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Modeling comparison of graphene nanoribbon field effect transistors with single vacancy defect

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ABSTRACT

In this paper, some important circuit parameters of a monolayer armchair graphene nanoribbon (GNR) field effect transistor (GNRFET) in different structures are studied. Also, these structures are Ideal with no defect, 1SVGNRFET with one single vacancy defect, and 3SVsGNRFET with three SV defects. Moreover, the circuit parameters are extracted based on Semi Classical Top of Barrier Modeling (SCTOBM) method. The I-V characteristics simulations of Ideal GNRFET, 1SVGNRFET and 3SVsGNRFET are used for comparing with SCTOBM method. These simulations are solved with Poisson-Schrodinger equation self-consistently by using Non- Equilibrium Green Function (NEGF) and in the real space approach. The energy band structure of nanoribbon is obtained by using nearest−neighbour interactions within an approximation tight-binding method. The modeling results show that 3SVsGNRFET in comparison to 1SVGNRFET has higher transconductance, cut-off frequency, electron average velocity, mobile charge, and quantum capacitance. Also, 3SVsGNRFET has smaller gate, drain and source capacitances than Ideal GNRFET. Furthermore, Drain-induced barrier lowering (DIBL) and sub-threshold swing (SS) of 3SVsGNRFET are smaller than 1SVGNRFET.

1. Introduction

Graphene has excited a great deal of consideration owing to its particular physical and electric characteristics since it was presented in 2004 [1]. Because graphene is a zero bandgap material [2], it could be laminated as narrow nanoribbons for opening bandgap [3]. Theoretical investigations have proved that graphene nanoribbons (GNRs) have energy gap which is inversely proportional to their width [4–6]. Defects in graphene nanoribbons can change bandgap and they can influence the characteristics of the GNR, such as energy band structure, carrier mobility, conductivity and so on [7]. Many works on modeling of graphene, graphene nanoribbon, and graphene nanoribbon field effect transistor were presented in recent years.

In Ref. [8], the application of the nonlocal continuum theory in modeling of carbon nanotubes and graphene sheets were studied. Also, a variety of nonlocal continuum models in modeling of the two materials under static and dynamic loadings were introduced and reviewed. In Ref. [9], the landscape of defects and their importance in both the electronic structure and the transport properties of graphene are presented using ab-initio and tight-binding simulations.

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In Ref. [10], a small-signal model for graphene barristor which is a promising device for the future nanoelectronics industry was presented. Moreover, transconductance, output resistance, and parasitic capacitances were discussed in this work. The backscattering phenomena during conduction for graphene nanoribbons of μm lengths, from single vacancy scatterers up to finite defect concentrations were studied by using ab-initio calibrated Hamiltonian models in Ref. [11].

In Ref. [12], a decoupled mode space approach based on the NEGF formalism coupled with a three dimensional Poisson-Schrodinger equation was described, which could be used to simulate GNRFETs. In Ref. [13], the multiphasic multiscale (MS) approaches required to model graphene-based materials and devices, presenting a comprehensive overview of the main physical models providing a quantitative understanding of the operation of nanoscale transistors, were reviewed. They especially focused on the ongoing efforts to consistently connect simulations at different levels of physical abstraction in order to evaluate materials, device, and circuit properties. Furthermore, they discussed various attempts to induce a gap in graphene-based materials and their impact on the operation of different transistor structures.

In Ref. [14], a graphene nanoribbon (GNR) field effect transistor (FET) using lightly doped drain and source (LDDS) between intrinsic channel region and highly doped source and drain regions was proposed. The represented structure is for minimizing tunneling leakage current and also it is used the non-equilibrium Green's function (NEGF) method to do simulations. Moreover, the LDDS-GNRFET has illustrated much less leakage current, larger on-current to off-current (I_{ON}/I_{OFF}) ratio and better sub-threshold-swing (SS). The first SPICE-compatible model of Schottky-barrier-GNRFETs (SB-GNRFETs) that takes various design parameters into account was presented in Ref. [15], which not only does it enable circuit-level simulations, but also it provides a way to evaluate process variation, including effects of channel length, transistor width, oxide thickness and graphene-specific edge roughness.

The potential integration of graphene nanoribbons field-effect transistor (GNRFET) into digital logic circuit through SPICE modeling was demonstrated in Ref. [16]. Also, the device model was based on the top-of-the-barrier ballistic device modeling approach. Furthermore, energy-delay product (EDP), and power-delay product (PDP) of logic circuits were investigated. In Ref. [17], a GNRFET structure with dual material gate or DMG-GNRFET was proposed. Also, the NEGF formalism with an uncoupled mode space has been used in order to simulate the electronic properties. Moreover, the simulated characteristics were compared with conventional GNRFET. In Ref. [18], a semi-analytical model has been presented by using "top-of-the-barrier" model, which is incorporating the effects of edge bond relaxation, the third nearest neighbour interactions, and edge scattering in graphene nanoribbon field effect transistors (GNRFETs) with armchair-edge GNR (AGNR) channels. In Ref. [19], the upper limit performance of CNR MOSFETs has been investigated by using a nearest neighbour tight-binding method for band structure calculation and a ballistic "top-of-the-barrier" model. In Ref. [20], a novel structure for a dual-gated graphene nanoribbon field-effect transistor (GNRFET) was offered. Also, in this work, some important circuit parameters such as capacitances, intrinsic delay time, power delay product (PDP), mobile charge and average velocity, Drain Induced Barrier Lowering (DIBL) and Sub-threshold Swing were studied by using a top-of-the-barrier two-dimensional circuit model.

In Ref. [21], our previous work, an armchair double-gated monolayer graphene nanoribbon (GNR) field effect transistors (GNRFET) which has one single vacancy (1SV) defect (so-called 1SVGNRFET), were simulated. Also, positions of defect in width and length of GNRFET channel were changed and a structure with three single vacancy (3SVs) defects (so-called 3SVsGNRFET) was suggested. Moreover, 3SVsGNRFET had higher I_{ON}/I_{OFF} ratio and lower sub-threshold swing than 1SVGNRFET.

But so far, in all of studies for graphene nanoribbon (GNR) field effect transistors (GNRFET) with SV defect, circuit properties such as transconductance, cut-off frequency, electron average velocity, mobile charge, quantum capacitance, lower, Drain-induced barrier lowering (DIBL) and sub-threshold swing (SS) and also gate and contacts capacitances have not been reported.

In this paper, in following of our previous work, an armchair double-gated monolayer graphene nanoribbon (GNR) field effect transistor (GNRFET) with no defect that is called Ideal, a double-gated monolayer armchair graphene nanoribbon (GNR) field effect transistor with one single vacancy (1SV) defect that is called 1SVGNRFET and a structure with three single vacancy (3SVs) defects that is called 3SVsGNRFET were studied. As mentioned in Ref. [22], the presence of vacancies significantly modifies the low-energy electronic properties of graphene and generates unusual phenomena. Vacancies cause resonant scattering at the Dirac points and are considered a major factor limiting graphene conductivity. In this work, the simulations were conducted based on self-consistent solution of the Poisson-Schrodinger equation with Non-Equilibrium Green Function (NEGF) formalism. Also, tight-binding Hamiltonian was assumed in the real space approach. Moreover, the energy band structure of nanoribbon was obtained by using nearest−neighbour interactions within an approximation tight-binding method [21].

According to performed simulations and I-V characteristics, some circuit parameters such as transconductance, cut-off frequency, electron average velocity, mobile charge, quantum capacitance, DIBL and sub-threshold swing (SS) are extracted by using Semi Classical Top of Barrier Modeling (SCTOBM model). Also, source, drain and gate capacitances for Ideal, 1SVGNRFET, and 3SVsGNRFET structures, are estimated.

2. Device structure and defect locations

The device structure schematic is shown in Fig. 1(a). The channel is 5-nm-long armchair-edge GNR (A-GNR), which has width of ~1 nm (N = 12). Transistor has two gate contacts in top and bottom, which are separated from nanoribbon by two oxide layers with a relative dielectric constant $\varepsilon_{ins} = 3.9$. The oxides are made of Sio_2 and have 1 nm thickness. The source and