Computational Materials Science 109 (2015) 240–247

Contents lists available at ScienceDirect

Computational Materials Science

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

Tunneling conductance of telescopic contacts between graphene layers with and without dielectric spacer

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ARTICLE INFO

Article history:
Received 26 April 2015
Received in revised form 22 June 2015
Accepted 4 July 2015
Available online 25 July 2015

Keywords:
Tunneling conductance
Graphene layers
Argon spacer
Negative differential resistance
Capacitance

ABSTRACT

The telescopic contact between graphene layers with a dielectric spacer is considered as a new type of graphene-based nanoelectronic devices. The tunneling current through the contacts with and without an argon spacer is calculated as a function of the overlap length, stacking of the graphene layers and voltage applied using non-equilibrium Green function formalism. A negative differential resistance (similar to semiconductor tunnel diode) is found with the peak to valley ratio up to 10 and up to 2 for the contacts without any spacer and with the argon spacer, respectively. The capacitance of the contacts between the graphene layers with the argon spacer is calculated as a function of temperature taking into account the quantum contribution. The related *RC* time constant is estimated to be about 3 ps, which allows elaboration of fast-response nanoelectronic devices. The possibility of application of the contacts as memory cells is discussed.

1. Introduction

Significant progress has been achieved recently in design of novel graphene-based heterostructures that offer great promise for application in nanoelectromechanical systems (NEMS) and nanoelectronic devices. Among such heterostructures there is double-layer graphene [1–4], a system comprising two graphene layers separated by a dielectric spacer. While in bilayer graphene the layers are located at the distance of about 3.4 Å, similar to graphite, in double-layer graphene the distance between the layers is controlled by the thickness of the dielectric spacer. Graphene-based field-effect transistors consisting of two graphene layers separated by a layer of adsorbed molecules [1] and by one or several layers of hexagonal boron nitride (h-BN) [2] have been realized recently and transport properties of such heterostructures have been measured [3,4]. The characteristics of the pressure sensor based on changes of interlayer tunneling conductance of the graphene/h-BN heterostructure have been calculated [5]. An idea of a high-speed memory cell based on relative rotation of layers of double-layer graphene with an argon spacer has been proposed [6]. In the present paper we consider the tunneling conductance of a telescopic contact between graphene layers with and without a monolayer argon spacer showing effects relevant both for traditional electronic devices and NEMS. We also analyze the capacitance of double-layer graphene with the argon spacer to estimate its characteristic response time in electronic devices based on this heterostructure.

The conductance between neighbor graphene layers has been addressed in a number of works [7–10]. The calculations show that the electronic structure of twisted bilayer graphene strongly depends on the twist angle [8]. The tunneling conductance of bilayer graphene can be modified by an order of magnitude upon atomic-scale in-plane relative displacement [7,9] or rotation [9] of the layers, similar to *c*-axis conductivity of graphite [10]. Significant variations in the band gap of bilayer graphene nanoribbons upon atomic-scale in-plane relative displacement of their layers are found using density functional theory (DFT) calculations [11,12]. Quasi one-dimensional transport in systems consisting of

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http://dx.doi.org/10.1016/j.commatsci.2015.07.006
0927-0256/

two overlapping layers [13–17] or a layer with an adsorbed graphene flake [16,18,19], both with a central bilayer region, has been recently a subject of extensive research. The tunneling conductance of such systems based on nanoribbons is found to change by an order of magnitude upon atomic-scale in-plane relative displacement of the layers [13]. Resonances and anti-resonances in the transmission as a function of the carrier energy and overlap length have been explained [16,17,19]. The case of crossed graphene nanoribbons has also been addressed [20,21]. Here we use the non-equilibrium Green function (NEGF) formalism on top of DFT calculations to investigate the influence of stacking and overlap length of graphene layers on the $k_\perp = 0$ component of the tunneling current between them. Such an approach also allows us to evaluate the effect of the argon spacer.

The effect of negative differential resistance is widely used in traditional electronic devices such as amplifiers, oscillators, frequency mixers and memory cells [22]. As for carbon-based nanoscale systems, up to now the negative differential resistance have been predicted for very narrow graphene nanoribbons [23], chemically doped [24] and field-effect doped [25] graphene nanoribbons, doped graphene monolayer with p–n junction [26], parallel graphene nanoribbons contacts [14,15] and parallel single-walled carbon nanotube contacts [27]. Here the negative differential resistance is found for contacts between graphene layers both with and without the argon spacer.

Extensive studies have been performed to demonstrate the possibility of using graphene layers as movable elements of NEMS. Fast mechanical response of such devices can be predicted from low Q-factor values obtained for relative vibrations [28,29] and self-retracting motion of graphene layers [29,30] observed experimentally [31]. Schemes and operational principles of a set of NEMS based on relative motion and interaction of graphene layers have been considered [7,11–13,29,32–35]. It is worth mentioning a nanorelay [29] and inertial sensor [32] based on telescopic motion of graphene layers [29], memory cells based on motion of a graphene flake on a graphene layer [33,34], nanoelectromechanical switches based on changes of the distance between graphene layers [35] and in-plane relative displacement of layers [11], various nanosensors based on measurements of conductance changes at the in-plane relative displacement of layers of bilayer graphene [7,11–13,35]. Operation of all these NEMS involves application of a bias and conductance measurements. Therefore, understanding of tunneling conductance between graphene layers, which can be gained through theoretical studies, holds the key to success of NEMS developments.

Nearly frictionless relative motion of graphene layers separated by an incommensurate spacer can be also used in fast-response nanoelectromechanical devices [6,36]. However, analysis of capacitance of such systems determining the characteristic time of their electronic response is still lacking. Experimental measurements [37] have shown that an important contribution to the capacitance of single-layer graphene [38] is provided by the two-dimensional electronic gas [39]. The influence of this quantum capacitance on the operation frequency of a radio-frequency device based on single-layer graphene has been studied [40]. Here we apply the approach [38] to obtain the total capacitance of double-layer graphene with the dielectric spacer including the quantum contribution. On the basis of these results and calculated tunneling conductance we estimate the RC time constant of double-layer graphene with the argon spacer.

The paper is organized in the following way. Methods of calculation of tunneling conductance are presented in Section 2. Section 3 is devoted to calculations of the tunneling conductance between graphene layers for telescopic contacts with and without the argon spacer and estimates of the capacitance and related RC time constant of the contact between the graphene layers with the argon spacer. Our conclusions are summarized in Section 4.

2. Methods

The tunneling conductance of telescopic contacts between graphene layers with and without the spacer has been obtained using the non-perturbative approach based on the Green function formalism for systems with semi-infinite periodic electrodes [16,41]. We use the localized basis set to divide the system along the current direction into segments that can only interact with the neighbor ones. In this way, the Hamiltonian of the system includes only Hamiltonians of separate segments and coupling matrices between adjacent segments. Thus, instead of considering the whole infinite system only electronic structures of several segments surrounded by their neighbors have to be calculated. As such segments, we take the contact area between the graphene layers and sufficiently long periodic segments of the electrodes (the size of the segments should be greater than the doubled cutoff radius of the orbitals). Therefore, we perform first-principles calculations for three relatively small structures. The periodic segments of the electrodes are considered under the periodic boundary conditions along the current direction. The third structure is the model of the tunneling contact between the graphene layers of a finite

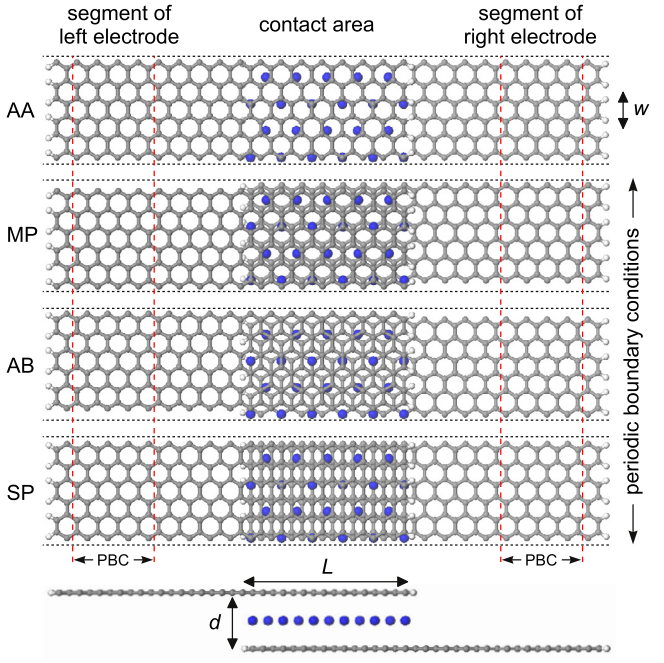

Fig. 1. The finite-length structures used for calculation of the electronic structure of the contact area between graphene layers with different stacking separated by the quasi-incommensurate argon layer (in position I) and coupling of the contact area to the graphene electrodes. Carbon, hydrogen and argon atoms are colored in gray, white and blue, respectively. The horizontal black dotted lines indicate boundaries of the simulation boxes with periodic conditions. The vertical red dashed lines denote the contact area and segments of the electrodes. The calculations of Green functions of the electrodes are performed for these segments with periodic boundary conditions (PBC) at the vertical dashed lines. The elementary unit cell width $w = \sqrt{3}a_0$, overlap length L of the graphene layers and distance d between them are shown, where $a_0 = \sqrt{3}a_{CC} = 2.466$ Å, and $a_{CC} = 1.424$ Å is the carbon–carbon bond length. Inequivalent AB and MP stackings for the systems with the argon spacer are referred to in the text as AB1, MP1, AB2 and MP2. The AB and MP stackings shown in the figure correspond to AB1 and MP1. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)