A Semiclassical Study of Carrier Transport combined with Atomistic Calculation of Subbands in Carbon Nanoribbon Transistors

D. Rondoni*, J. Hoekstra*, M. Lenzi** and R. Grassi**

* Delft Technical University, Electronics Research Laboratory
Faculty of Electrical Engineering, Mathematics and Computer Science
mikelweg 4, 2628CD Delft, The Netherlands, D.Rondoni@tudelft.nl
** ARCES and DEIS, University of Bologna, Viale Risorgimento 2, 40136, Bologna, Italy

ABSTRACT

In this paper we present a deterministic approach to the study of one-dimensional carrier transport in CNR devices, both in the ballistic regime and when phonon scattering is taken into account. The energy subbands and the potential energy profiles along the longitudinal coordinate are obtained through the atomistic slab-by-slab solution of the transverse Schrödinger equation. The longitudinal transport is modeled through a deterministic solution of the Boltzmann transport equation. Finally, these equations are solved self-consistently with the Poisson equation in order to obtain the electrostatic potential, the charge density and the electrical currents at different biases. Results are presented for different channel widths and transistor geometries and the impact of phonon scattering is discussed.

Keywords: carbon nanoribbons, carrier transport, Boltzmann equation, phonon scattering.

1 INTRODUCTION

Carbon Nanotubes (CNTs) have received a very large attention from the nanoelectronic research community during the last years. In fact, CNT-FETs exhibit very promising performances, with very high mobilities and carrier velocities [1]. However, despite the big amount of research in the last few decades, many serious technology issues are still to be solved (control on the chirality of the tubes, mixing of planar deposition and cylindrical geometry, circuit patterning, amongst the others). Therefore, at present, it appears that the feasibility of large scale integration of CNT devices will require the development of revolutionary techniques in process technology.

Carbon Nanoribbons (CNRs) exhibit properties similar to CNTs [2], [3], together with a planar geometry that appears in principle more feasible for integration with SiC substrates through high performance lithography techniques. Therefore, in the last few years CNRs are being addressed as a valid alternative to CNTs [4]–[6] and simulation studies of CNR-FETs are becoming very important in order to evaluate the performances of such nanodevices.

Figure 1: Example of a basic cell for a (12,0) armchair nanoribbon (note that the chiral vector formalism is 90 degrees rotated for CNRs compared to CNTs). The dimers are numbered from left to right.

In this paper we simulate and evaluate the performance of nanometric planar FETs whose channel is made of a narrow (few nanometers wide) armchair semiconducting single-layer nanoribbon. The CNR is treated as a 2D-channel and 1D transport is obtained through the confinement in the transverse direction. The nanoribbon is considered as a series of basic cells, called slabs (see Fig. 1).

We separate the 2D problem in the transverse and longitudinal directions and solve it self-consistently with the 3D Poisson’s equation. In the transverse direction (quantum confinement), a Tight-Binding (TB) Hamiltonian is used to find the energy subbands in each slab of the CNR. The 1D problem of transport along the longitudinal direction is then solved with a deterministic solution of the Boltzmann Transport Equation (BTE), both in the ballistic regime and when scattering is taken into account, based on a simplified dispersion relation that includes first order non-parabolic effects.

2 CONFINEMENT: TRANSVERSE SOLUTION

In this section we describe the TB model used for the transverse solution (lateral confinement). In principle, for every slab $l$ of the ribbon, the energy dispersion relations (subbands) $\varepsilon(k)$, with $k$ the longitudinal wavevector, should be calculated starting from the full TB Hamiltonian and solving the transverse Schrödinger equation with the potential energy repeated periodically throughout the device.
In our recent work [7], we show that the dispersion relations obtained with the non-parabolic expression

$$(\varepsilon_b - \frac{E^\circ_b}{2})/2 - \frac{\varepsilon_b}{E^\circ_b} = \frac{\hbar^2 k^2}{2m^*_b}$$

(1)

where b is the subband index, $E^\circ_b = E^b_c - E^b_v$ is the energy gap and $m^*_b$ the effective mass, match with excellent agreement, over an extended range of energies, the dispersion relations obtained with a full TB approach. The results described in [7] show that we can perform our calculations over a simplified version of the transverse problem. For a given width, the full subband structure is calculated only once for a slab with flat zero potential, from which the effective masses of the lowest desired subbands are extracted. The eigenvalue TB calculation is then repeated in every slab of the device only for $k = 0$, in order to obtain $E^b_n$ and $E^b_v$, as well as the eigenfunction $\chi^b$, as a function of the longitudinal coordinate $z$. Subsequently, the potential profile along $z$, obtained from the energy minima of the calculated bands, is used, together with the effective masses and non-parabolicities, as the input of the BTE solver.

### 3 TRANSPORT: DETERMINISTIC SOLUTION OF THE BTE

The transport problem along the longitudinal direction is treated with a semi-classical approach. In this work we simulate carrier transport only in the conduction band, therefore we consider only electrons as carriers. In the next future we intend to include holes and extend the model to the valence band.

The electronic current along the device is described by a system of BTEs, having as unknowns the electron distribution functions $f_b(z,k)$, where $b$ is the subband index. The steady-state BTE of the $b$-th subband is written in the form

$$u_b \frac{\partial f_b}{\partial z} - \frac{1}{\hbar} \frac{dE_b}{dz} \frac{\partial f_b}{\partial k} = C^b_{in} - C^b_{out}$$

(2)

where $u_b = 1/\hbar(d\varepsilon_b/dk)$ is the group velocity, with $\varepsilon_b(k)$ the energy-dispersion relation. $C^b_{in}$ and $C^b_{out}$ are the in- and out-scattering integrals, respectively, relative to the state $k$ of the $b$-th subband, and are integrals of the scattering probabilities, which are written in accordance to Fermi’s Golden Rule [8], [9]. Both acoustic (elastic) and optical scattering is considered, intrasubband and intersubband.

For acoustic scattering, in the high temperature and isotropic approximation [9], the scattering probability from state $k$ in band $b$ to $k'$ in band $b'$ is

$$S_{ac}^{bb'}(k,k') = \frac{2\pi D^2_{ac}k_BT}{\hbar v^2_s\rho} \delta[\varepsilon_b(k') - \varepsilon_b(k)]$$

(3)

with $D_{ac}$ the acoustic deformation potential, $v_s$ the sound velocity in graphene, $\rho$ the graphene superficial mass density, $\delta[x]$ the Dirac delta-function, and $I^{bb'}$ the form factor. For optical phonons, the scattering probability from state $k$ in band $b$ to $k'$ in band $b'$ is

$$S_{op}^{bb'}(k,k') = \frac{\pi D^2_{op}I^{bb'}}{\rho\omega_{op}} [N_{op}(\hbar\omega_{op}) + \frac{1}{2} \mp \frac{1}{2}]$$

(4)

with $D_{op}$ the optical deformation potential, $\omega_{op}$ the phonon angular frequency and $N_{op}(\hbar\omega_{op})$ the phonon number given by Bose statistics. The upper and lower signs correspond, respectively, to phonon absorption and emission processes.

The values of the physical constants for the scattering processes are taken from recent literature. Since research on scattering in CNRs is at its very beginning, reliable values are still not available, and therefore some of them have been extrapolated from analogous values of CNTs. In particular, for acoustic phonons the reader may refer to [10], while for optical phonons we focus on longitudinal optical phonons (see [2], [5], [10]) and the value of the energy quantum associated with the optical scattering is $E_{op} = \hbar\omega_{op} = 160$ meV (taken from CNTs values [11], [12]). Finally, the form factors $I^{bb'}$ in equations (3) and (4) are defined, in agreement with [8], as

$$I^{bb'} = \int_0^w |\chi^b(x)|^2 |\chi^{b'}(x)|^2 dx \simeq \left\{ \begin{array}{ll} 3/2w & \text{if } b = b' \\ 1/w & \text{if } b \neq b' \end{array} \right.$$  

(5)

where $w$ is the ribbon width.

The distribution functions and the charge densities obtained from the BTE are fed into the Poisson’s equation to calculate the new electrostatic potential and the whole procedure is iterated until the self-consistent global solution is reached.

### 4 RESULTS

Simulations have been carried out for CNR-FETs with the structure shown in Fig. 2. Two types of arm-...
Figure 3: 2D contour plots (in log-scale and \((z, E)\) space) of carrier distribution functions in ballistic transport conditions for the most populated subband of a 12-dimers (top) and 19-dimers (bottom) armchair nanoribbon, positive (left) and negative (right) flows, with \(V_{DS} = 0.4V\) and \(V_{GS} = 0.4V\). Values of the distribution function go from \(10^{-6}\) (deep blue) to 1 (red).

Armchair nanoribbons have been considered, one with \(N = 12\) (about 1.35 nm wide) and the other with \(N = 19\) (about 2.2 nm wide), \(N\) the number of dimers in the basic cell. The length of both nanoribbons is 83 slabs, equal to about 35 nm of which 15 nm of undoped channel and about 10 nm source and drain extensions. It is important to point out that the subbands calculated with the TB approach in [7] allow us to restrict ourselves to the two most populated subbands because the third conduction subband of the nanoribbons considered here results very far from the bottom of the conduction band and doesn’t contribute to the conduction. Therefore only the two most populated subbands are simulated in the BTE and considered in the transport problem.

The distribution functions in the ballistic case for the most populated subband of the two types of CNR-FETs are depicted in Fig. 3. In the case of flow in the positive direction, at the drain side it can be clearly noticed a population of carriers in equilibrium with the drain and a population of hot carriers coming from the source. In the case of negative flow the carriers coming from the drain cannot overcome the potential barrier and hot carriers at the source are not present. The net flow, calculated amongst all the subbands considered, will give the total current of the device.

In Fig. 4 the effect of scattering is highlighted in the case of the 19-dimers nanoribbon, for positive flow and different subbands. In the case of acoustic scattering only, the carrier density coming from the source decreases towards the drain because the carriers are backscattered either in the same subband or in the other subband. However the energy level of the carriers stays the same. Viceversa, if we consider in our calculations also optical scattering, we can notice the effect of energy spreading due to the optical phonon absorption/emission process.

The \(V_{DS} - I_{DS}\) output characteristics for ballistic CNR-FETs are depicted in Fig. 5. Both 12-dimers and 19-dimers FETs are reported for a comparison. Results (for similar widths and bias conditions) are in good agreement with calculations performed in other papers [3], [4].

Fig. 6 shows the output characteristics of the 19-dimers FET when \(V_{GS}\) is varied and different phonons.
are considered. It is evident that acoustic scattering is the main cause of current degradation and only when the channel is sufficiently open (\(V_{GS} = 0.6\) V) optical scattering plays an appreciable role. This is due to the fact that only when there are available states inside the channel optical scattering is able to backscatter the carriers towards the source, while carriers which are scattered by optical emission after the channel are sooner or later collected by the drain (see Fig. 4).

5 CONCLUSIONS

A computational method for the solution of carrier transport in CNR-FETs has been presented. The problem is solved through a deterministic solution of BTEs coupled with an atomistic TB transverse solution of the Schrödinger equation, self-consistently solved with Poisson’s equation. The approach exhibits short simulation times compared to Monte-Carlo, where the computational times are quite long due to the statistical noise. In fact, in the case of carrier transport in CNRs the one-dimensionality of the problem makes direct solutions of Boltzmann Equations more convenient, particularly when the number of subbands to consider is limited.

Future work will have to include the transport of positive carriers (solving the BTEs for the valence band) and the edge-roughness scattering, that, especially in very narrow ribbons, plays a strong (if not major [3]) role. Moreover, a study of the device mobility will be useful to further evaluate the reliability and the accuracy of the model.

ACKNOWLEDGEMENTS

This research project has been supported by a Marie Curie Early Stage Research Training Fellowship of the European Community’s Sixth Framework Programme under contract number 504195-EDITH.

REFERENCES