Electron-phonon scattering and ballistic behavior in semiconducting carbon nanotubes

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We study the steady-state and ballistic transport properties of semiconducting zig-zag carbon nanotubes (CNTs) using semiclassical Monte Carlo simulation. Electron-phonon scattering is the only type of interaction included in the model. The band structure and phonon dispersion are derived from that of graphene by the zone folding method. Steady-state drift velocity and low-field mobility are calculated in CNTs with wrapping index ranging from \( n = 10 \) to \( n = 59 \), i.e., for a diameter range of \( 0.78 - 4.62 \) nm. Principally, a transient analysis of transport under uniform driving field is realized and gives the fraction of ballistic electrons as a function of CNT length and the mean free path (MFP) for acoustic and optical phonons scattering. The probability to have ballistic electrons on a given distance appears to be higher for nanotubes of large diameter and depends on the field applied. © 2005 American Institute of Physics. [DOI: 10.1063/1.2119421]

Electronic transport through single-wall carbon nanotubes (SWNTs) generated considerable interest in the past few years for both fundamental and science technology.1 Taking advantage of its extraordinary electrical properties, such individual nanotube can be used as the channel of nanotube field-effect transistors (CNTFETs) which have recently reached a high level of performance.2,3 Such devices may operate with either Ohmic or Schottky source and drain contacts.4,5 CMOS-like logic circuits using \( n \)-type and \( p \)-type MOS-like FETs have been demonstrated.6,7 Several groups have observed ballistic transport in carbon nanotubes. In metallic tubes, the MFP has been experimentally found to be about \( 1 \) \( \mu \)m at low field and in the range \( 10 - 100 \) \( \mu \)m at high field.8,9 For semiconducting tubes, values close to \( 300 - 500 \) \( \mu \)m and \( 10 - 100 \) \( \mu \)m have been obtained at low-field and high field, respectively.1,4,10

To investigate the transport properties of usual semiconductors and devices, simulation techniques based on the solution of the Boltzmann equation have been widely and successfully applied, especially using the Monte Carlo method11 which consists of a statistical description of classical trajectories of individual carriers as a succession of free flights and instantaneous scattering events. It was recently used to calculate the steady-state velocity-field characteristics of semiconducting CNTs.12 In the present work, we use our Monte Carlo code13 to analyze both steady-state and transient regimes of transport for “perfect” single-wall zig-zag semiconducting CNTs of diameter \( d \), ranging from 0.78 nm to 4.62 nm. The only type of scattering mechanism under consideration is the electron-phonon interaction. We focus on the intrinsic ballistic transport properties which is a debated question in the community. In particular, we evaluate the mean free path as a function of field and length for several tube diameters, which is the average distance traveled by a carrier between two scattering events. The particle Monte Carlo technique requires the knowledge of material band structure, phonon energies and scattering rates which are briefly described below.

The structure of a CNT can be seen as the result of the rolling up of a graphene sheet.14 The rolling up is geometrically characterized by the indices \( (n, m) \) which specify the diameter and the chiral angle of the CNT and determine its fundamental properties. In this work, we study zig-zag CNTs (i.e., \( m = 0 \)) having semiconducting properties (i.e., \( n + 2 \) or \( n + 1 \) is multiple of 3), with wrapping index \( n \) ranging from 10 to 59.

The energy dispersion of the nanotube is here considered to arise directly from that of graphene calculated by the tight-binding approximation. Depending on how the sheet is rolled up, the periodic boundary conditions impose restrictions on available states, which results in a discrete set of allowed wave vectors. Each electron wave vector is characterized by a quantum number \( \eta \) which specifies the confinement along the tube circumference and by a continuous component \( k_z \) along the tube axis. Finally, this zone-folding method breaks up each band of graphene into 2\( n \) subbands. For the CNT, among the 2\( n \) subbands, \( n - 1 \) of them are twofold degenerate. This degeneracy leads to two equivalent valleys in the subband structure, each centered near a graphene K point. For this study of transport, we focus our interest on subbands resulting from the \( \pi \)-antibonding bands of graphene. We consider the same band structure as that calculated in Ref. 12. In this paper, a convenient analytical approximation is proposed to describe the energy of the first three subbands of each valley for semiconducting zig-zag CNTs, which is amply sufficient considering the range of field applied in the present work \((E < 100 \) kV/cm\). The general expression of energy dispersion is finally

\[
\frac{\hbar^2 k_z^2}{2m_b(n)} = \left[ E_b - E_b^n(n) \right] \left[ 1 + \alpha_b(n)(E_b - E_b^o(n)) \right],
\]

where \( E_b^n(n) \), \( m_b(n) \), and \( \alpha_b(n) \) are the minimum of energy, the effective mass, and the nonparabolicity coefficient of subband \( b \), respectively.

Similarly, the phonon spectrum of CNTs can be well described by zone folding the phonon dispersion curves of 2D graphene sheet. Each of the 6 phonon branches of graphene are broken in 2\( n \) subbands. Longitudinal acoustic

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and optical modes are considered to be dominant for electrons scattering within the first three subbands of both valleys.\textsuperscript{15} For the acoustic mode, we use the same phonon energies as in Ref. 12. For intervalley and intersubband acoustic phonon transitions, we make an approximation considering that the branches are flat with a constant energy equal to the minimum value of each mode $\hbar \omega = E_p z(0)$. Moreover, the phonons resulting from the longitudinal optical branch of graphene are included, with energy values of 180 meV and 200 meV. They induce additional intervalley/ intersubband transitions.\textsuperscript{16}

The scattering rates are calculated using the first-order perturbation theory within the usual deformation potential model. For zig-zag tubes, the deformation potential $D$ can be considered constant and equal to 9 eV.\textsuperscript{17} We treat the intrasubband acoustic scattering as an elastic process and each intersubband transition is considered via its corresponding constant energy phonon $E_p z$.

Now, we present the results obtained with Monte Carlo simulation of electron transport, at room temperature, for zig-zag semiconducting CNTs with wrapping index $n=10, 22, 34, 49, 58$.

To validate the model and the approximations, we first calculated some steady state velocity-field characteristics (not shown). We find that the velocity increases with the tube diameter $d_v$ and the peak velocity reaches $3.43 \times 10^7$ cm/s for $n=10$ ($d_v = 0.783 \text{ nm}$) and $4.88 \times 10^7$ cm/s for $n=58$ ($d_v = 4.62 \text{ nm}$). Similar results have been reported.\textsuperscript{18} The critical field $E_{0\text{sat}}$ associated with the peak velocity falls as the tube diameter increases. Indeed, the intersubband energy spacing is all the smaller as diameter is larger, which makes intersubband and intervalley transitions possible and effective at lower field.

The calculated low-field mobilities are in the range $2800-141200 \text{ cm}^2/\text{V s}$, which is consistent with experimental mobilities.\textsuperscript{19}

In Fig. 1, we plot together the subband occupation (solid lines) and the electron velocity (dashed line) as a function of field for a tube of index $n=49$ ($d_v = 3.83 \text{ nm}$). It allows us to understand the origin of the “saturation” peak velocity and the change of slope in the velocity-field characteristics. Field-induced electron heating makes subband transfer possible which is reflected on the velocity because the effective mass and the total scattering rates increase with the subband index. The change of slope observed for $E \approx 0.1 \text{ kV/cm}$ is due to transfer between the two first subbands of the same valley. The velocity peak (for $E = 7 \text{ kV/cm}$) and velocity saturation occur when intervalley subband transfer becomes possible and significant.

Now, considering an electron gas initially at equilibrium under $E=0$, we study its transient behavior in response to a field step of height $E_s$ applied at time $t=0$. We use the possibility of counting the number of scattering events experienced by each carrier between the positions $z=0$ and $z=L$.\textsuperscript{20}

As shown in Fig. 2 (for $n=22, d_v = 1.72 \text{ nm}, E_s = 8 \text{ kV/cm}$), the spectroscopy of scattering events for various tube lengths illustrates very well the process of relaxation. The distribution is very sharp and decays exponentially for small length ($L < 200 \text{ nm}$ in this case) with a high fraction of ballistic electrons. For larger length the distribution becomes a bell-curve and the number of ballistic electrons vanishes rapidly. For larger tubes, the curves are similar but with a smaller fraction of scattering events.

We have access to the number of purely ballistic electrons as a function of the length $L$, as shown in Figs. 3(a) and 3(b) for various CNTs with a field step of 0.6 and 8 kV, respectively. For $E=0.6 \text{ kV/cm}$, the main scattering event corresponds to electron-phonon acoustic scattering. The
curves decay slowly for large tubes \((d_{\text{t}}=4.6 \text{ nm})\) with 50% of electrons which are still ballistic at \(L=1 \mu \text{m}\). For small tubes, the electron ballisticity decreases rapidly on the first 200 nm. Now, considering a higher field \((E=8 \text{ kV/cm})\), for each curve, there is an abrupt fall in the fraction of ballistic electrons [Fig. 3(b)]. The length \(L_F\) at which this fall occurs is approximately the same for all CNTs \((L_F\approx 180 \text{ nm})\). It corresponds to the distance needed for a ballistic electron to reach the minimum kinetic energy which makes possible an intervalley phonon emission \((\hbar \omega=160 \text{ meV and } 180 \text{ meV})\). Thus \(L_F\) is roughly defined by \(k_B \times T/2 + E \times L_F = \hbar \omega\). As soon as this phonon emission is possible, the emission rate is so high that the ballistic probability vanishes rapidly.

The probability to have ballistic electrons on a given distance is all the higher that the diameter is larger, which is strongly related to the diameter-dependence of effective mass. For \(d_{\text{t}}=1.72 \text{ nm}\) and a field-step of 8 kV/cm, the fraction of ballistic carriers is greater than 90% for a tube length of 10 nm, and is still 50% for a length of 200 nm. It should be noted that for a higher field step, like \(E_{\text{t}}=60 \text{ kV/cm}\), the fraction of ballistic electrons falls to 50% for a length of only 60 nm (not shown). We illustrate in Fig. 3(b) the high performance of CNTs by comparing them to undoped Si. In the latter material, half electrons have already scattered at \(L=25 \text{ nm}\) and almost none of them are still ballistic at \(L=100 \text{ nm}\).

We now focus on the average length traveled by electrons before being scattered by acoustic and optical phonons. Thus, we performed simulation in stationary transport and obtained the MFP for each scattering process (Fig. 4). Our results show that the MFP for electron-phonon acoustic scattering depends on tube diameter and is in the range 100–600 nm for diameter between 1.72 and 4.62 nm. The MFP for electron-phonon intervalley scattering decreases as the electric field increases and we find \(L_{\text{MFP}}=20 \text{ nm for } E=100 \text{ kV/cm}\), which is consistent with other works. In particular, it is striking that for each tube, the range of field in which acoustic and intervalley curves intersect corresponds to the region where the velocity saturation occurs.

In conclusion, we have shown that large tubes exhibit a high level of performance. They are likely to reach high mobility and peak velocity with a good potential for quasi ballistic transport. However, the band gap energy of large-diameter CNT is very small, e.g., \(E_G=0.186 \text{ eV for } d_{\text{t}}=4.62 \text{ nm}\). For practical application, the choice of the CNT to be used should result from a compromise between high mobility/ballisticity and large band gap.

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