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Numerical study of localization length in disordered graphene nanoribbons

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ABSTRACT

In this work, we study quantum transport properties of a defective graphene nanoribbon (DGNR) attached to two semi-infinite metallic armchair graphene nanoribbon (AGNR) leads. A line of defects is considered in the GNR device with different configurations, which affects on the energy spectrum of the system. The calculations are based on the tight-binding model and Green's function method, in which localization length of the system is investigated, numerically. By controlling disorder concentration, the extended states can be separated from the localized states in the system. Our results may have important applications for building blocks in the nano-electronic devices based on GNRs.

1. Introduction

The discovery of graphene sheets has created huge interests in studying their transport properties [1,2]. Graphenes, a two-dimensional sheet of graphite with honeycomb structure, exhibits some extraordinary properties much different compared with ordinary 2D materials; its charge carriers mimic relativistic particles and can be described by the Dirac equation [1–3]. Furthermore, it has shown a high mobility both at room temperature and at a high degree of doping [4]. The latter makes graphene nanoribbons (GNRs), as a strong candidate for building blocks in nano-electronic devices [5,6]. The energy gap is necessary to control electronic and transport properties of the nano-devices. Therefore, the narrow GNRs are useful to control of the properties. The tight-binding calculations or solutions of Dirac's equation show that the width of the energy gap depends sensitively on the

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geometry of edges and the width of the nanoribbons [7,8]. The energy gap in patterned graphene nanoribbons can be tuned during fabrication with the appropriate choice of ribbon width. Ribbon dimension and orientation are controllable parameters for the electrical properties of graphene structures [9]. Depending on their edges, the GNRs can be classified either as zigzag or armchair type. The width of GNR is denoted by N_A, which represents the number of zigzag lines for zigzag ribbons and the number of dimer lines for armchair ribbons. The tight-binding method predicts the zigzag ribbons to be conducting for all N_A and the armchair ribbons to be either conducting or semiconducting, depending on their width N_A [8]. According to this method, the armchair ribbon is metallic only for $N_A = 3m - 1$ (m: integer) otherwise, the armchair ribbon is semiconducting [10]. Authors of Ref. [11] have shown that with controlling a line of hopping integrals, one can modify electronic properties of a system.

In our recent works, we have introduced a simple method to investigate electronic transport in quasi one-dimensional systems (such as superlattice and superlattice-like disordered carbon nanotubes) by mapping of its real-space to one-dimensional mode space [12,13]. In the mentioned systems, the disorder is distributed in direction of the nanotube axis.

In the present work, we concentrate on the localization length of a defective graphene nanoribbon (DGNR) device attached to metallic AGNR leads taking into account a line of defects. The study of these defects can help us to understand the structure and electronic properties of GNR materials under different conditions. Our calculations are based on the tight-binding model and Green's function method within the nearest-neighbor approximation. Our results can serve as a base for developments of GNRs in designing nano-electronic devices.

The paper is organized as follows: In Section 2, the DGNR system is briefly defined and the proposed model for calculating the localization length is described. In Section 3, the numerical results and discussion is presented. The last section of the paper is devoted to the discussion and the conclusion of our findings.

2. Description of the model and method

In this section, we study the electronic quantum transport in a quasi-one-dimensional structure formed by M AGNR unit cells connected to two semi-infinite metallic AGNR leads. The carbon slices of the leads are assumed comprised between $(-\infty, 0] \bigcup [N+1, +\infty)$. The sandwiched spacer is known as a DGNR device (see Fig. 1).

We consider that the DGNR device consists of two types of carbon and impurity atoms with diagonal on-site energies, ε_c and ε_i, respectively. In Fig. 1 we have depicted the structure of a DGNR in the real space. Each disordered unit cell has one impurity atom. The disordered length of the device is $X(= N_{\text{impurity}})$, where N_{impurity} is the number of impurity atoms. In this study, we ignore the

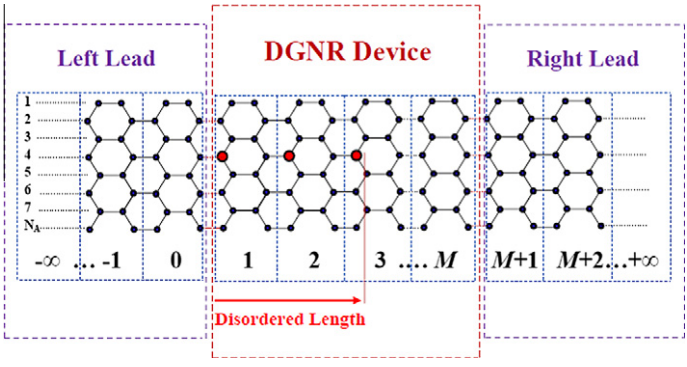

Fig. 1. Schematic representation of the DGNR composed of $M = 4$ unit cells bonded to two ideal leads. Here, the system width and the disordered length are $N_A = 8$ and $X = 3$, respectively.