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Tuning the analog and digital performance of Germanene nanoribbon field effect transistors with engineering the width and geometry of source, channel and drain region in the ballistic regime

Hossein Fatholah nejad[a], Daryoosh Dideban[a,b,*], Abbas Ketabi[b], Mehran Vali[a], Amir Hossein Bayani[a], Hadi Heidari[c]

[a] Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan, Iran
[b] Department of Electrical and Computer Engineering, University of Kashan, Kashan, Iran
[c] Electronics and Nanoscale Engineering Research Division, School of Engineering, University of Glasgow, Glasgow, UK

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ABSTRACT

In this paper, with taking advantage of electrical properties of a germanene nanoribbon, we propose a germanene nanoribbon field effect transistor (GeNR-FET). Here by tuning the width and geometry of the germanene nanoribbon in the source, drain and channel regions, we investigate theoretically the transistor characteristics, analog and digital performances of these several different GeNR-FETs at room temperature. Our simulations are obtained using density functional theory (DFT) combined withnon-equilibrium Green's function (NEGF) method. The simulation results show that for digital applications, by tuning the width of the germanene nanoribbon a GeNR-FET with a finite band gap in the channel region and small band gap in the source and drain regions shows a better I_{on}/I_{off} ratio in transfer characteristics. However, for the analog applications, if the band gap of the channel region has small value and the band gap of the source and drain regions have a finite value, the output characteristic shows a higher peak to valley (PVR) ratio which is an important figure of merit in analog applications. Also from the output characteristics, we find that the T-shape channel shows more desirable (PVR) compared with other devices and it reaches to 17.28 in this case.

1. Introduction

Since the experimental fabrication of two-dimensional honeycomb structures of carbon atoms named as Graphene [1–3] and due to its promising electronic and mechanical properties, there has been a vast extent of experimental and theoretical research on such 2D materials [4–6]. Among them, there are atomically thin structures of Si and Ge which are called Silicene and Germanene, respectively [7–10]. As Graphene, These are also honeycomb structures with a Dirac-point electronic band structure. Although planar Germanene is reported to be unstable and metallic but the buckled structure is stable and behaves as a semi-metal [11].

In terms of transistor performance, a single layer of graphene or germanene has zero bandgap which does not allow proper cut-off in the graphene and germanene FETs. We can overcome this issue by confining such materials in one dimension and making nanoribbons or nanotubes. Graphene nanoribbons show considerable electronic properties such as the dependence of the electronic bandgap on the width of the ribbon [12,13]. As the width of the ribbon increases in Graphene, the electrical bandgap decreases [14]. A similar width dependence behavior has been also investigated in Silicene and Germanene nanoribbons [15]. Electrical band gap existence [16,17] and other properties such as high carrier mobility [18,19] and high current density [20] of Graphene and Germanene makes them as excellent candidates in transistor [21] and sensor applications [17]. By changing the width of the nanoribbon and building a field effect transistor whose band gap in the channel is different from the source and drain regions, it will be possible to obtain a non-linear effect such as negative differential resistance (NDR). This phenomenon is interesting for designing high-speed analog devices [22]. Although investigations have been carried out on graphene nanoribbon FETs [23,24], but no study is yet performed to utilize germanene nanoribbons on this kind of field effect transistors.

In this paper, we study the transistor performance of germanene nanoribbons with different widths in the channel and leads by the combination of density functional theory (DFT) and Non-equilibrium Green's function (NEGF) method. The output and transfer characteristics of the proposed FETs are investigated and then analyzed for both

* Corresponding author at: Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan, Iran.
E-mail address: dideban@kashanu.ac.ir (D. Dideban).

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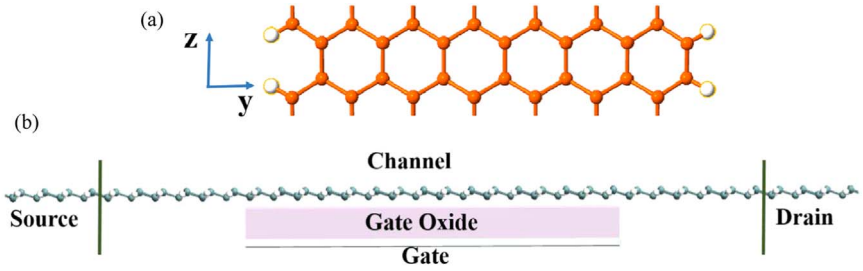

Fig. 1. (a) The unit cell of germanene nanoribbon with hydrogen passivation. (b) Schematic sketch of the considered field effect transistor.

analog and digital applications.

2. Device structure and simulation procedure

The open-source ab initio package named TranSIESTA [25] based on density functional method and non-equilibrium Green's function (NEGF) formalism is used to obtain the electronic structure and current-voltage characteristics of germanene nanoribbons (GeNRs) with different widths. Double-ζ plus polarization (DZP) sets are employed as the linear combination of atomic orbitals (LCAO) basis sets with Perdew, Burke, and Ernzerhof (PBE) [26,27]exchange-correlation functional. Orbitals of Kohn-Sham are expanded up to 150 Ry and a vacuum thickness of 15 Å and 25 Å are applied in the x and y-directions to eliminate the artificial nanoribbons. All atoms in the unit cell of the ribbon are relaxed until a force convergence of 0.02 eV/Å is achieved. A sampling of 1 × 1 × 11 and 1 × 1 × 101 k-mesh are used to optimize the structures and obtain the accurate ground state structures, respectively.

Fig. 1(a) shows the unit cell of an armchair GeNR with n = 14 and Δ = 0.65 Å buckling parameter which is used as leads of the proposed field-effect transistors (FETs) which shows schematically in Fig. 1(b). In order to utilize bandgap engineering of the channel, germanene nanoribbons with n = 12 and 16 are used. Hydrogen atoms are attached to the ribbon edges of the GeNRs to saturate the dangling bonds.

Investigation of electron transport through the device is performed by self-consistent calculation of DFT and NEGF.

We consider a 10 nm GeNR as the channel of the proposed devices. Fig. 2 shows the gated proposed GeNR-FETs with different channel widths. We consider three different configurations for the channel of the FETs which are named thin (n = 12), thick (n = 16) and T-shape (n = 16) structures. Landauer-Buttiker formula [28] with self-consistent approach is employed to calculate electron transport through the channel of the devices, (Eq. (1)):

$$I(V_g, V_{bias}) = \frac{2e}{h}\int_{-\infty}^{+\infty}\{T(E,V_g, V_{bias})[f_L(E-\mu_L) - f_R(E-\mu_R)]\}dE \quad (1)$$

Where T (E, V_g, V_{bias}), Vg, V_{bias}, $f_{L/R}$and μ_L/μ_R are the transmission probability, gate voltage, Drain-Sourcebias voltage, Fermi-Dirac distribution function for the left (L)/right (*R*) electrode and the electrochemical potential of the L/R electrodes, respectively.

3. Results and discussion

In this section, we analyze the obtained results from two point of views: analog and digital applications. Hence, we present the transfer characteristics and output characteristics of the simulated devices at room temperature and we investigate three different figures of merit including I_{on}/I_{off} ratio,negative differential conductance and peak-to-valley (PVR) ratio.

3.1. Transfer characteristics

In this subsection, we investigate and compare the transfer characteristics of three simulated devices at the ballistic regime. In all devices, we consider a germanene nanoribbon as source and drain leads where both have the same width with N = 14 germanium atoms. While the channel region includes a germanene nanoribbon with N = 12 and 16 germanium atoms as depicted in Fig. 2. In the case of the channel with N = 16 atoms, we consider two configurations; T-shape and wide (symmetric) channels.

Fig. 3 illustrates the current through the channel as a function of the gate voltage for all three simulated Ge-NRFETs with thin, wide and T-shape channels. The figure shows that each current curve displays a minimum value at almost the same value of the gate voltage i.e. $V_g \sim$ 0.1 V.Moreover, it reflects two points about the ON- and OFF- current for all three devices. As can be seen, the maximum value of the current has not changed significantly,while the minimum current decreases by changing the width and shape of the channel region from T-shape to thick and then thin cases.

As ref. [15] demonstrates, the relationship between the band gap and width of an armchair Ge-nanoribbon can be classified in three categories: N = 3 m, N = 3 m + 1 and N = 3 m + 2; where N denotes

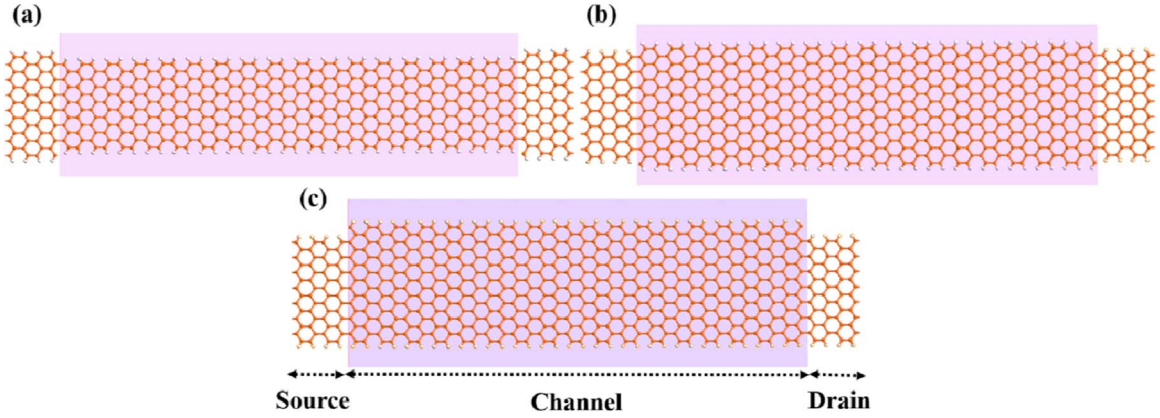

Fig. 2. Configurations of channel; thin (a), thick (b) and T (c). The pink square behind the structures is metal gate.