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Study of Nitrogen terminated doped zigzag GNR FET exhibiting negative differential resistance

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ABSTRACT

This paper presents the study of Gallium and Aluminum doped Nitrogen terminated zigzag Graphene Nano Ribbon (GNR) FET with high-k dielectric. The GNR FET structure has been designed and simulated using Quantumwise Atomistix Toolkit software package. The presented GNR FET with n-type (Nitrogen doped) electrodes and p-type (Gallium or Aluminum doped) scattering region are simulated and analyzed using Density Functional Theory combined with NEGF formalism and Device Density of States (DDOS). The device shows a negative differential resistance phenomenon which can be controlled by the gate of the zigzag GNR FET. It is found that doping of Gallium and Aluminum in scattering region provides higher drain current, higher I_{ON}/I_{OFF} and I_P/I_V ratios as compared to that of Boron doped zigzag GNR FET. The potential applications of the device are in logical, high frequency, and memory devices.

1. Introduction

The continuous miniaturization of Si devices based on CMOS technology is reaching its physical and geometrical limits so we are moving on other materials. Graphene, a two dimensional honey comb layer of carbon atoms in which carbon atoms form three σ bonds in the plane of Graphene in sp^2 configuration while another orbital p_z, which is perpendicular to the Graphene plane makes π covalent bond, has shown the capability to become the novel material for nano-electronics because of its extraordinary properties [1–3]. This includes ultrahigh carrier mobility, thermal conductivity, electron–hole symmetry and quantum hall effect [4].

Graphene, being a zero band gap material, is not suitable for semiconductor electronics to fabricate FETs. However, formation of Graphene nanostructure of less than 10 nm can induce a band gap [5]. These nanostructures are called Graphene Nano Ribbon (GNR). Confining Graphene in one direction results in zigzag type GNR which shows metallic properties due to wave function localization at the zigzag edges and confining Graphene in other direction results in Arm chair type GNR which shows semiconducting properties due to both quantum confinement and the edge states. The induced band gap depends upon the width of the ribbon [6]. This band gap is not sufficient for Graphene to be used in digital logical applications. Arm chair type GNR has been used to simulate various high frequency GNR FETs [7]. Fabrication of GNRs requires atomically precise edges. Such a technique of fabricating GNRs has been proposed and this opens way for GNR to be used in future high-performance electronics applications [8].

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Various methods have been reported to open a band gap in zigzag GNR e.g. selective doping [9], edge modulation (defective boundaries and edge disorder) [10,11], enabling each edge Carbon (C) atom to two Hydrogen (H) atoms [12], terminating the edge C atoms of the ribbon by Nitrogen (N) atoms [13].

In this paper we present a study on N (Nitrogen) terminated zigzag GNR FET. The binding energy created by the passivation of Nitrogen molecule (N_2) on unpassivated zigzag GNR is always positive. Thus the formation of such ribbons is energetically favorable. The passivation of N can transform zigzag GNR (arm chair GNR) from metal (semiconductor) to semiconductor (metal). Band gap engineering by terminating edge C atoms with N atoms has the advantage that neither it requires any controlled manufacturing, which can be crucial in the case of defective boundaries nor it loses sp^2 hybridization of edge C atoms, therefore, the resulting ribbon does not lose its planarity as is the case with H loading [12], where sp^3 atoms are present along the edges [13].

In this paper we present a FET structure in which the scattering region (channel) is made of Nitrogen (N) terminated zigzag GNR and is doped with either Aluminum (Al) or Gallium (Ga), electrodes are made of N terminated zigzag GNR and are doped with Nitrogen. The device has been simulated and its electrical characteristics are described using Density Functional Theory (DFT) based on quantum transport calculations and device Density of States (DDOS). Based on these simulations we found that it exhibits negative differential resistance (NDR) in the voltage range of 0.1–0.25 V and provides better ON current compared to the N-passivated zigzag GNR proposed by Kumar et al. [13].

Negative differential resistance implies that for an increasing range of voltage the current will be decreasing. NDR can be either current controlled or voltage controlled. Due to ambipolar transport behavior of Graphene, NDR has been observed and reported in various three terminal GNR devices [14]. Previously single-gate Graphene sheet junctions have also shown negative differential resistance [15]. Negative differential resistance was also discovered in arm chair GNR junction [16,17], and the arm chair GNR junction has been examined for its suitability in tunneling diodes [17]. It has also been reported that $p+/p$ zigzag GNR junction also exhibit NDR with high peak-to-valley current ratio (I_P/I_V) [18]. GNR FETs have been extensively investigated for their suitability at high frequency electronics [19,20]. Maximum frequency of oscillation (f_{max}) and cut off frequency (f_c) of the proposed device is in the range of Giga-hertz; so, the NDR phenomenon in the proposed device is quite useful for high-frequency applications.

2. FET structure

The semiconducting N-passivated zigzag GNR proposed in [13] has been used to realize GNR FET in the present work. The GNR FET is comprised of N-passivated (2, 2) zigzag GNR of which scattering region is doped with Al or Ga as shown in Fig. 1. The length and width of the scattering regions are 2.39 nm and 0.94 nm respectively. A high-k material has been used as gate dielectric to increase the gate control over the scattering region (channel). A typical dielectric constant of $24\varepsilon_0$ corresponding to that of Hafnium oxide (HfO_2) with thickness of 0.36 nm has been considered [21]. Since both the electrodes and the scattering region are parts of the same N-passivated (2, 2) zigzag GNR, such device structure can be useful for increasing the device density together with simplifying the fabrication process. The dopant atoms (N, Al, Ga) are substituted for C atoms in carbon materials similar to that of dopant added in Carbon Nano Tubes (CNTs) [22].

In the GNR FET, the two electrodes are doped using penta-valent N atoms with a doping concentration of 1 N atom for every 16 C atoms. Doping the N passivated zigzag GNR with N causes it to be n-type semiconductor. The scattering region is doped with trivalent Al or Ga atoms with a doping concentration of 1 dopant atom for every 80 C atoms. Doping the N passivated zigzag GNR with Al or Ga causes it to be p-type semiconductor. Doping with Aluminum (Al) and Gallium (Ga) is preferred because Al and Ga belong to the same group and also both Al and Ga are more reactive than Boron (B) [13]. The band structures of the N doped drain/source, scattering region doped with Al or Ga are shown in Fig. 2(a), (b) and (c) respectively.

The Bloch functions for valance band maximum (VBM) and conduction band minimum (CBM) along with the projected density of states are analyzed to get the opening of band-gap. The band gap value for Nitrogen doped drain/source region is 0.62 eV, for Al doped scattering region is 0.35 eV, and for Ga doped scattering region it is 0.37 eV as shown by blue lines in

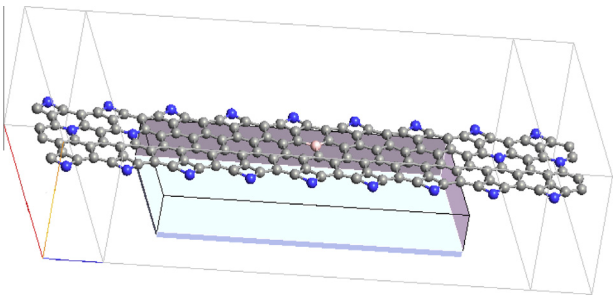

Fig. 1. Structure of the N-passivated (2, 2) zigzag GNR FET, where the box region at the two sides indicate the contacts region and blue (pink) ball represents the N (Ga/Al) atoms. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)