Superlattices and Microstructures xxx (2017) 1–9

Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

Electron transport in graphene/h-BN lateral hybrids: Rhombus and bowtie domains

Ali Mehri [a, *], Maryam Jamaati [b], Afshin Namiranian [b]

[a] Department of Physics, Faculty of Science, Babol Noshirvani University of Technology, Babol, Iran
[b] Department of Physics, Iran University of Science and Technology, Narmak, 16345, Tehran, Iran

ARTICLE INFO

Article history:
Received 7 April 2017
Received in revised form 29 April 2017
Accepted 3 May 2017
Available online xxx

Keywords:
Graphene/hBN hybrid
Nanoflake
Electronic transport
Non-equilibrium Green's function

ABSTRACT

Electron transport in graphene/h-BN lateral hybrids with rhombus and bowtie domains is investigated. We apply non-equilibrium Green's function method under tight binding approximation to calculate electrical transmission in mentioned hybrid monolayers. Our findings reveal the importance of size and shape of doped regions in the transport through hybrid systems. Generally, we find that boron and nitrogen doping in zigzag graphene nanoflake, with both rhombus and bowtie patterns, improves its conductance. Growing size of the doped segments, in fixed system size, leads to a stable conductance level. Moreover, carbon doping in h-BN can also make a tunable semiconducting behavior. In the latter case, when the system size is kept constant, enlarging the doped carbon domains exponentially rise up the transmission.

1. Introduction

Graphene, as an important member of two dimensional layered materials family, has received extensive scientific and industrial attention due to its unique electronic, mechanical and thermal properties [1–3]. Since pristine graphene is a zero-gap semimetal, tailoring its conductive properties is desirable to open band gap for applications such as electronic devices [4–6].

Among different strategies, exploring techniques to achieve this goal gave rise to a novel class of two dimensional materials, referred to as "graphene hybrids" [7,8]. As a close analog of graphene, hexagonal boron nitride (h-BN) known as white graphene, is a large band gap semiconductor. It has shown the possibility to transform graphene and h-BN from their intrinsic nature to n-type or p-type semiconductors by substituting carbon (C) atoms with boron (B) and nitrogen (N) atoms to make graphene/h-BN (h-CBN) hybrids [9–11], and by doping C atoms in h-BN (h-BNC) [12,13]. Despite the similarities between lattice parameters and the bond length of graphene and h-BN, the electronic properties of h-BN is drastically different from those of graphene [8]. Since h-BN is a wide band gap compound [14], h-CBN and h-BNC hybrid structures provide the diversity and flexibility to develope electronic devices [15–17].

Recently, the possibility of directly merging graphene and h-BN into in-plane (lateral) graphene/h-BN (h-CBN and h-BNC) hybrids with well controlled shape and size of doping domains has been experimentally realized by various groups [18–22]. Experimental works has been also confirmed improved device performance suitable for wide applications in modern electronics using h-CBN and h-BNC hybrids [5,23–25]. Furtheremore, extensive theoretical calculations have been investigated

* Corresponding author.
E-mail address: alimehri@nit.ac.ir (A. Mehri).

http://dx.doi.org/10.1016/j.spmi.2017.05.005
0749-6036/

the electronic [12,26–28], transport [13,29], magnetic [30,31], thermal [32], and optoelectronic [33] properties and stability of lateral graphene/h-BN hybrid systems [11]. The relative predominance of C—N or C—B bonds [34], the shapes and size of the h-BN segments [35] and carbon domains [33,36], or the presence of isolated B and N atoms [37] play a crucial role in determining the physical properties of these hybrid systems [7].

The aim of this work is to give a better understanding of the electronic and transport properties of lateral h-CBN and h-BNC hybrid systems. We study triangle shaped h-BN islands dispersed in a graphene host lattice and also the inverse type of hybrid in which finite graphene segments are confined in a h-BN lattice. The influence of h-BN or graphene segment position at the corner (rhombus pattern) or middle (bowtie pattern) of zigzag edges of the studied system and their percentages on the conductance are investigated in detail. Furtheremore, we will check density of states to gain a deeper insight into the role of existance of doped atoms and their structure in the electron transport of graphene/h-BN hybrid systems. The electrical conductance of these systems was calculated using non-equilibrium Green's function method (NEGF) using nearest neighbor tight binding model to describe the atomic interactions.

The remaining sections are structured as follows. In section 2 we will briefly introduce the NEGF method employed for conductance calculation. Section 3 is dedicated to illustrate and discuss the obtained result. Finally, we conclude and give a summary of our main points in section 4.

2. Numerical modeling

In this section we illustrate computational procedure of our study. Transport properties of graphene/h-BN hybrid is investigated through solving Schrödinger equation using the non-equilibrium Green's function (NEGF) formalism [38,39]. The NEGF approach is proved to be a powerful simulation tool, which can be used to analyze quantum transport in a variety of nanoscale devices [40]. It is also one of the best widely used techniques for investigation of electrical properties in graphene/h-BN hybrid systems [41–43].

In the NEGF theory, the structure is partitioned into three parts including the central device and two semi-infinite electrodes, which can be completely described using four main equations. These equations involve several matrices to give an explanation of central device, and the interaction between the central device and the reservoirs. The first out of four NEGF equations defines the retarded Green's function as below:

$$G^r(E) = \left[(E + i\eta)I - H_{device} - \Sigma_L^r - \Sigma_R^r\right]^{-1}, \tag{1}$$

where E is the energy of the particle, η is a positive infinitely-small real number, and I represents the identity matrix. Hamiltonian of the device, H_{device}, can be obtained using a tight-binding model with P_z orbital basis set.

Hence, the Hamiltonian can be written as:

$$H_{device} = \sum_{i=1}^{N}(|i> \varepsilon_i <i|) + \sum_{<i,j>}\left(|i> t_{i,j} <j|\right), \tag{2}$$

where ε_i is the on-site energy, and $t_{i,j}$ is the hopping energy between nearest neighbor lattice points i and j. $\sum_{<i,j>}$ refers to a sum over the nearest-neighbor sites. The values of on-site energies of carbon, boron, and nitrogen atoms and hopping energies are chosen to be $\varepsilon_C = 0$, $\varepsilon_B = +2.33eV$, $\varepsilon_N = -2.5eV$ and $t_{C,C} = -3eV$, $t_{B,N} = -2.81eV$, $t_{B,C} = -2.7eV$, $t_{N,C} = -3.14eV$, respectively [44]. $\Sigma_{L/R} = \tau_{L/R}^{\dagger} g_{L/R} \tau_{L/R}$ are the self energy matrix for left and right reservoir respectively, which describe the effect of scattering by the contacts on the Hamiltonian of the system. $\tau_{L/R}$ is the coupling matrix, which shows the hopping of electron from the left/right electrode to the device.

The τ is calculated using nearest neighbor tight-binding Hamiltonian with the above mentioned parameters to describe hopping strengths. And, $g_{L/R}$ is the surface Green's function of leads evaluated by a recursive iteration technique [45,46]:

$$g_{L/R}(E) = \left[(E + i\eta)I - H_0 - H_1 g_{L/R}(E) H_1^{\dagger}\right]^{-1}, \tag{3}$$

here, H_0 and H_1 denote the Hamiltonian of single isolated layer in the lead and the hopping between neighboring layers, respectively. It should be noted that, the above equation can be solved iteratively starting in the first step by choosing $g_{L/R}(E) = [(E + i\eta)I - H_0]^{-1}$.

The third equation represents the coupling term, which describes the energy level broadening due to the interaction between central device and the source (drain) contacts and can be obtained from the self energy terms via the below formula:

$$\Gamma_{L/R}(E) = i\left[\Sigma_{L/R}^r(E) - \Sigma_{L/R}^a(E)\right]. \tag{4}$$

Please cite this article in press as: A. Mehri et al., Electron transport in graphene/h-BN lateral hybrids: Rhombus and bowtie domains, Superlattices and Microstructures (2017), http://dx.doi.org/10.1016/j.spmi.2017.05.005