Numerical Modeling of a Deep Submicron Gas Sensor Based on Double-Gate Graphene Nanoribbon Field-Effect Transistor

K. Tamersit, F. Djeffal and M. Meguellati

***Abstract*—In this paper, a new gas sensor based on Double-Gate Graphene Nano-Ribbon Field Effect Transistor (DG GNRFET) for high performance gas sensing applications is proposed. The sensor is simulated by self-consistently solving the Schrödinger equation using the non-equilibrium Green's function formalism (NEGF) with two-dimensional (2D) Poisson equation, under ballistic limits. The sensor response in a gaseous environment is studied and the sensitivity behavior is analyzed for different regimes of DG GNRFET working. It has been found that the high sensitivity can be achieved when the GNRFET-based gas sensor is operated in the subthreshold domain. The obtained results make the proposed DG GNRFET-based gas sensor a promising candidate for nanoscale, low power and high sensitivity multi-gas sensing applications.**

***Index Terms*— Graphene nanoribbon (GNR), non-equilibrium Green's function formalism (NEGF), gas sensor, sensitivity.**

I. Introduction

Graphene is a two-dimensional zero-bandgap crystal with atomic thickness, its carbon atoms are arranged in a honeycomb lattice [1]. This material has attracted a significant amount of attention in physics, chemistry and nanomaterials science since its discovery in 2004. It is considered one of the most attractive candidates for future nanoelectronic applications owing to its unique and interesting properties such as the high carrier velocity, linear energy dispersion relation, large surface-to-volume ratio, extremely high mobility (~10^5 cm^2/V.s) and low manufacturing costs [1-4]. The main drawback of graphene as a channel in field effect transistor is the absence of a gap that limits seriously its usefulness in digital applications [5]. The graphene nanoribbon (GNR), which has almost all of the interesting properties of the carbon nanotube (CNT) and sheet of graphene, has the additional benefit of a tunable bandgap through varying the carbon dimers along the width direction [10] and/or applying uniaxial and shears strains. Therefore, many recent studies have been performed to exploit the GNR as a channel material for field effect transistor to overcome the limitations previously encountered with silicon-based channel [6-11].

Moreover, MOSFET-based gas sensors have attracted enormous attention due to their excellent characteristics such as high sensitivity, low cost, high reliability, low power consumption, CMOS compatibility, and small size which leads to a possibility of integration in microsystems [14-20]. In addition, the MOSFET-based gas sensors have given beneficial impulses to different major fields such as chemical and pharmaceutical industries, automotive, environmental area and biomedical diagnostics. Therefore, significant efforts have been made to improve the main characteristics of such sensors. The conducting polymers (CPs) and catalytic metals (CMs) are considered as attractive candidates to be used as receptors and/or transducers in MOSFET-based gas sensors [14-20]. The CPs are advantageous than the CMs, because of their porosity which can be easily penetrated by gases that can profoundly change their electronic properties especially the work function (WF). The second advantage of CPs that considered as an interesting bonus is the tunability. The practical consequence of work-function tuning is the possibility of constructing multisensing microfabricated arrays [14,19]. In this study, a new gas sensor based on graphene nanoribbon field effect transistor (GNRFET) is proposed and simulated by self-consistently solving the Schrödinger equation using the non-equilibrium Green's function formalism with two-dimensional Poisson equation. The high sensitivity of GNR to its electrostatic environment [1-3], the good gate control of GNRFET [6-10] and the interesting chemical modulation of the CP's work function [14] make the proposed GNRFET-based gas sensor a promising candidate for high-performance gas sensing applications.

This paper is organized as follows. In Sect. 2, we present a brief description of the simulation approach which is based on self-consistent solutions of the 2D Poisson equation coupled with the Non-Equilibrium Green's Function formalism in mode space representation. In Sect. 3, we investigate and analyze the sensor performance and sensitivity behavior. The conclusions will be drawn in Sect. 4.

II. SIMULATION APPROACH

Fig. 1.(a) shows the 2D cross-sectional view of the DG GNRFET-based gas sensor where the whole graphene nanoribbon is embedded between two dielectric layers. The

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catalytic metal or conducting polymer can be used as gates (sensing elements) which are attached to the dielectrics over and under the intrinsic GNR without overlap. $L_{S(D)}$, L_C and t_{OX} are the length of source (drain) extension, length of intrinsic GNR channel and the thickness of the gate oxide, respectively.

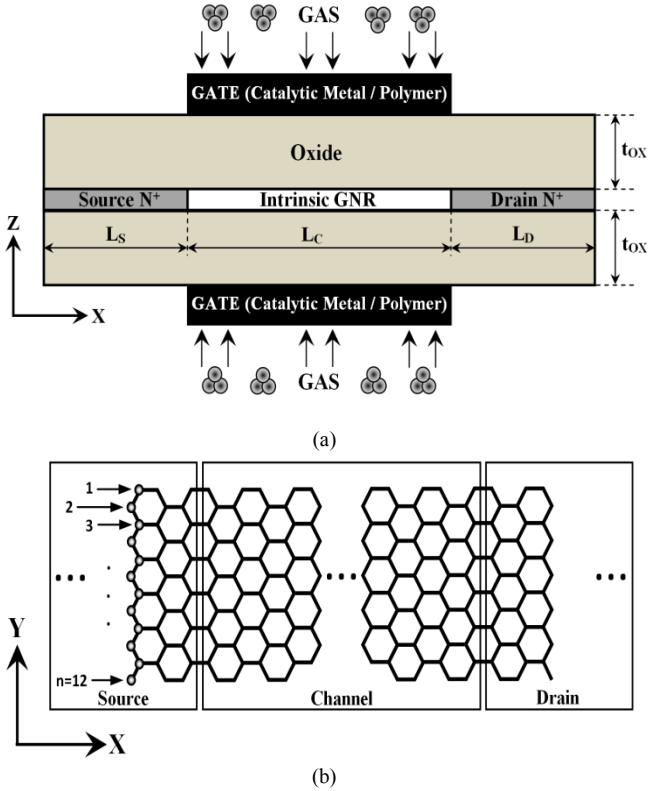

Fig. 1. (a) Cross-sectional view of the proposed double-gated GNRFET-based gas sensor (b) Schematic sketch of an armchair N=12 GNR channel with the source and drain extensions.

Fig. 1.(b) shows an armchair graphene nanoribbon with 12 carbon dimers along the width direction which correspond to a width equal to 1.35 nm and bandgap of EG≈0.60 eV. It should be noted that there are two conformations of graphene nanoribbon, zigzag and armchair GNR. We used the second conformation because the bandgap collapses at a finite source-drain bias in the case of zigzag GNR, this is not appropriate for the MOSFET-type device [7]. The channel is assumed intrinsic and the source and drain extensions are heavily n-type doped (N+) with 5×10-3 dopant/atom. The sensing mechanism is defined by the adsorption of gas molecules at the catalytic metal or conducting polymer surface and thereby diffusion of some atomic gas into membrane, which changes the gate work function and hence modulate the electrostatic gating and sensor characteristics [14-20].

The GNRFET-based gas sensor is simulated by self-consistently solving the Schrödinger equation using the non-equilibrium Green's function formalism with two-dimensional Poisson equation under the ballistic limits [12,13]. The mode space approach is used in the simulation of the proposed gas sensor for the computational saving and low complexity, because the MS decouples the 2D real space GNR lattice to one-dimensional lattice, which significantly reduces the size of the Hamiltonian matrix leading to a decrease in computational cost by orders of magnitude [6-8]. It is sufficient to include only the first subband (mode) in the simulation because the remaining subbands contribute little to the carrier transport [7]. It is to note that, the mode space approach including the effects of edge bond relaxation can excellently reproduce accurate results with respect to real space approach [7].

The basis of the NEGF method was on obtaining the retarded Green's function given by [12]

$$G(E) = \left[(E + i\eta^+)I - H - \Sigma_S - \Sigma_D\right]^{-1} \quad (1)$$

where E is the energy, η is an infinitesimal positive value, I is the identity matrix, H is the Hamiltonian of the GNR, and ΣS and ΣD are the self-energies of the source and drain contacts respectively, which can be computed analytically using the expressions described in [7]. The source (drain) density of states that lead us to the charge density can be calculated using:

$$D_{S(D)} = G\Gamma_{S(D)}G^+ \quad (2)$$

where ΓS(D) is the energy level broadening due to the source (drain) contact and is given by

$$\Gamma_{S(D)} = i(\Sigma_{S(D)} - \Sigma^+_{S(D)}) \quad (3)$$

Using the above equations, the charge density in the channel can be computed as [7,8]

$$Ne = \int_{-\infty}^{+\infty} dE\ sgn[E - E_N]\{D_S(E)f(sgn[E - E_N](E - E_{FS})) + D_D(E)f(sgn[E - E_N](E - E_{FD}))\} \quad (4)$$

where sgn is the sign function, DS(D) is the source (drain) density of states and f(sgn[E-EN].(E-EFS(D))) represents the source (drain) Fermi function corresponding to the Fermi level EFS(D). The charge neutrality level EN is at the middle of the band gap because the valence band and the conduction band are symmetric in GNR [7].

The above equations for obtaining the charge density Ne demand knowledge about the on-site potential energy U which is derived by solving the Poisson equation given by

$$\nabla^2 U = \frac{-q}{\varepsilon}\rho \quad (5)$$

where U is the electrostatic potential, ε is the dielectric constant, and ρ is the net charge density counting the doping concentration. The Poisson equation is solved in 2D coordinates using the Finite Difference Method (FDM) assuming that the potential in the width direction is invariant. In the contacts between GNR and gate, the potential V is computed by Dirichlet boundary condition given by

$$eV = eV_G + \Phi_{GNR} - \Phi_{G(SENSING)} \quad (6)$$

where VG is the gate voltage, ΦGNR and ΦG is the work function of GNR and gate electrode (sensing element), respectively. The Neumann boundary condition is applied to the remaining boundaries of GNRFET-based gas sensor. Starting from an initial guess for the on-site potential energy profile U, the equation (4) is solved and the resulting charge density Ne is fed back into the Poisson equation for obtaining the new on site electrostatic potential. This cycle is repeated until the self-consistency is achieved for a stop criterion. After convergence, the channel current can be calculated using the Landauer-Büttiker formula given by

$$I = \frac{2e}{h}\int dE\ T(E)\left[f(E - E_{FS}) - f(E - E_{FD})\right] \quad (7)$$

where e is the electron charge, h is Planck's constant and

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T(E) is the transmission coefficient computed as [12,13]

$$T(E) = Tr(\Gamma_S G \Gamma_D G^+) \quad (8)$$

Where Tr is the trace operator.

III. Results and Discussion

In order to test the accuracy and the predictive behavior of the drain current versus gate voltage, we compare the I_{DS}-V_{GS} transfer characteristics obtained from our simulation with the results given in [14,16], as shown in Fig. 2. The good agreement is observed for both structures GNRFET and GNRTFET with and without the edge effect.

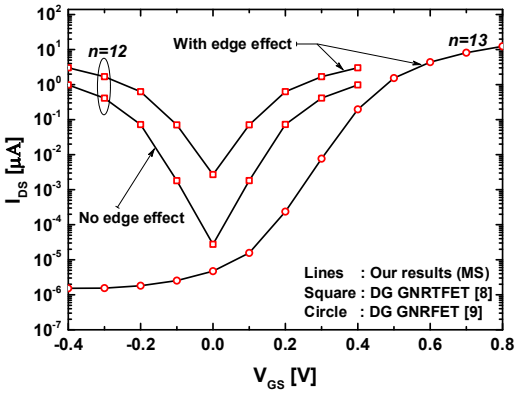
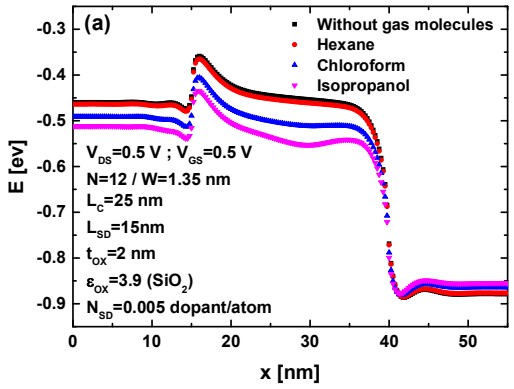


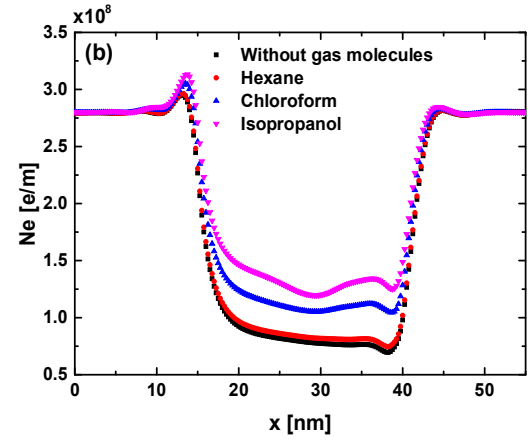
Fig. 2. Comparison between I_{DS} versus V_{GS} characteristics of our simulator with the simulated results given in [8,9].

The GNRFET is used as a transducer which translates the work-function responses ($\Delta\Phi_{CP/CM}$) of CPs or CMs to a change in the drain-source current. Fig. 3. shows the effect of the different gases on the potential profile and charge density through the conducting polymer (sensing element) which acts as gates. The reason for the use of CP is its capability to be sensitive to several gases, this makes it an interesting material for sensing applications.

It is also clear that the variation of potential profile and charge density is important in the active region (intrinsic GNR under gate) reflecting the effect of ΔWF on the electrostatic gating.

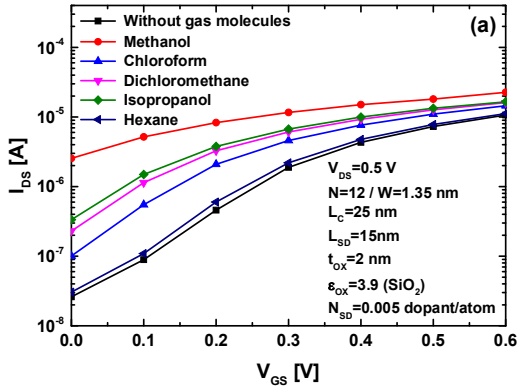


(a)

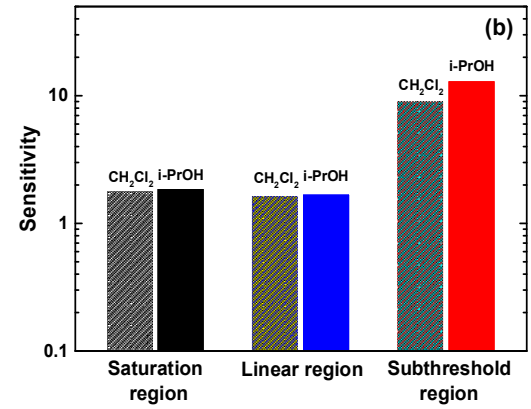


(b)

Fig. 3. (a) Variation of potential profile and (b) charge density for different gases.



(a)



(b)

Fig. 4. (a) Transfer characteristics of GNRFET-based gas sensor under different gases, (b) Comparison between sensitivity obtained in saturation, linear and subthreshold regions for two different gases: Dichloromethane (CH2Cl2) and Isopropanol (i-PrOH).

Fig. 4.(a) shows the simulated IDS-VGS transfer characteristics of GNRFET-based gas sensor under different gases. The values of the parameters used in the simulation are shown in the same figure. The changes of CP work function that correspond to the exposed gases are extracted from the experimental results [14,16]. The amounts of exposed vapors are: Methanol (4.6 mM), Chloroform (1.2

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mM), Dichloromethane (8.5 mM), Isopropanol (0.8 mM) and Hexane (1.6 mM). Fig. 4.(b) shows the sensitivity comparison in terms of order of change in drain current, (i.e., ratio of IDS after and before the gas exposure). The sensitivity is calculated in saturation, linear and subthreshold regions in order to find the suitable location of sensitivity parameter. It has been found that the high sensitivity can be achieved when the GNRFET-based gas sensor is operated in the subthreshold domain.

IV. Conclusion

In this paper, a new nanoscale multi-gas sensor based on Double-Gate Graphene Nano-Ribbon Field Effect Transistor is proposed and simulated by self-consistently solving the Schrödinger equation using the non-equilibrium Green's function formalism in mode space with two-dimensional Poisson equation under the ballistic limits. This simulation method can take into account the majority of quantum and electrostatic effects which can affect the sensor performance. The GNRFET is endowed of a particular gate which allows it to be able to nose different vapors. It has been found that the high sensitivity can be achieved when the GNRFET-based gas sensor is operated in the subthreshold regime. The high sensitivity and the excellent gate control of GNRFET, provided by the investigated device, make the proposed GNRFET-based gas sensor a promising candidate for high performance and low power multi-gas sensing applications.

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