarrow{a_2} \quad (1)$$

The values of (m,n) are the chiral indices defining the CNT. In this study, the CNTs are taken to be metallic armchair ($n = m$) tubes. While the results presented are for a (10,10) armchair SWCNT, the technique used can be modified to simulate CNTs of different chiralities.

Driving a current through a single walled carbon nanotube (SWCNT) is often described by a ballistic transport [3,4,7,8]. While it can be approximated to behave in such a regime, the interactions between conduction electrons and the rest of the lattice have a non-negligible contribution to the electrical and mechanical characteristics of SWCNTs. To describe the transport behavior of SWCNTs, we use a quasi-ballistic [9] approach in which momentum is exchanged between charge carriers and the lattice.

In Quantum Mechanics, the amount of momentum that is carried by an electron with wavevector $\mathbf{k}$ is given by the formula:

$$\mathbf{p} = mhboxh\mathbf{k} \quad (2)$$

If the electron is scattered by an ion on the lattice, its wavevector will change, and as a result the amount of momentum carried by the electron will change to $\hbar\mathbf{k}'$, where $\mathbf{k}'$ represents

* *Corresponding author:* Fax: +1 716 645 5402.
E-mail addresses: gautreau@buffalo.edu (P. Gautreau), cjb@buffalo.edu (C. Basaran).
0008-6223/$ - see front matter
http://dx.doi.org/10.1016/j.carbon.2013.01.031

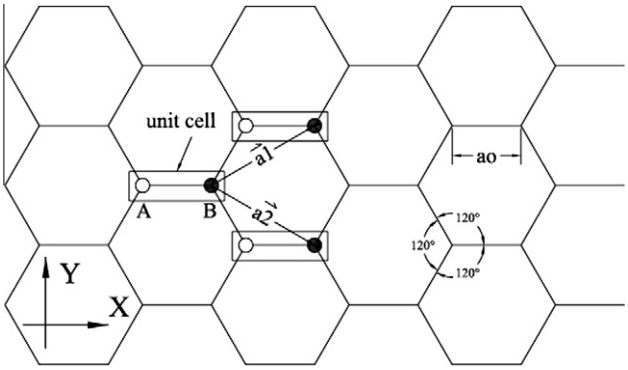

Fig. 1 – Lattice structure of graphene before it is rolled up into a CNT.

the wavevector of the scattered state. Based on the principle of momentum conservation, the difference in momentum between the electron states before and after the scattering event is transferred to the lattice through the absorption or emission of a phonon of wavevector **q** as shown in Fig. 2.

According to Newton's second law, the rate of momentum transfer to the lattice is the electron wind force. The goal of this study is to calculate the influence of hot phonons on the wind force. To this date, very few research groups have studied the wind force effect, but the interest in knowing the magnitude of these forces and the need to control them for nano-electronic applications have created a need for further study.

Ref. [11] demonstrates the possibility of a motor driven by wind forces for possible application in nanoelectromechanical structures (NEMS). The authors of Ref. [11], used a semi-classical approach to model the momentum transfer to the lattice. They find a linear relationship between the force exerted on the lattice and the group velocity of the electrons. The wind force effect in (10,10) carbon nanotubes has also been studied by Ragab and Basaran [12] with a quantum mechanical treatment of momentum transfer. In Ref. [12], Ragab and Basaran show that a linear relationship exists between the wind force and applied electric force field. This study is based on the model developed by Ragab and Basaran with the addition of the treatment of hot phonons in (10,10) single walled carbon nanotubes.

2. Modeling

Under an applied electric force field, many scattering mechanisms occur between electrons and phonons. Phonons can be subdivided into several modes. They can be longitudinal or transverse depending on the direction of propagation as compared to the longitudinal axis of the carbon nanotube. Additionally, phonons can be acoustic (similar to sound waves, TA and LA) or optical (similar to light waves, TO and LO). While TA, LA, TO, and LO phonons all scatter with electrons, only LA and LO are considered in this study, because the scattering rates of LA and LO are high compared to TA and TO [13–15]. Scattering between electrons also occurs in metallic CNTs, but these scattering mechanisms do not directly transfer momentum to the lattice and, therefore, can be neglected during the simulation. Making use of the deformation potential approximation and Fermi's golden rule, the scattering rates S for LA and LO scattering mechanisms are given by [14],

$$S((k,v),(k',v')) = \frac{\hbar D_{LA}^2 (q^2 + (2\mu/d)^2)}{2\rho E_P^{LA}(q,\mu)} \left(N(E_P^{LA}(q,\mu)) + \frac{1}{2} \pm \frac{1}{2} \right) \left| \frac{dE}{dk} \right|^{-1}_{(k',v')} \quad (3)$$

and

$$S((k,v),(k',v')) = \frac{\hbar D_{LO}^2}{2\rho E_P^{LO}(q,\mu)} \left(N(E_P^{LO}(q,\mu)) + \frac{1}{2} \pm \frac{1}{2} \right) \left| \frac{dE}{dk} \right|^{-1}_{(k',v')}. \quad (4)$$

D_{LA} and D_{LO} are the deformation potential constants. $E_P(q,\mu)$ is the energy of the phonon with wavevector q in sub-band μ. ρ is the linear mass density of the SWCNT. 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.

Once the scattering probabilities are known, we can calculate the average force applied on the lattice due to momentum transfer from electron–phonon scattering events. Summing over all the scattering mechanisms and all the sub-bands of the CNT, we obtain the following formula [12]:

$$F = \frac{1}{\pi} \sum_m \sum_v \int (\hbar k - \hbar k') \times S_m((k,v),(k',v')) \times f(k,v) \times (1 - f(k',v'))dk \quad (5)$$

where $\hbar k - \hbar k'$ represents the momentum transferred during a scattering event, S_m is the scattering probability of a given scattering mechanism m, and $f(k,v)$ is the probability of state (k,v) to be occupied and $1 - f(k',v')$ is the probability of state

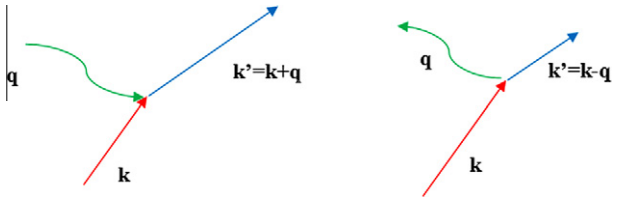

Fig. 2 – Electron–phonon scattering [10].

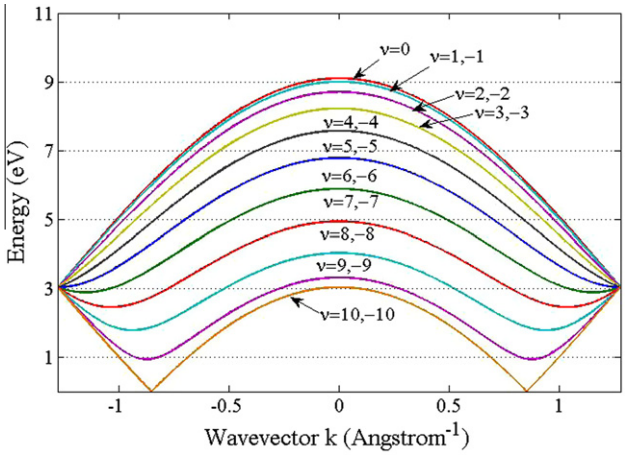

Fig. 3 – Energy dispersion relation of the conduction band for (10,10) CNT in the first BZs.