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Improving performance of armchair graphene nanoribbon field effect transistors via boron nitride doping

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ABSTRACT

Device performance of 10 nm length armchair graphene nanoribbon field effect transistors with 1.5 nm and 4 nm width (13 and 33 atoms in width respectively) are compared in terms of I_{on}/I_{off}, trans-conductance, and sub-threshold swing. While narrow devices suffer from edge roughness wider devices are subject to more substrate surface roughness and reduced bandgap. Boron Nitride doping is employed to compensate reduced bandgap in wider devices. Simultaneous effects of edge and substrate surface roughness are considered. Results show that in the presence of both the edge and substrate surface roughness the 4 nm wide device with boron nitride doping shows improved performance with respect to the 1.5 nm one (both of which incorporate the same bandgap AGNR as channel material). Electronic simulations are performed via NEGF method along with tight-binding Hamiltonian. Edge and surface roughness are created by means of one and two dimensional auto correlation functions respectively. Electronic characteristics are averaged over a large number of devices due to statistic nature of both the edge and surface roughness.

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1. Introduction

The discovery of graphene, a single layer of carbon atoms arranged in a honeycomb lattice structure, has opened a promising alternative to silicon electronics [1,2]. Observed charge mobilities at room temperature in pristine graphene are indeed orders of magnitude larger than those of silicon [3–5]. Nevertheless, the maximum achievable on- to off-current ratio, an important device figure in digital applications, in graphene devices cannot compete with that of silicon devices due to lack of an energy bandgap in graphene [2,6,7]. Cutting graphene into narrow strips, graphene nanoribbons (GNRs), laterally confines the movement of carriers, inducing an energy gap inversely proportional to the ribbon width [8,9]. Unfortunately, electronic transport properties of GNRs suffer from edge roughness (ER) [10,11]. ER defined as lack of or excess carbon atoms at GNR edges, due to fabrication process, plays more deteriorating role in electronic transport properties as GNR width reduces [6,12,13]. It has been proved that ER deteriorates the device performance of GNR field effect transistors (GNRFETs) [6,12,13].

Another way to open a gap in graphene band-structure is to confine the transport of carriers by doping graphene edges parallel to the transport direction via a high energy bandgap material such as boron nitride (BN) [14]. As a result, one can alleviate the effect of ER by making use of wider AGNRs while maintaining large enough the energy bandgap by BN doping of GNR edges. Nevertheless, one must take care of the substrate surface roughness (SSR) effects, an area dependent scattering source, when the channel dimensions increases [15–17]. To have a better insight into the operation of such devices a comprehensive study considering simultaneous effects of ER and SSR proves inevitable. In this work simultaneous effect of BN doping, ER and SSR on the performance figures of BN doped armchair GNRFETs (AGNRFETs) is studied. Symmetrical BN doping of GNR edges is employed to open required bandgap, hence, make it possible to use wider GNRs which are less sensible to the ER and benefit from larger on current. ER and SSR are modeled via one- and two-dimensional auto correlation functions (ACF) respectively. Electronic transport is performed by means of non-equilibrium green's function (NEGF) formalism along with the first nearest neighbor tight-binding Hamiltonian. The paper is organized as follows: in the next section the employed models and methods are reviewed. Section 3 is devoted to results and discussions and conclusion remarks are listed in Section 4.

2. Model and methods

In the Tight-Binding scheme the electronic properties of graphene can be modeled by only considering p_Z orbital of carbon atoms [18]. The Hamiltonian in the second quantized representation is written as:

$$H = \epsilon_i \sum_i c_i^+ c_i + t_{ij} \sum_{i \neq j} (c_i^+ c_j + h.c.) \tag{1}$$

Here ϵ_i and t_{ij} represent the on-site energy and hoping parameter respectively and $c^+(c)$ is fermion creation (annihilation) operator. The hoping parameters and on-site energies of perfect GNRs used to construct tight-binding Hamiltonian are chosen according to Ref. [19].

The hoping parameter between p_Z orbitals depends on the C–C bond length. SSR modulates the Tight-binding parameters of AGNR both through the bending of the p_Z orbitals and stretching of C–C bond lengths. While the effect of orbital bending is much smaller than that of the bond length stretching, it can be neglected without notable loss of accuracy [20]. The hoping parameters of graphene lattice are related to the C–C bond length via [21,22]:

$$t(l) = t_0 \exp(-3.37(l/l_0 - 1)) \tag{2}$$

where l_0 and t_0 denote the C–C bond length and hoping parameter of flat GNR and l represents the distance between two carbon atoms. Because of slight lattice mismatch of graphene and BN one can apply Eq. (2) with proper t_0 to compute the modulation of hoping parameter between BN, BC and NC bonds due to SSR [23,24]. Experimental data on the surface roughness of graphene over most