The prediction of the effective charge number in single-walled carbon nanotubes using Monte Carlo simulation

Tarek Ragab a,b, Cemal Basaran b,*

a Alexandria University, Egypt
b Electronic Packaging Lab, State University of New York at Buffalo, 102 Ketter Hall, North Campus, Buffalo, NY 14260, United States

ABSTRACT

The ensemble Monte Carlo simulation is used to calculate the electron-wind forces per unit length of single-walled carbon nanotubes under an electric field applied through the nanotube axis. The electronic system and the ionic system are decoupled from each other. The rate of momentum transferred from the electronic system to the ionic system in the form of the emission or absorption of longitudinal acoustic and longitudinal optical phonons is calculated stochastically to determine the electron-wind forces. Complete unabridged energy and phonon dispersion relations are included in order to obtain more accurate results. The effect of the temperature and the electric field magnitude on the induced forces is also taken into account. Results are compared with a prediction based on quantum mechanical integral form that calculates the electron occupation probability based on a modified Fermi–Dirac distribution. Results show a quantitative agreement between the two methods, however, the method proposed in here we believe is more accurate, because it does not make simplifications for the electron occupation probability as in the modified Fermi–Dirac distribution.

1. Introduction

Carbon nanotubes are one of the materials that gained huge interest during the current decade due to their extraordinary mechanical [1–3], thermal [4–6] and electrical [7] properties. Furthermore the insatiable demand for miniaturized electronics requires decreasing the size of the electronic interconnects leads to higher current densities in these components. The increase in current densities is far beyond the current carrying capacity of traditional metals and semiconductors currently used [8,9]. Research has shown that carbon nanotubes (CNTs) are a strong candidate for replacing traditional metals and semiconductors [10] due to their high current carrying capacity and insensitivity to failure mechanisms like electromigration and thermomigration [11]. However, due to their novelty and their nanoscale dimensions, important properties affecting their electromigration and thermomigration reliability (e.g. the effective charge number; the force induced on the atomic lattice due to a unit electric field force) are still not yet established. In an earlier study [12], authors quantified the electron-induced wind forces in single-walled CNT using a quantum mechanical model that is based on the momentum transfer between the electronic system and the lattice vibration modeled by both longitudinal acoustic (LA) and longitudinal optical phonons (LO). In that study, the occupation probability of the electron states in the presence of an electric field was approximated using a modified Fermi–Dirac distribution [13]. Monte Carlo simulation is known to be a reliable method for accurately solving the Boltzmann transport equation (BTE) for calculating the electron state occupation probability in semiconductor CNTs [14–20]. Javey et al. [21] used ensemble Monte Carlo (EMC)

* Corresponding author: Fax: +1 716 645 3733.
E-mail address: cjb@buffalo.edu (C. Basaran).

© 2010 Elsevier Ltd. All rights reserved.

simulations to calculate the mean free path of electrons in metallic CNTs, where only the lowest energy sub-band was included with an assumed linear relationship and also scattering to higher sub-bands was neglected. Moreover, the authors ignored the full details of the phonon dispersion relation.

In this study, a quantum mechanical model used in our earlier study is integrated within an ensemble Monte Carlo simulator for eliminating the errors from roughly approximating the electron occupation probability with all the details of the energy and phonon dispersion relations taken into account which are presented in Sections 2 and 3 of this paper, respectively. The calculations of the scattering rates are presented in Section 4. The model used in the study along with the EMC simulation description are given in Section 6. In Section 7, the electron-induced wind forces are calculated for an armchair metallic (10, 10) single-walled CNT at different electric field forces and temperatures. The results are compared with the values obtained using the modified Fermi-Dirac distribution for the electron occupation probability.

2. Energy dispersion relation

We use the zone folding technique [22] to obtain the energy and phonon dispersion relations for CNT from values that were obtained for graphene. In the zone folding technique, periodic boundary conditions are imposed in the circumferential direction of the CNT; this implies that in the reciprocal space of the CNT, the wavevector \( \vec{k} \) corresponding to the circumferential direction is quantized, by imposing the following equation,

\[
\vec{k} \cdot \vec{C}_n = 2\pi n
\]

(1)

where, \( n \) is an integer quantum number, and \( \vec{C}_n \) is the chirality vector which gives the direction and the magnitude of the folding direction. Eq. (1) defines a series of parallel lines (sub-bands), each corresponding to a different quantum number \( n \). For convenience, the wavevector \( \vec{k}(k_x, k_y) \) is represented as

\[
\vec{k}(k_x, k_y) \equiv \vec{k}(n, \Delta k_x, k_y),
\]

(2)

where the value of \( \Delta k_x \) depends on the chirality of the CNT, and \( \vec{k}_x, \vec{k}_y \) are the reciprocal lattice vectors along the CNT circumference and axis, respectively. We show the first and the second Brillouin zones (BZ) of a (10, 10) armchair CNT, which is the case modeled in this study, along with the BZ of graphene in Fig. 1.

Using an accurate energy dispersion relation is one of the key points for having a good MC simulation. The energy dispersion relation used for CNTs can be an analytical approximation of the exact energy dispersion relation [14,16]. In this study, the full exact energy dispersion relation is calculated at 1000 grid points in each sub-band. The energy dispersion relation of graphene is calculated first using the tight binding method with the electron wave-function of the \( 2p \) electrons used as the basis for the Bloch function using nearest-neighbor interaction only [22]. Each unit cell of graphene has two carbon atoms thus resulting in a bonding \( \sigma \) (positive) and anti-bonding \( \sigma^* \) (negative) (with respect to the energy of the \( 2p_z \) level) energy bands. Neglecting the overlap integral, these are given by

\[
E(k) = \pm t \times \sqrt{1 + 4 \cos \left(\frac{3k_x a_0}{2}\right) \cos \left(\frac{\sqrt{3}k_y a_0}{2}\right) + 4 \cos^2 \left(\frac{\sqrt{3}k_y a_0}{2}\right)}
\]

(3)

where, \( t \) is the transfer integral and is equal to 3.033 eV, \( a_0 \) is the atomic separation distance between two carbon atoms and is equal to 1.42 Å, \( k_x \) and \( k_y \) are the wave-vectors in the \( x \) and \( y \) directions, respectively.

Using Eq. (2) along with Eq. (3), the energy dispersion relation for the different sub-bands for (10, 10) CNT can be written as

\[
E(k, \nu) = \pm t \times \sqrt{1 + 4 \cos \left(\frac{\nu \pi}{10}\right) \cos \left(\frac{\sqrt{3}k_y a_0}{2}\right) + 4 \cos^2 \left(\frac{\sqrt{3}k_y a_0}{2}\right)}
\]

(4)

These are plotted in Fig. 2, where the positive energies give the conduction bands and the negative energies give the valence bands with no energy gap for sub-band \( \nu = 10 \) thus giving the (10, 10) CNT its metallic characteristics.

3. Phonon dispersion relation

For the phonon dispersion relation, the letters \( \mu, q \) are used instead of \( \nu, k \) that were used for the energy dispersion relation to differentiate them from each other. In order to find the phonon dispersion relation of graphene, a Laplace transform of time and a discrete Fourier transform of the lattice equation of motion in the real space given by Eq. (5), yields Eq. (6) in the frequency domain.

\[
\begin{align*}
\end{align*}
\]
\[
|M|\{\dot{u}_n(t)\} = \sum_{n=1}^{N} [K_{n,n}]\{\ddot{u}_n(t) - \ddot{u}_0(t)\}
\]
\[
(\omega^2(q)|M| + \hat{K}(q)|\dot{u}(q, \omega) = 0,
\]
where \(|M|\) is the mass matrix, \(\dot{u}_n(t), \ddot{u}_n(t)\) are the time-dependent acceleration and displacement of atom \(n\), respectively, \([K_{n,n}]\) is the stiffness matrix (which is diagonal in the local coordinates of the bond between atom \(n\) and \(n_0\), \(\omega(q)\) is the frequency of the phonon mode and \(\hat{K}(q)\) is the discrete Fourier transform of the stiffness matrix given as
\[
\hat{K}(q) = \sum_{n=0}^{N} [K_{n,n}] e^{-i2\pi r_n q},
\]
where \(r_n\) is the position vector of atom \(n\). Since only interactions up to the fourth neighboring atom (which is necessary to get accurate results [23]) is used with a harmonic inter-atomic potential between the atoms [24], the associate cell that is used in the calculation of \(\hat{K}(q)\) has a total number of graphene unit cells of seventeen as shown in Fig. 3.

\[\text{Fig. 2 – Energy dispersion relation of the valence and conduction bands for (10, 10) CNT in the first and second BZs.}\]

\[\text{Fig. 3 – The associate cell that is used in the calculation of } \hat{K}(q). \text{ The dotted circles show the first, second, third and fourth atoms for atom A0, while the solid circles show them for atom B0.}\]

\[\text{Fig. 4 – LA and LO phonon dispersion relation for (10, 10) CNT in the first BZ. The lower labeled sub-bands are for the LA mode, and the upper unlabeled sub-bands are the LO modes.}\]

Solving the Eigenvalue problem of Eq. (6), gives the phonon dispersion relation of graphene. The zone folding technique is then used to find the phonon dispersion relation of the LA and LO phonons only for the (10, 10) CNT (Fig. 4). Using the zone folding technique has proven to give accurate results for the longitudinal modes of the CNT but have some deficiencies in predicting the transverse modes [22] which are not used in this study.

\[\text{4. Scattering rates}\]

For calculating the scattering rates of an electron in a certain state, both LA and LO phonon absorption and emission are allowed as well as forward scattering and backward scatterings, thus giving 8 different scattering mechanisms for interaction with a specific phonon branch \(\mu\). Moreover, an electron in a specific sub-band is allowed to scatter to a state in any of the other sub-bands (inter-band scattering), thus for the case of the (10, 10) CNT under consideration in this study, there are a total of 160 scattering events to be taken into account. These are illustrated in Fig. 5. Also electrons in the first BZ are allowed to scatter to both states in the first BZ (normal scattering) as well as states in the second BZ (Umklapp scattering).

In this study the CNT is assumed to be infinitely long, perfect and un-doped, and thus scattering off potential barriers and scattering with defects or impurities are not included. Moreover, electron–electron scattering as well as scattering with transverse phonons are ignored because electron–electron scattering has no effect on the momentum transferred to the lattice and scattering with transverse phonons is less likely to happen in CNT as well as it has trivial effect on the electronic structure of the CNT [25,26].

The selection rules are that, for an electron in state \((k, \nu)\) with energy \(E(k, \nu)\) scattering to another state \((k', \nu')\), it should emit or absorb a phonon with energy \(E_\nu(q, \mu)\) that satisfies energy conservation as well as momentum conservation in both the axial and circumferential directions. This is imposed through the following equations respectively
of $10^{13}$ and $10^{14}$ s$^{-1}$ for LA and LO phonons backscattering, respectively. The peaks in the scattering rates shown in Fig. 6 are due to electrons scattering near the bottom of a sub-band whether this scattering is inter-sub-band or intra-sub-band scattering. The density of the final states was calculated numerically to avoid the singularities corresponding to scattering to states at the bottom of the sub-bands.

Also from Fig. 6, it is clear that increasing the temperature results in an increase in the scattering rate due to the increase in the Bose–Einstein occupation number, but the percentage of that increase is not equal for all the states. For 300 K, for sub-band 10, the scattering rate at the bottom of the scattering-well centered about the zero energy point at $k = 0.8515\, \text{Å}$ is about 17 and 666 times less than the value just outside the well for LA and LO phonons, respectively. These factors are only 2.4 and 6 for 1200 K, thus the preference for electrons to stay in the states in the scattering-well is less for higher temperatures than for lower temperatures. The initial distribution of the electrons among the different states in the EMC simulations is calculated according to Fermi–Dirac distribution of the electrons among the different states in the temperatures at high temperatures. The initial distribution for electrons to be located in the scattering-well is decreased. As a result, at high temperatures, the electrons are spread over more final states that are on sub-bands, other than sub-band 10. Therefore, including all the sub-bands in the EMC simulations is critical for obtaining accurate results at high temperatures.

5. Momentum transfer quantum model

Only electrons scattering with LA or LO phonons (which represent the vibration of the lattice atoms) gives rise to the electron-wind force exerted on the atoms. For an electron initially in state $(k, v)$ and scattering by LA or LO phonons to a final state $(k', v')$, the momentum transferred to or from the lattice in the circumferential direction in this event will be $\hbar (v - v') k_x$, while the momentum transferred in the direction of the tube axis would be $\hbar k$. Thus from Newton’s second law, the average force, referred as “electron-wind force”, acting on the lattice in the longitudinal direction (momentum transferred per unit time) due to this scattering event can be written as $(\hbar k - \hbar k') \times S(k, v, (k', v'))$. Taking into account the probability that state $(k, v)$ is occupied and the probability that state $(k', v')$ is empty and integrating over all the states in the first BZ, the total force per unit length $(F)$ of CNT can be expressed as

$$ F = \frac{2}{\pi} \sum_{k} \sum_{v} \int (\hbar k - \hbar k') \times S_m((k, v), (k', v')) \times f(k, v) \times (1 - f(k', v')) \, dk, $$

where $f(k, v)$ calculated according to a modified Fermi–Dirac distribution function in the presence of an electric field $E$ given as

$$ f(k, v) = \frac{f_0(E(k, v) - e\nu_{ik}, - E),}
In this study, only electric fields applied along the direction of the tube axis is considered. In Eq. (14), only the integration over the initial states in the axial direction of the CNT is performed, while integration over the final states $dk_0$ is replaced by summation over all the scattering mechanisms $m$. This is because for every initial electron state $(k, m)$ interacting with a phonon sub-band $l$, there can be only a maximum of one final state, for each of the 8 scattering mechanisms mentioned above.

This model has been verified in a previous study [12] by comparing the I–V curve to experimental results [21,27]. However, it is important to note that the distribution function given by Eq. (15) is an approximation of the exact occupation probabilities that cannot be calculated in a direct manner. As the temperature and the applied electric field increase, the occupation probabilities from Eq. (15) diverges from the expected exact value [13]. In order to calculate the occupation probability exactly, two methods in the literature are always used, namely the Boltzmann transport equation (BTE) and the Monte Carlo simulation. Using these two methods for calculating the occupation probability is well established and there is no need to argue about their validity. Thus, in order to quantify the integral given by Eq. (14), we use an EMC simulator (Section 6) to integrate the equation stochastically without the need to calculate the occupation probability initially in a separate step. Using the EMC simulation has two advantages over using the BTE, these are, eliminating the need to calculate the occupation probability initially and then feed it into the integral, and secondly using the EMC gives a better description of the electron dynamics, and thus help us to have a better understanding of the physical phenomenon occurring.

6. Monte Carlo simulation

The MC simulation method is a semi-classical transport method for simulating the electron dynamics, where the electrons drift due to an electric field classically according to Newton’s second law according to

$$\frac{d}{dt} \mathbf{k} = F_{\text{drift}} = e\mathbf{E}, \quad (17)$$

but scatter stochastically according to the scattering rates calculated quantum mechanically (Section 4).

The parameters governing the use of Eq. (17) are the electric field (E) which is constant throughout every single simulation and the scattering rates for all the states which are

![Fig. 6 – Scattering rates for LA and LO modes at different temperatures. (A) LA scattering for sub-band 10. (B) LA scattering for sub-band 9. (C) LO scattering for sub-band 10. (D) LO scattering for sub-band 9.](image)
calculated in Section 4. During the simulation random numbers that are uniformly distributed from zero to one are generated and compared to the ratio of the total drift time to the scattering rate at the state under consideration. The specific scattering mechanism is also selected randomly among all the scattering mechanisms for a specific state.

To calculate the electron-wind force, EMC are run according to Eq. (17) and the momentum transfer to the lattice during the scattering events is calculated and summed over the total scattering time and finally divided by the total simulation time to yield the electron-wind force.

For each of the EMC carried out, 100 pseudo-charge carriers were simulated for 100,000 time steps. Time steps were 0.1 Femto Second (FS) which is one tenth of the shortest scattering time calculated in Section 4. The electric charge of these pseudo-charge carriers were chosen to represent only the number of electrons in the conduction band of 1 Å long (10, 10) CNT. The pseudo-charges were distributed in the initial step among the energy sub-bands according to Fermi–Dirac distribution.

Electrons were only simulated in the conduction band, and no scattering or drifting to or from the valence band was taken into account. From Fig. 2, it is clear that only electrons at the top of sub-band 0 of the valence band can scatter or drift to states in the conduction band or the opposite (electrons at the bottom of sub-band 10 of the conduction band can scatter or drift to states in the valence band). The justification for not including these mechanisms is that, for drifting, it is clear that electrons can move from the valence to the conduction band and vice versa, due to the degeneracy at wavevector value $k = \pm 0.8515$ Å.

In CNTs, this degeneracy is lifted, thus prohibiting electrons from drifting from the valence to the conduction band and vice versa. The lifting of the degeneracy in CNTs is because the transverse acoustic phonon mode in CNTs unlike graphene does not preserve symmetry, and thus zone folding gives rise to a small energy gap at these $k$ points in the order of 1 meV at zero temperature accompanied by a parabolic curving of the sub-bands [29,30]. On the other hand for scattering between the valence and the conduction bands, as mentioned before, only scattering with LA and LO phonons are considered which have a maximum energy of 0.196 eV (Fig. 4). For approximation, in that energy range, we can assume that scatterings of electrons from the valence band to the conduction band is nearly compensated by scatterings in the opposite direction. This is because the probability of a state in the conduction band being full $f_c(E = 0 - 0.196 \text{ eV})$ is nearly one order of magnitude less than the probability of a state in the valence band being full $f_v(E = 0 - 0.196 \text{ eV})$, also the probability of a state in the valence band being empty $(1 - f_v)$ is one order of magnitude less than the probability of a state in the conduction band being empty $(1 - f_c)$, but on the other hand, the probability of an electron in the valence band scattering to a state in the conduction band $S(V \rightarrow C)$ is two orders of magnitude less than the opposite way scattering $S(C \rightarrow V)$ because the scattering rate when absorbing a phonon is proportional to $N(E_v(q, \mu))$ the Bose–Einstein occupation number for that phonon while it is proportional to $N(E_c(q, \mu)) + 1$ for the case of emitting a phonon. Thus due to these three factors, it is fair to state that both way scattering compensate for each other.

For calculating the electron-induced wind forces, the momentum difference before and after any scattering events at each time step is added up for all the charge carriers and its cumulative value is plotted against the simulation time for the different temperatures. By definition, the slope of these lines for each temperature and electric field yield the electron-induced wind forces per unit length of CNT.

7. Results and discussion

In this study, EMC simulations were carried out at temperatures of 300 K, 600 K, 900 K and 1200 K and for electric fields of 0.25, 0.5, 0.75, 1, 1.25, 1.5, 2, 4, 6, 8, 10, 15 and 20 kV/cm for each temperature. Electrons were allowed to scatter to states in the second BZ. Fig. 7 shows the time history of the location of a charge carrier in the wavevector space at the two extreme temperatures simulated. From parts A and B of the figure, which shows the evolution of the wavevector of the sample pseudo-electron reduced to the equivalent state in the first BZ, it is clear that electrons at 300 K is limited to states in the scattering-well of Fig. 6A and C and that electrons at 1200 K are distributed over the wider scattering-well from 0.75 to 0.95 Å$^{-1}$. This later finding supports the argument presented earlier in Section 4. Parts C and D show the location of the sample pseudo-electron among the first and second BZs as a function of temperature. This shows the importance of accounting for scatterings to the second BZ that cannot be ignored. As the temperature increase to 1200 K the frequency of scattering across the two BZs increases dramatically compared to that at 300 K. Parts E and F show the location of the sample pseudo-electron among the different sub-bands (reduced to the first BZ). At 300 K all the electrons are strictly distributed among the lowest sub-band ($\nu = 10$) but as the temperature increases electrons scatter to higher sub-bands and stay there for short periods of time. Thus, it is important to include the higher energy sub-bands for high temperatures, while for 300 K including all the energy sub-bands is just a computational burden without any increase in the accuracy of the results, but since the electrons scatter to the states in sub-band 0 in the second BZ (equivalent to sub-band 10 in the first BZ) both sub-bands 0 and 10 of the phonon dispersion relation must be taken into account to allow for this type of scattering, even at 300 K.

The cumulative momentum transferred to a unit length of the lattice $h\text{k} - h\text{k}'$ for all the simulated pseudo-electrons is plotted as a function of the simulation time and presented in Fig. 8 for different temperatures. In this figure, it is clear that as the temperature increases, the amplitude of the fluctuations in the momentum transferred per unit length is increased. This is due to the increase in the scattering rates for both forward and backward scatterings. At higher temperatures, the momentum transferred to the lattice increases. This is due to the fact that at higher temperatures the difference between forward and backward scattering increase. Also from the figure, it can be observed that the relationship between the cumulative momentum transferred per unit length and simulation time is linear (excluding the consistent...
fluctuations) for 300 K, 600 K and 900 K. For 1200 K, this linearity is interrupted by some random bumps due to the stepwise transfer of an electron that reached sub-band zero of the second BZ to higher sub-bands by emitting optical phonons until reaching sub-band 10 or vice versa. This mechanism is illustrated in Fig. 7F at around 80% of the simulation time.

For calculating the force generated per unit length of the CNT, the curves plotted in Fig. 8 should be differentiated with respect to time. In order to eliminate the fluctuations in the curves, they were linearly fitted and the slope of the curves were used to determine the electron-wind forces. The calculated force per unit length of the CNT is plotted for 300 K and compared with that calculated using Eq. (14) at different electric fields in Fig. 9. The non-linear behavior of the results obtained by the integral form can be explained that, initially, as the electric field increases, according to the approximation given by Eq. (15), the probability of the occupation of the right

Fig. 7 – Time evolution of a sample electron location at 300 K and 1200 K. (A) Wavevector for 300 K. (B) Wavevector for 1200 K. (C) BZ index for 300 K. (D) BZ index for 1200 K. (E) Sub-band index for 300 K. (F) Sub-band index for 1200 K.
moving electron states \(f(k > 0.855, \nu = 10)\) starts to increase, while the probability of the occupation of the left moving electron states \(f(k < 0.855, 10)\) decreases, and thus force will increase rapidly, explaining the behavior till an electric field force of around 1.5 kV/cm. By increasing the electric field force more, \(f(k < 0.855, 10)\) continue decreasing and \(f(k > 0.855, 10)\) continue increasing till they saturate at an electric field force around 2 kV/cm. Saturation for \(f(k < 0.855, 10)\) happens when it reaches a value of zero and thus cannot decrease anymore, while saturation for \(f(k > 0.855, 10)\) is due to the step in the scattering rates at 0.875 Å⁻¹ shown in Fig. 6, thus the increase of the electric field force at that point has a little impact on \(f(k)\) and thus on the calculated value of the force, resulting in the observed saturation between 2 and 6 kV/cm. Increasing the electric field more than 6 kV/cm starts to increase the probability \(f(k, 10)\) more over the range of the next peaks in the scattering rates around the wavevector values of 0.875 and 1 Å⁻¹. These jumps are due scattering to states near the bottom of sub-bands -9, +9 that have energy values that are close to that of the initial states, and thus the increase in the probability \(f(k, 10)\) at these states is compensated by the nearly equal decrease in the probability \(1 - f(k', \pm9)\), thus preventing the force from growing exponentially to extremely high value. From this explanation it is clear that the approximation of the electron occupation probability has a major effect on the calculation of the electron-induced wind forces.

On the other hand, the linear behavior exhibited by the EMC simulations can be explained through Eq. (17) where as an electric field is applied, the electrons at the bottom of sub-band 10 start to drift toward the states of higher wavevector till they reach 0.875 Å⁻¹. After that value, the scattering rate increases by orders of magnitude thus increasing the probability of the electrons scattering by phonons (mostly backwards), thus gives rise to the induced forces transferred to the lattice. Increasing the electric field will only make the electrons reach that scattering step faster and thus backward scatter more frequently and thus increasing the induced forces and since the rate of change in the wavevector of the electrons is linearly proportional to the electric field force; the change in the induced forces will also be linearly proportional to it. The linear behavior observed in Figs. 9 and 10 is the same as electron-wind force formulation suggested by Fiks in 1959 [31], and widely used in electromigration literature since, where the electron-wind force in metals is given by \(Z' eE\), where \(Z'\) is the effective charge number. The EMC simulations give a more correct view of the electron dynamics than the approximation used in the integral form, and it is clear that using the modified Fermi–Dirac distribution approximation

![Image](https://example.com/image.png)

**Fig. 8 –** Cumulative momentum transferred from the electron to the lattice during the simulation time for all the electric fields simulated.
is not capable of completely capturing the correct behavior. This behavior calculated here for the (10, 10) CNT should be the same for any armchair CNT regardless of the diameter due to exhibiting the same energy and phonon dispersions but with different number of sub-bands.

For studying the effect of the temperature, the electron-induced forces are plotted at different electric fields for the temperatures simulated in Fig. 10. All of the curves show the same linear behavior, but the noise in the data increases as the temperature increase. This noise can be eliminated by extending the simulation time. Also, as the temperature increases, the forces increase due to the increase in the difference between the backward and the forward scattering rates.

Finally, the value of the effective charge number at different temperatures \( Z' \) can be calculated from the slopes of the curves in Fig. 10 giving values of 3.46E–3, 9.18E–3, 0.0127 and 0.015 for 300, 600, 900 and 1200 K, respectively.

8. Conclusions

In this study, an analytical method using the ensemble Monte Carlo simulations is presented for calculating the effective charge number and the electron-induced wind forces in armchair (10, 10) carbon nanotubes. It was found that for 300 K including the lowest energy sub-band along with the lowest and the highest phonon sub-bands is enough for the simulations. For 1200 K, it is important to include all the energy sub-bands. The electron-induced wind force is found to be linearly dependent on the electric field. The effect of the temperature on the effective charge number \( Z' \) was studied. The effective charge number value for CNT was found to vary between 4.65E–3 and 15E–3. Results was compared with an integral solution based on an approximation of the electron occupation probability, and showed that the modified Fermi–Dirac approximation in not reliable in calculating effective charge number and the electron-induced wind forces. The model presented in this paper can be extended to take into account the hot phonon effect through continuous update of the phonon occupation number and the scattering rates in every simulation step based on the previous scattering events.

Acknowledgments

The authors are grateful to Professor Peihong Zhang of the Physics Department at the University at Buffalo, SUNY for his valuable discussions. This project has been sponsored by NSF CMS division Grant No. CMS-0508854 and ONR Advanced Electrical Power Systems Division by program director Terry Ericsen.

REFERENCES