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Investigation of the width-dependent static characteristics of graphene nanoribbon field effect transistors using non-parabolic quantum-based model

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ABSTRACT

The performance of graphene nanoribbon field effect transistor (GNR FET) is investigated from a numerical model based on self-consistent non-equilibrium Green's Function (NEGF) formulism in mode-space with position-dependent effective mass model and tight-binding model. The model accounts for the tunneling currents on the static performance of GNR FETs in two semiconducting families of armchair GNRs (3p,0) and (3p+1,0).

We conclude that increasing the GNR width in both GNR families increases the leakage current and subthreshold swing, and decreases I_{ON}/I_{OFF} ratio. In this scenario, GNR group (3p+1,0) leads to superior off-state performance such that GNR (7,0) has off-state current close to 2.5×10^{-16} A, five orders of magnitude lower than GNR (6,0) as well as 67 mV/decade subthreshold swing which is much smaller than that of 90 mV/decade in GNR (6,0).

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1. Introduction

Moore's law for MOSFET scaling has been on track and has reached to a limit that further scaling MOSFET may not be practically feasible [1]. This has resulted in search of other materials to replace silicon in near future [2,3]. The discovery of novel carbon-based materials such as carbon nanotube [4] and graphene [5] has already introduced merit materials for next-generation electronics. Graphene is one atomic layer of carbon sheet in a honeycomb lattice, which can outperform state-of-the-art silicon in many applications [6,7] due to its exceptional properties such as large carrier motility, high carrier concentration, high thermal conductivity and atomically thin planar structure [8,9]. However, large-area graphene is a semimetal with zero bandgap, which cannot be fully switched off and consequently not a proper material for digital applications [10]. The quantum confinement of graphene sheet in the form of one-dimensional (1D) nanoribbon with very narrow width (∼1–3 nm) provides the energy gap of several hundred meV required for FET operation in digital applications [11,12]. In addition to ribbon width, the size of induced bandgap depends on the atomic structure of nanoribbon, such that the armchair-edged graphene nanoribbon (GNR) has larger bandgap and consequently higher performance potential for logic applications [13]. The bandgap can significantly change by removing or adding one edge atom along the nanoribbon, such that two thirds of armchair GNRs can be categorized as semiconducting, indicating the precise control of the ribbon width down to the nanometer size as an important unsolved technical problem in the experimental characterization of GNR FET [8]. Thus, a precise simulation study is required to explore theoretical performance and limitation of GNR FETs for future integrated circuits.

There is not much reported work on the width-dependent study of GNR FET with respect to GNR index. In 2007, Ouyang et al. [14] showed the scaling behavior of GNR FETs considering only one semiconducting family of armchair GNRs. In 2008, Raza and Kan [15] extracted analytical expressions for bandgap and effective mass of first subband versus GNR width by categorizing them into three families. In 2011, Sako et al. [13] investigated the effects of edge bond relaxation in device performance using top-of-the barrier model for the 10 nm gate length by incorporating the effective mass of first subband. More recently, in 2013, Kliros [16] studied the effect of width-dependent performance of GNR FETs using an analytical model. However, performance studies of armchair GNR families with channel length below 10 nm is to be researched, and a more comprehensive investigation is thus warranted based on more sophisticated approaches. In this work, we have made an attempt to study GNR FET as a post-CMOS emerging device by the year 2025 as reported in International Technology Roadmap for Semiconductors (ITRS) [3].

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In recent years, hexagonal boron nitride (h-BN) with 2D atomic structure similar to graphene has been proposed as a promising complementary insulator layer [17]. As atomic thick graphene is susceptible to environmental conditions of growth, h-BN promotes the growth of uniform and charge trapping free high-*k* gate insulator [18,19]. It introduces significant device performance as its operation approaches quantum capacitance limit (QCL) [20]. In addition, first principle method predicts that the difference in interaction energy between the carbon–nitrogen and carbon–boron can open the bandgap of 50 meV [21], however, there is no experimental evidence of such a bandgap due to the lack of control on crystallographic alignment [19]. The effects of such induced bandgap have been studied in this work considering the fact that the h-BN buffer layer can make the ballistic transport assumption more accurate than SiO_2 dielectric layer in earlier studies.

To evaluate the performance of GNRFETs, different current transport models can be used including either simplified semi-classical transport models [13,22,23] or quantum transport models [14,24]. The former methods cannot treat short gate-length electrostatic effects and quantum tunneling effects such as direct source-to-drain tunneling in short channel GNR FET or band-to-band tunneling at the source and drain junctions [25]. Thus, the method is inaccurate for investigating the role of GNR width as a key attribute in static performance of GNR FETs. In addition, the existence of mismatch between the parabolic band approximation and the exact dispersion relation in analytical models [16], top-of-the-barrier model [26] or semi-analytical model [27] can have an erroneous estimation of actual concentration of carriers in the channel. The accurate results and deeper physical insight can be achieved by atomistic quantum transport models at the expense of long computational times. Yet, a considerable computational advantage and relatively accurate results can be achieved by solving the self-consistent non-equilibrium Green's Function (NEGF) formulism in mode space basis as has been already demonstrated for conventional MOS FETs [28,29], carbon nanotube FETs [9,30] and GNR FETs [31,32]. In addition, the application of non-parabolic effective mass (NPEM) correction [33] and the proper selection of contributing subbands in self-consistent loop can lead to a considerable decrease in simulation time.

In this paper, we simulate the GNRFET by self-consistently solving the 3D Poisson and the 1D Schrödinger wave equations within the NEGF formulism. The energy-position dependent Hamiltonian model with non-parabolic effective mass correction is used in order to precisely calculate the off-state attributes of GNR FET like band-to-band tunneling as has been demonstrated in [33]. The device features of GNRFETs with different GNR widths are investigated in terms of transfer characteristic, output characteristic, leakage current, I_{ON}/I_{OFF} ratio and subthreshold swing, which have been compared with ITRS projections by the year 2025.

2. Device structure

The GNR FET structure used in our simulation is shown in Fig. 1. In this structure, the GNR is sandwiched between two thin insulator layers in a double metal gate topology in order to maximize the electrostatic control of the gate electrode over the GNR channel. A h-BN layer has been used as a buffer layer [34], leading to the growth of uniform and charge trapping free high-*k* gate insulator due to protection of GNR against environmental influence [18]. The proposed GNR FET has the HfO_2 dielectric layer with the relative dielectric permittivity $\varepsilon_r = 24$ and the oxide thickness $t_{ox} = 1.2$ nm, while the dielectric permittivity of h-BN layers is $\varepsilon_r = 4$ and the interlayer spacing between graphene and h-BN layer is assumed 3 Å [35]. Thus, the insulator combination of h-BN and HfO_2 dielectrics result in an approximate equivalent oxide thickness (EOT) of 0.5 nm, leading to ultimate gate control over the GNR channel [36], which fulfills the criterion of ITRS. In addition, the length of intrinsic GNR channel, $L_G = 7.5$ nm and power supply voltage are based on scaling criteria as in ITRS for commercial high-performance and low power FET for digital integrated circuits. The symmetric regions of GNR channel is heavily doped with the concentration of 0.01 n-type dopants per carbon atom as extensions of source and drain regions and connected to two large contacts.

3. Simulation approach

We simulate the proposed DG-GNRFET by converging an iterative procedure between electrostatic and quantum transport solutions, where the 3D Poisson and the 1D Schrödinger equations are solved self-consistently within the NEGF formulism. The quantum transport calculation based on NEGF formulism is a strength simulation approach to treat quantum–mechanical confinement as well as the effects of contacts on the carriers transport in the

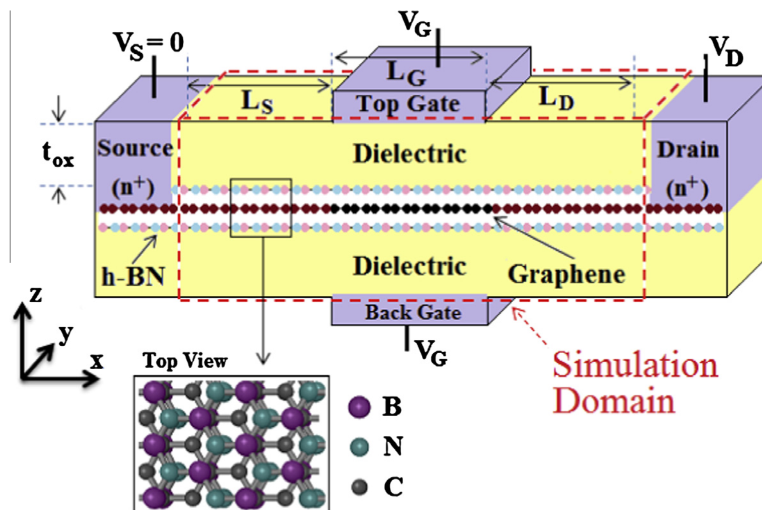

Fig. 1. 3D schematic view of the proposed double gate (DG) GNR FET. Note: The armchair GNR channel under the gate area is un-doped and the source and drain regions are n-type doped. Simulation domain which contains the source, gate, and drain regions in longitudinal direction are shown with the dashed line. The top view of GNR sandwiched between two h-BN layers is also shown.

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