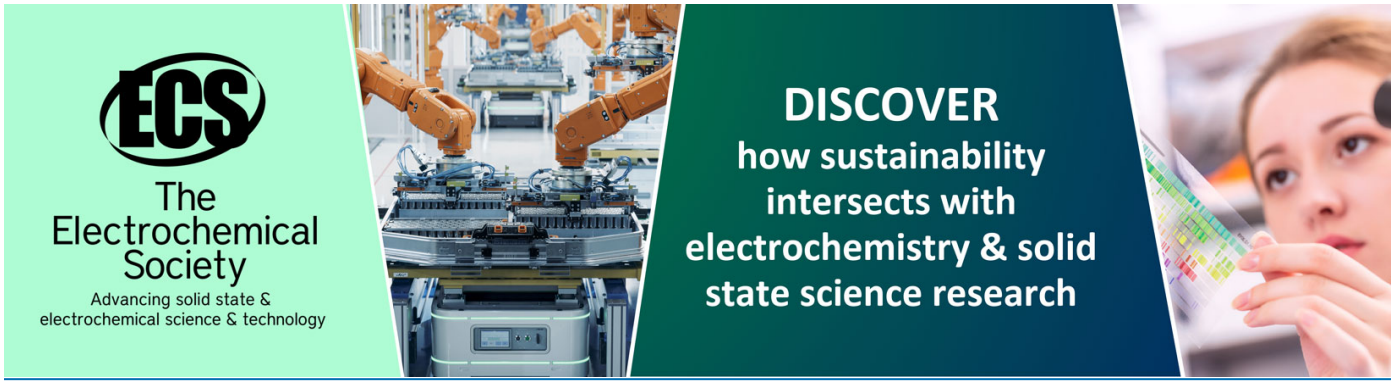
Bilayer graphenes with antidots: structures, properties and applications



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Bilayer graphenes with antidots: structures, properties and applications

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Abstract. We consider structures, properties and possible applications of next bilayer graphene (BLG) materials with nanoholes. Formation of folded nanoholes in bilayer graphene: modelling and comparison with experiments will discussed. The most advantageous shape of the BLG holes was determined in a manner analogous to the method used by Woolf to find the optimal shape of the crystals, unlike the method, the edge energy depends not only on the direction, but also on the cut along the direction. This suggests that the optimal shape of the holes depends on their size. The comparisons with the experiments of M.Takeguchi group (Japan) was carried out. The holes in single and few-layer graphene films can be the impacts of heavy high-energy ions. To carry out the comparison with the experiments, a collaboration with N. Nebogatikova group (Russia), was carried out. We have studied the atomic structures of nanoholes in both bilayer and multilayer graphene using two-temperature molecular dynamics simulations requires proper treating of dynamic energy exchange between electronic and ionic subsystems in the irradiated system. Different stable forms of nanoholes with closed edges are considered in BLG structures of AA, AB and Moiré stacking's. We have found stable BLG nanomeshs with both semimetal, metal and semiconductor properties. Some applications of similar BLG structures are proposed.

1. Introduction

Successful synthesis and intensive investigation of graphene [1-3] yields many outstanding properties of this materials which can be used in the various fields of science and technology. Like graphene monolayer bilayered graphene (BLG) also attracts a lot of attention to the worldwide scientific community. In BLG the Dirac cone transforms to parabolic bands in which small band gap (~10 meV) can be opened by molecular doping or applying an external electric field [3-6]. Very recently, for the first time for a purely carbon structure on a graphene with Muar structure, a superconductivity was discovered [7].

One of the promising way of the opening of band gap in graphene monolayer by formation of periodically arranged antidots (nanoholes) [8] significantly increases the speed of development of BLG structures [9]. Unlike graphene monolayer where holes have open edges which are unstable and passivated another atoms, holes in bilayered graphene tend to closing edges [10–12]. Moreover, ab initio calculations predicted that the connection of the edges even does not require overcoming of any barrier

[11] and therefore hollow sp2-hybridized graphene structure forms spontaneously. The possibility of formation of such structures was confirmed in the experiments [13, 14]. Also, it is worth noting that, bilayer graphene with periodically located holes is a very interesting and promising object for use in the field of semiconductor optoelectronics. Presence of the holes in the structure of hollow sp2 carbon structures drastically changed the electronic properties of BLG by appearance of additional mini-bands in the vicinity of Fermi energy level. Such changes in the band structure could be explained in the terms of the redistribution of the electron density directly on the newly formed topological defects. In the report we consider structures, properties and possible applications of next bilayer graphene materials with nanoholes.

2. Formation of folded nanoholes in BLG

Other paragraphs Different stable forms of nanoholes with closed edges are studied in BLG structures of AA, AB and Moiré stacking's. The modeling examples and their comparisons with experiments are shown in papers [10-12, 14, 16].

The most advantageous shape of the BLG holes was determined in a manner analogous to the method used by G. Wulff to find the optimal shape of the crystals, which can also be used to determine the shape of the pores for two-dimensional crystals [17,18]. However, in our case, unlike the Wulff method, the edge energy depends not only on the direction, but also on the cut along the direction. This suggests that the optimal shape of the holes depends on their size. A certain size leaves only one definite optimal cut for any direction. Some examples of such constructions are shown in figure1: There are AA (a) and twisted 5°tBG (b), and predicted optimal shape comparison with the observed nanoholes by electron beam preparation in 5°tBG (Japanise M.Takeguchi group [14]).

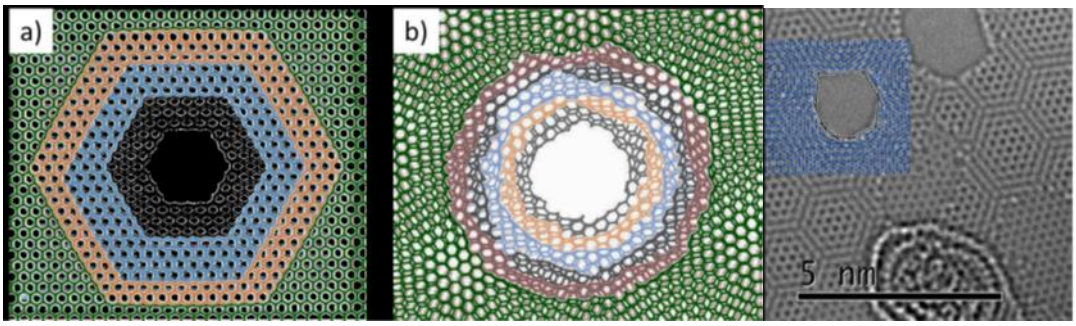


Figure1. Dependences of the shape of the holes on the size for a random point of its nucleation in a BLG and predicted optimal shape comparison with the observed nanoholes. [14]

3. The holes in single and few-layer graphene films

Some The holes in single and few-layer graphene films can be the impacts of heavy high-energy ions. To carry out the comparison with the experiments of N. Nebogatikova group (Novosibirsk, RF) [15], we have studied the atomic structures of nanoholes in both bilayer and multilayer graphene films. To interpretation of the experimental results through atomistic simulations requires proper treating of dynamic energy exchange between electronic and ionic subsystems in the irradiated system. We used two-temperature molecular dynamics model in which atomic subsystem is described by classical molecular dynamics simulations, whereas electronic subsystem is characterized by local electronic temperature and treated as a continuum on a regular grid. The model account for energy transfer between these subsystems. For the calculations we used the LAMMPS code.

In the Fig. 2 are shown: a) hole size as a function of the number of Xe ions irradiated considered region; the range of experimental values of the pore size is denoted by orange; upper and down series of the insets (relatively to the data) represent atomic structures of holes formed by ions with energy 167 and 26 MeV, respectively; b) temperature and structural changes of three-layered graphene in MD simulations after the irradiation at Xe^{+} energy 100 MeV; the evolution of the graphene structure at the

chosen steps is shown. In the inset the zoomed side view connected edges is shown; c) band gap of the infinite ribbon with connected edges as a function of the distance between connected regions.

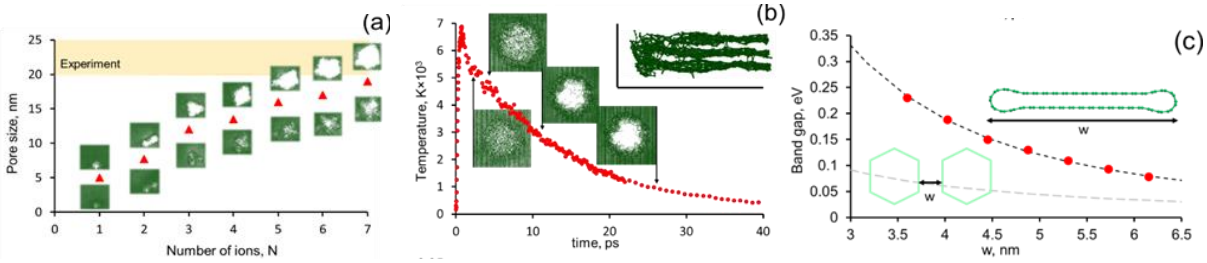
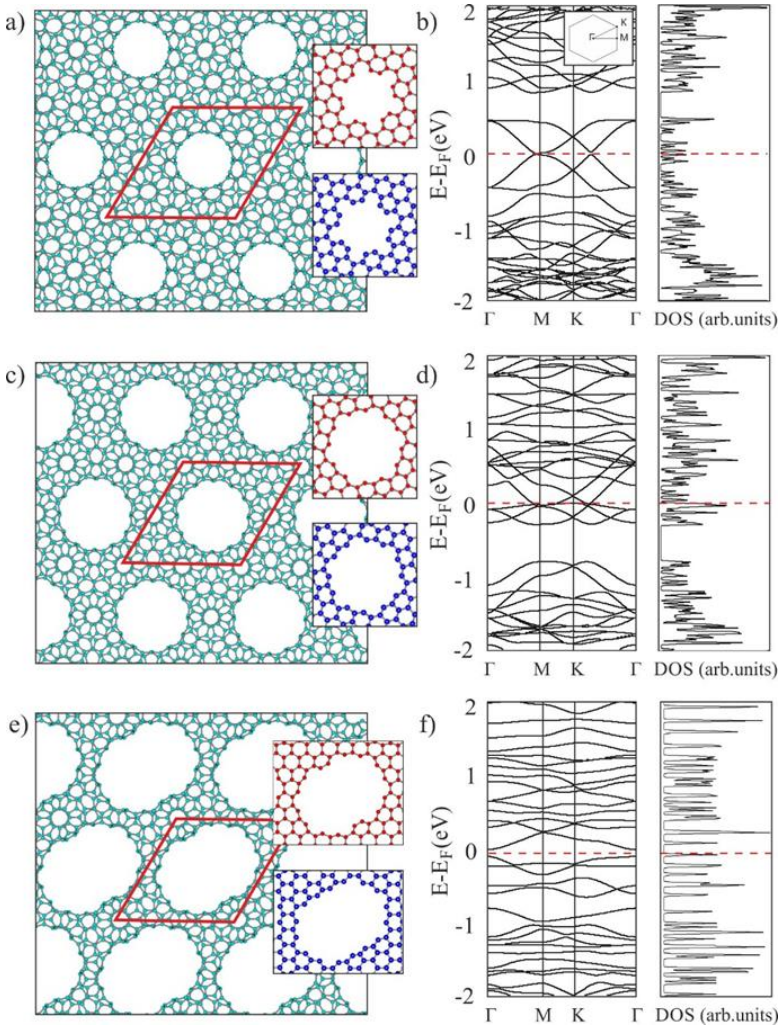


Figure 2. The schematic views of corresponding hole formation structures and the band gap dependence via the region W between folded pores in bilayer graphene.

4. Examples of 30ºtBG nanomeshes

We have modeled different stable types of BGNMs and found stable BLG nanomesh structures with both semi metal, metal and semiconductor properties [10-12,14,16].



Fugure 3. Perforated moiré 30°tBG with round holes (a, c) and oval holes (e), their electronic spectra and the density of electronic states (DOS) (b, d, f).

Some their examples of 30°BG nanomeshes [16] are shown in figure 3: a) a structure with a period of l = 17.7Å and a smallest hole radius r_1 = 0.4 nm, c) a structure with l = 17.6Å and a radius of r_2 = 0.6 nm., e) periodic "oval 1" 30°tBG structure with l = 16.91Å, (b, d, f) electronic spectrum and the density of electronic states (DOS) of each nanomeshes. A parallelogram designates a unit cell; a dashed line is the Fermi level. On the inset - fragments of the upper and lower layers of the structure

5. Conclusion

Thus, we considered examples of a new class of bi-graphite nanostructures with different shapes and sizes of holes with closed boundaries. These structures are multiply connected systems of completely sp2-hybridized carbon atoms with inherent features in electronic spectra. So the band structures of BGNM nano-networks differ sharply from the spectra of monographene meshes, whose pairs, bound along the edges of the holes, constitute these bi-graphene meshes.

We note that applying a transverse voltage to semimetallic nanoscreens 30°tGNMr1 and 30°tGNMr2, will result in a shift of the Fermi level, analogous to the shift in graphene [1]. Thus, it is possible to obtain a conduction-change effect on the semiconductor, and, consequently, to use these nanoscale as switching elements in nanoelectronics. The result of the presence in all tGNM meshes of quasi-local modes in the electronic spectrum, the number of doubly larger modes localized near similar holes in single-layer graphene nanomeshes. This leads to the appearance in a wide range of peak energies of electronic states. In this connection, there appears the prospect of effective use of the considered 30°tGNMs in photovoltaics and optoelectronics, as well as in thermoelectric elements like the use of moiré twisted BG structures [19, 20]. Obtained structure with close edges holes can display "p- or n-doped" metallic or semiconductor conductivity. Note that, because of the absence of a center of symmetry, the similar BLG nanomeshes should display significant piezoelectric effect, which increases the interest in the use of these structures in electro- or opto- mechanical nanodevices.

Acknowledgments
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