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Direct Simulation of Charge Transport in Graphene Nanoribbons

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Abstract. Graphene nanoribbons are considered as one of the most promising ways to design electron devices where the active area is made of graphene. In fact, graphene nanoribbons present a gap between the valence and the conduction bands as in standard semiconductors such as Si or GaAs, at variance with large area graphene which is gapless, a feature that hampers a good performance of graphene field effect transistors.

To use graphene nanoribbons as a semiconductor, an accurate analysis of their electron properties is needed. Here, electron transport in graphene nanoribbons is investigated by solving the semiclassical Boltzmann equation with a discontinuous Galerkin method. All the electron-phonon scattering mechanisms are included. The adopted energy band structure is that devised in [1] while according to [2] the edge effects are described as an additional scattering stemming from the Berry-Mondragon model which is valid in presence of edge disorder. With this approach a spacial 1D transport problem has been solved, even if it remains two dimensional in the wave-vector space. A degradation of charge velocities, and consequently of the mobilities, is found by reducing the nanoribbon width due mainly to the edge scattering.

AMS subject classifications: 82D37, 82C70, 65M60, 82C80

Key words: Graphene nanoribbons, bipolar charge transport, discontinuous Galerkin method.

1 Introduction

Graphene has received a lot of attention because of its peculiar features [3] which make it very appealing in nano-electronics. In particular, large area graphene sheet possesses very high mobility and good conductivity. However large area graphene is a semimetal.

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This limits the use of graphene in field effect transistors (FETs) because there exists a restricted current-off region as a consequence of the zero gap, which produces a relevant current due to the minority charges when the gate voltage decreases below a threshold value [4]. Graphene nanoribbons (GNRs) represent a possible way to overcome such a drawback; in fact, the spatial confinement induces a band gap [1, 5], even if the mobility reduces with respect to the large area graphene sheet. Preliminary analyses often assume ballistic transport, e.g. in [2], but it is necessary to take into account scatterings in order to give an accurate assessment of the performance of GNRs for their applications to nano-electronic devices.

A sufficiently accurate model for charge flow in GNR is the semiclassical Boltzmann equation for electrons and holes. Here, edge roughness, which in principle enters as boundary condition, has to be also considered. Alternative approaches are based on hydrodynamical models [6–14]. For approaches based on the Wigner function see [15,16].

Usually the energy dispersion relation is split in subbands and it is related to the shape of the boundary, e.g. armchair or zigzag, and to the width of the ribbon. Here as energy bands we adopt those formulated in [1] which are in good agreement with DFT calculations up to energy of 1 eV, high enough for device applications. Following [2], the edge effects are included as an additional scattering stemming from the Berry-Mondragon model which is valid in presence of edge disorder. In this way it is possible to consider the average along the longitudinal direction which gives rise to a spacial 1D transport problem (observe that the problem remains 2D in the wave-vector domain).

The Boltzmann equation is numerically solved by the discontinuous Galerkin (DG) method proposed in [17, 18] (for methods based on finite difference see [19], for Monte Carlo approaches see [18, 20–23]) with a proper inclusion of the dispersion relation for GNRs and edge scattering.

We simulate the electron transport in GNRs and study the degradation of the mobility due to the confinement and the edge effects. A reduction of the carrier velocity, and as a consequence of the current degradation, is found by decreasing the nanoribbons width.

The plan of the paper is as follows. In Section 2 the mathematical model is presented while in Section 3 the numerical scheme for solving the Boltzmann equation is introduced. The numerical simulations are shown in the last section where the effects of the confinement and edge roughness are studied. Some details are reported in the appendices for the sake of completeness.

2 Mathematical model for GNRs

In large area graphene the energy band $\varepsilon(\mathbf{k})$ around the Dirac point has a conical shape

$$\varepsilon(\mathbf{k}) = \alpha\hbar v_F\sqrt{k_x^2+k_y^2}, \tag{2.1}$$

where v_F is the (constant) Fermi velocity, $\hbar$ the reduced Planck constant and $\mathbf{k}=(k_x,k_y)$ is the wave-vector, we assume to vary in $\mathbb{R}^2$. The parameters $\alpha=1$ and $\alpha=-1$ refer