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Analytical expressions for electrostatics of graphene structures

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HIGHLIGHTS

- An atomistic moment method is applied for the estimation of graphene structures electrostatics.
- New analytical equations are obtained for the prediction of total charge or capacitance of graphene structures.
- The lowest point charges are found at the center of a graphene structure, while the maximum charges are found at its corners.
- The maximal charge enhancement increases as the size of the graphene structure is increased as well.

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ABSTRACT

This study focuses on electrostatics of various graphene structures as graphene monolayer, graphene nanoribbons, as well as multi-layer graphene or graphene flakes. An atomistic moment method based on classical electrostatics is utilized in order to evaluate the charge distribution in each nanostructure. Assuming a freestanding graphene structure in an infinite or in a semi-infinite space limited by a grounded infinite plane, the effect of the length, width, number of layers and position of the nanostructure on its electrostatic charge distributions and total charge and capacitance is examined through a parametric analysis. The results of the present show good agreement with corresponding available data in the literature, obtained from different theoretical approaches. Performing nonlinear regression analysis on the numerical results, where it is possible, simple analytical expressions are proposed for the total charge and charge distribution prediction based on structure geometry.

1. Introduction

Graphene is the well-known flat monolayer of covalently bonded carbon atoms tightly packed into a two dimensional (2D) honeycomb crystal lattice. Although graphene was presumed not to exist in a free state, the free-standing graphene was unexpectedly discovered almost a decade ago [1,2]. Graphene constitutes the building block of other nanostructures such as single layer graphene sheets, graphene nanoribbons, and multi-layer graphene sheets or graphite flakes [3]. Graphene has been observed to present unusual band structure [4] leading to unique electronic properties and making it an ideal candidate for numerous applications in nanoelectronics and nanoelectromechanical systems (NEMS) [5–9]. Simultaneously, graphene presents exceptional mechanical properties having a Young's modulus of almost 1 TPa and an intrinsic strength of approximately 130 GPa, and thus it is one of the strongest material ever measured, also having a low weight [10,11].

Recently, Ray [12] published a comprehensive work presenting various applications of graphene and graphene-oxide based nanomaterials. Electromechanical coupling plays a significant role in the applications of graphene structures in NEMSs. Therefore, beyond their mechanical performance, the modeling and prediction of their electrical behavior is also a fundamental goal. Wang and Scharstein, in their excellent theoretical work [13], studied the distribution of net electric charge in graphene, using both a constitutive atomic charge–dipole interaction model and an approximate analytical solution to Laplace's equation. It was found that their analytical model gave a good description of the charge distribution, except for the very edge atoms because of the atomic edge state, which could instead be treated by their numerical model. Fang et al. [14] derived fundamental results for carrier statistics in graphene two-dimensional sheets and nanoscale ribbons. Guinea [15] considered the charge distribution induced by external fields in finite stacks of graphene planes, or in semi-

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infinite graphite and calculated the charge induced by the self-consistent electrostatic potential using the linear response theory (random phase approximation). Silvestrov and Efetov [16] analytically investigated the distribution of charge induced by a gate voltage in a graphene strip. They demonstrated a strong macroscopic charge accumulation along the boundaries of a micrometer-wide strip and noted that this charge inhomogeneity is especially important in the quantum Hall regime.

An important quantity is the capacitance of graphene. Carbon nanomaterials, including 1D carbon nanotubes, 2D graphene, and 3D mesoporous carbon, are promising as electrode materials for flexible supercapacitors due to their extremely large surface area, excellent mechanical and electrical properties, and high electrochemical stability. Recently, Mombeshora and Nyamori [17] published a review on the use of carbon nanostructured materials in electrochemical capacitors. They explored set platforms for a variety of carbon nanomaterial based designs with high prospective specific capacitance. Xia et al. [18] reported a direct measurement of the quantum capacitance of graphene as a function of gate potential using a three-electrode electrochemical configuration. Their results demonstrated that the quantum capacitance has a nonzero minimum at the Dirac point and a linear increase on both sides of the minimum with relatively small slopes. Chen and Dai [19] provided an overview of recent progress towards the development of advanced flexible supercapacitors based on carbon nanomaterials discussing the challenges and perspectives in this emerging field. Nawaz and Tahir [20] derived the quantum capacitance in monolayers of silicene and related buckled materials as a function of the Fermi energy as well as temperature concerning electron-hole puddles through a Gaussian broadening distribution. Their predicted results are very interesting concerning future applications in spintronic and valleytronic devices.

In the present paper, the electrostatic behavior of various graphene structures, i.e. graphene nanoribbons and multilayer graphene configurations, is studied. To the author's best knowledge, it is the first time that the atomistic moment method is utilized in order to obtain the charge distribution of graphene structures assuming that stand in an infinite space or in a semi-infinite space limited by an infinite grounded plane. Using the results, the total charge as well as the capacitance of the nanostructure under investigation may be evaluated. Performing regression analysis, new and simple analytical expressions are extracted concerning the total charge and capacitance of various graphene structures.

2. Electrostatics of graphene structures

Assume a charge which is uniformly distributed in a region around a carbon atom. The electric potential of graphene results on a further distribution of charges. It is assumed that the charge can be accumulated in the corresponding atom as a point charge. Thus, graphene becomes the carrier of point charges located on carbon atomic positions. Here, we examine two different boundary conditions as presents. Firstly, graphene is assumed to be in an ideal electric field, i.e., the electric potential on the surface of graphene is V_0 and the reference point tends to the infinite. Thus, the only boundary condition is that the whole external surface of the graphene is kept at a potential V_0. Secondly, as Fig. 1 depicts, graphene behavior is examined when the potential V_0 has a reference point in a semi-infinite space. The distance between graphene layers of is $t=0.34$ nm, while L is the distance from the grounded plane. When $L\rightarrow\infty$ the graphene is considered to exist in an infinite space.

To evaluate the charge distribution of graphene, the atomistic moment method is adopted. According to this method, the classic

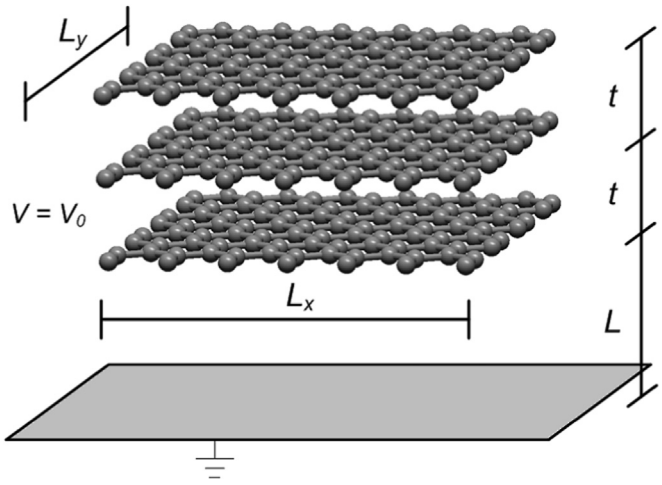

Fig. 1. Multi-layer graphene in a semi-infinite space. Graphene structure is considered in an infinite space when $L\rightarrow\infty$ or $L=L_\infty$.

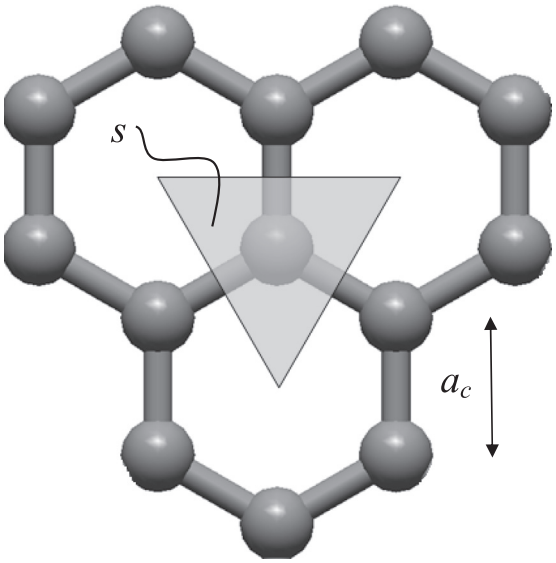

Fig. 2. Triangular area around a carbon atomic position where the electric charge is distributed.

electrostatic theory is actually applied on the atomistic structure of graphene in nanoscale. As Fig. 2 illustrates, the surface of graphene is divided in triangular areas, in such a way that a single carbon atom is always located at the center of them. The charge is assumed to be distributed uniformly in each divided area and concentrated as a point charge at atomic positions. The point charges at all atomic positions may be estimated by solving a system of algebraic equations, which are determined in terms of equipotential surface.

2.1. Electrostatics of graphene in an infinite space

The atomistic moment method based on classic electrostatic theory for the charge distribution evaluation of carbon nanotubes [21–23] will be adjusted here for graphene structures and presented in detail. It is noticed that some works have already used the atomistic moment method to calculate the charge distribution in graphene. In their excellent work, Hao et al. [24] proposed a modified atomistic moment method based on the classical electrostatics theory to obtain the distribution of extra charges induced by an external electric field and net electric charges stored in a freestanding graphene monolayer in an infinite space and