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# Voltage-dependent parameter extraction for graphene nanoribbon interconnect model through ab initio approach

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ABSTRACT

This paper presents electrical parameter extraction for metallic graphene nanoribbon (GNR) interconnects utilizing ab initio approach. Unlike the studies taking the kinetic inductance, quantum capacitance and Fermi velocity as constant values, voltage-dependencies of these parameters are obtained for GNR transmission line model. The variations of the kinetic energy and the current by the applied voltage are taken as bases for voltage-dependent kinetic inductance calculation. Quantum capacitance and the Fermi velocity are also computed from the kinetic inductance variation. It is concluded that voltage-dependencies of the kinetic inductance and the quantum capacitance have to be taken into account for accurate GNR modelling in nanoelectronic design.



## 1. Introduction

Power and ground lines, clock pulse and other signals are transported among circuit components via interconnects inside the integrated circuits (ICs). Copper, gold and aluminium interconnects are conventional structures for the transmission of these signals. However, as the scaling down of the IC technology node continues, the resistances of conventional bulk interconnects increase due to grain-boundary and surface scattering mechanisms because the interconnect dimensions become comparable to electron wavelength [1–3]. These disadvantages of bulk interconnects lead the research to various feasible alternatives. Nano scale interconnects such as metallic carbon nanotubes (CNTs), graphene nano ribbons (GNRs) and gold nanowires are promising alternatives according to theoretical and experimental studies [4–6]. From the fabrication viewpoint, GNRs are advantageous [5]. However in order to utilize metallic GNRs as interconnects in the future IC technology, their accurate models have to be developed.

There are various circuit models for GNR interconnects in the literature [7–11] and the transmission line model shown in Fig. 1 is the backbone of these studies. In the GNR transmission line model of Fig. 1, the $\delta$ symbol denotes the infinitesimal of the corresponding parameter. $R_q$ is the contact resistance that is generally taken as the resistance quantum value, 12.9 k, for good quality contacts [7]. $L_m$ is the magnetic inductance that is obtained from the classical electromagnetic analyses [7,8]. $C_e$ is the electrostatic capacitance which is also calculated using classical electrostatic arguments. $L_m$ and $C_e$ are material and geometry dependent parameters; therefore, they are calculated using the classical methods in the same way as the calculation utilized for the conventional bulk interconnects [11]. Hence, $L_m$ and $C_e$ are well-defined. On the other hand, there are two other parameters in the GNR transmission line model, namely the kinetic inductance, $L_k$, and the quantum capacitance, $C_q$. These two parameters arise from quantum effects during the electron transport in nano scale interconnects [12–14] and they do not have classical counterparts. Therefore $L_k$ and $C_q$ have to be obtained using quantum mechanical arguments.

Quantum capacitance and kinetic inductance of metallic GNR interconnects are generally taken as having constant and voltage-independent values in the literature. For example in [11], $L_k$ and $C_q$ of GNR interconnects are taken as 8 nH/μm and 200 aF/μm, respectively. Similarly another study takes $L_k$ and $C_q$ as having the values of 16.1 mH/m and 96.8 pF/m, respectively [9]. In [15], an analysis on the kinetic inductance is given and assuming that the Fermi velocity, $v_F$, is $8.10^5$ m/s in GNRs, kinetic inductance is calculated as 4 nH/μm. It is worth noting that in [15], the obtained $L_k$ value is valid only under the assumption that the Fermi velocity has the mentioned value, which is not an exact value. In other studies, the average value for $v_F$ is also taken around $10^6$ m/s for GNR interconnects [11,16,17]. [8] and [16] also give expressions for $L_k$ and $C_q$ dependent on an average value for $v_F$; however, it does not discuss the accurate quantum mechanical calculation of $L_k$, $C_q$ or $v_F$. The relation of $v_F$ and $L_k$ is also discussed in [17] and a kinetic

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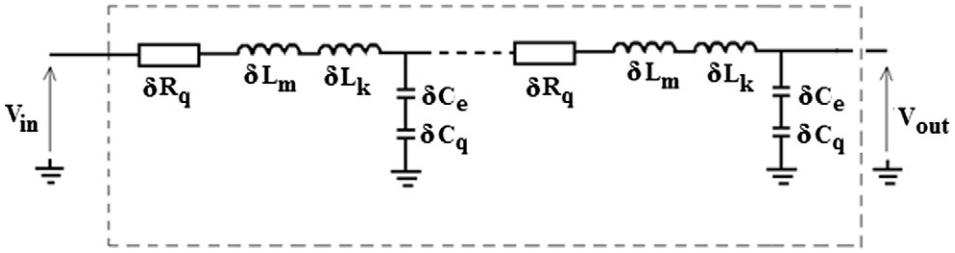


**Fig. 1.** The generic graphene nanoribbon interconnect transmission line model.

inductance of 16 nH/μm is calculated using an average value for $v_F$. In [7], $L_k$ and $C_q$ are discussed in the case of parallel GNR interconnects and again taking $v_F$ as having an average constant value, $L_k$ and $C_q$ are found to be 8 nH/μm and 200 aF/μm, respectively. As summarized above, in the studies considering the kinetic inductance and quantum capacitance of GNR interconnects in the literature, various $L_k$ and $C_q$ values are calculated under the assumption of average and constant Fermi velocity values. However, Fermi velocity of electrons which are being transported in a nano scale interconnect is expected to have a voltage-dependent orbias-dependent characteristics due to the modulation of the transmission spectrum in nano scale conductance channels, which is analysed in detail in various studies in the literature[1,13,18,19]. Hence, in order to obtain accurate voltage-dependent $L_k$ and $C_q$ characteristics, quantum mechanical simulations need to be performed which take the transmission spectrum modulation and kinetic energy variations into consideration. There is only one study in the literature for the accurate calculation of the quantum capacitance value in this manner [20]; however, it considers only metallic CNTs and not GNRs. Moreover, it is limited to the quantum capacitance computation and does not consider the calculation of the kinetic inductance.

In this study, accurate voltage-dependent variations of the kinetic inductance and the quantum capacitance of a GNR interconnect sample are obtained in the quasi-static regime using ab initio quantum mechanical simulations. The variation of the Fermi velocity is also discussed. It is concluded that the voltage-dependencies of the kinetic inductance and quantum capacitance have to be taken into account for accurate GNR interconnect transmission line modelling.

## 2. The relations among kinetic energy, current, kinetic inductance, quantum capacitance and the Fermi velocity

The relation between the kinetic energy $E_k$ at voltage $V$, and the current $I$ at voltage $V$, passing through a nano scale interconnect is given by (1) in the quasi-static regime [14,21].

$$E_K(V) = \frac{1}{2} L_K(V).[I(V)]^2 \tag{1}$$

where $L_k(V)$ denotes the voltage-dependent kinetic inductance. Taking the derivatives of both sides and arranging the equation, the expression for the accurate voltage-dependent kinetic inductance is given by (2).

$$L_K(V) = \frac{1}{I(V)} \frac{dE_K(V)}{dI(V)} \tag{2}$$

In (2), $dE_k(V)$ is the change of the kinetic energy and $dI(V)$ is the change in the current passing through the interconnect. Hence, accurate voltage-dependent kinetic inductance can be computed if the change in the kinetic energy and the current by the voltage applied to the interconnect is obtained by quantum mechanical simulations. In this study, ab initio simulations of a sample GNR interconnect are performed using Quantumwise ATK® software package in order to compute $dE_k$ and $dI$ for use in the calculation of the kinetic inductance. In addition, the relation of $v_F$–$L_k$ and $v_F$–$C_q$ can be given as in (3) and (4), respectively [10].

$$L_K(V) = \frac{h}{4q^2 v_F(V)} \frac{1}{N_{ch}} \tag{3}$$

$$C_q(V) = N_{ch} \frac{4q^2}{h v_F(V)} \tag{4}$$

where $q$ is the electron charge, $h$ is Planck's constant and $N_{ch}$ is the number of transmission channels. Using (3) and (4), the relation between $C_q$ and $L_k$ can be found as in (5).

$$C_q(V) = N_{ch}^2 \frac{16q^4 L_K(V)}{h^2} \tag{5}$$

Hence, voltage-dependent quantum capacitance can also be computed when voltage-dependent kinetic inductance is obtained. Voltage-dependent $v_F$ can also be obtained from (3) as follows.

$$v_F(V) = \frac{h}{4q^2 L_K(V)} \frac{1}{N_{ch}} \tag{6}$$

## 3. Ab initio quantum mechanical simulations of the GNR interconnect sample

Ab initio simulations of nano scale devices provide accurate results for the electronic behaviours of various structures such as CNTs [20], metal nanowires [22] and GNRs [23]. First principle quantum mechanical simulations have several types that are used for different aims. The voltage-dependent variations of $E_k$ and $I$ are needed in this study; hence, a quantum mechanical simulator capable of calculating voltage-dependent variations is required. Quantumwise ATK® is an ab initio simulator utilizing density functional theory (DFT) to solve Kohn–Sham equations in conjunction with non-equilibrium Green's function formalism (NEGF) to provide voltage-dependent variations of electronic parameters [24]. ATK® can also be used for accurate computations of GNR structures in consistent with experimental results [25]. Therefore, this software package is used in this work.

The metallic 5 atom wide zigzag GNR (5-ZZGNR) interconnect shown in Fig. 2 is simulated in ATK® in order to obtain $E_k$–$I$ variations for computing $L_k$, $C_q$ and $v_F$. The simulated GNR interconnect sample is 4.79 nm long which is a realistic length for nanometre scale ICs. In addition, the sample GNR is chosen as 5 atoms wide which is asymmetric since asymmetric GNRs have linear $I$–$V$ characteristics without a transmission pinch off by the applied voltage permitting to be utilized as conductors [26]. The GNR sample provides also a trade-off between the width and the simulation cost. The GNR interconnect considered in our study is consistent with the GNRs utilized in the previous studies by having hydrogen terminated edges and asymmetric structure.