Analysis of transport in a graphene ribbon with an antidot lattice, based on the scattering matrix solution of the Dirac equation

Paolo Marconcini\textsuperscript{1} and Massimo Macucci\textsuperscript{2}

\textbf{Abstract}—We have performed a simplified numerical simulation of the transport properties of a graphene ribbon with an antidot lattice. We have used an envelope function model for graphene, in which a space-dependent mass term approximately reproduces the effect of the regions of the ribbon where the carbon atoms are absent. The envelope function equation has been solved in proper subregions of the ribbon and then the results have been composed using a scattering matrix approach. Our simulator has been used to study the dependence of the energy gap and of the conductance of the ribbon on the different geometrical parameters of the antidot lattice, such as the size of the antidots, the distance between them and the tilt angle of the antidot lattice.

I. INTRODUCTION

In the last decade, the scientific community has devoted a large effort to the study of graphene [1]–[8], a two-dimensional material made up of a hexagonal planar lattice of carbon atoms, for which many different applications have been proposed. One of the most active research fields has been focused on the possibility to exploit its high mobility, one-atom thickness, and planar nature for the fabrication of electronic nanodevices [9], [10]. From this point of view, however, in unconfined monolayer graphene the absence of an energy gap prevents its application in digital electronics, where a large enough gap is necessary in order to achieve a sufficient $I_{on}/I_{off}$ ratio. Different approaches have been proposed to open up an energy gap in graphene, without however achieving values that are suitable for proper operation of digital circuits. One of such approaches is based on lateral confinement, i.e. defining with lithography or other techniques a graphene nanoribbon; another one consists of introducing an antidot lattice in the graphene sheet. An antidot lattice is a regular pattern of holes, i.e. regions where the carbon atoms are missing, defined antidots. Such lattices have been fabricated using several techniques, among which e-beam lithography [11], diblock copolymer templates [12] and nanoimprint lithography [13]. It has been shown that the presence of an antidot lattice introduces an energy gap in graphene, with a value that depends both on the number of removed atoms with respect to the total number of atoms in pristine graphene and on the specific shape of the holes and geometry of the antidot lattice [14]–[20]. Here we present our approach to the investigation of the transport properties of graphene antidot lattices and the results we have obtained as a function of different geometric parameters.

II. NUMERICAL METHOD

We have performed a generalization of the envelope-function based code that we have previously developed [21], [22] and applied [23], [24] for the simulation of transport in armchair ribbons with a generic potential. In analogy with what we have previously done for the simulation of 2DEG-based structures [25], [26], the device is divided into a series of sections; then the scattering matrices coupling adjacent sections are computed and composed in order to obtain the total transmission through the device. Since an exact treatment of the boundary conditions at the edges of the antidots would require considering sections with a length of the order of the interatomic distance, thereby making the problem computationally very complex, here we have chosen to simulate the effect of the antidots by introducing a space-dependent term $m(\vec{r})v_F^2$ ($m$ is a mass, $\vec{r}$ is the position, and $v_F$ is the graphene Fermi velocity) into the envelope function (Dirac) equation [27], [28]. This term is assumed equal to zero outside the antidots and equal to a value much larger than the considered injection energies inside the antidots, in such a way as to prevent charge carriers from entering the antidots [29], [30]. While this approach neglects the valley mixing introduced by the antidots, it has been shown that, in the absence of extended zigzag edges (along which it would not be able to reproduce the localized edge states), it provides a good representation of the main transport properties at low energies [17]. More in detail, we divide the $\tilde{W}$-wide ribbon into a cascade of transverse sections, in each of which both

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the potential (which in the present simulations is assumed as null inside the ribbon) and the mass term can be approximated as longitudinally constant. Within a section, each of the four envelope functions of graphene can be expressed as a transversally confined function \( \Phi(y) \) multiplied by a plane wave propagating in the longitudinal direction \( x \) with wave number \( k_y \). We can then compute enforcing the continuity at the interface the Dirac equation with the Dirichlet boundary conditions enforced at the edges of the armchair ribbon. In particular, we have solved this eigenproblem [with periodic boundary conditions for \( e^{-i k_y \varphi(y)} \)] in the reciprocal domain, obtaining the longitudinal wave vectors \( k_y \) and the Fourier coefficients of the transverse components \( \Phi(y) \). We have numerically observed that the \( Z_2 \times Z_2 \) symmetry in the Gauss plane of the wave vectors \( k_y \), valid in the absence of the mass term [31], is preserved also when a nonzero mass term is present. Once we have solved the Dirac equation in each section, the scattering matrices which relate adjacent sections can be computed enforcing the continuity at the interface of the wave function on the two graphene sublattices. This can be done efficiently in terms of the Fourier coefficients projecting the continuity relations on a proper basis of sines. In all the calculation a sufficiently large number of modes has to be considered, in order to properly reproduce the envelope functions in the regions where the presence of holes divides the ribbon into several decoupled channels in parallel. Finally, by composing all the scattering matrices, we can obtain the transmission matrix and, from it, the conductance \( G \) of the graphene ribbon using the Landauer-Büttiker approach.

\[
\begin{align*}
\left\{ \begin{array}{l}
(\sigma_y \partial_y + \sigma_y f(y) - i \sigma_y q(y)) \varphi(y) = -k_y \varphi(y) \\
- (\sigma_y \partial_y + \sigma_y f(y) - i \sigma_y q(y)) \varphi(y) = -k_y \varphi(y) \\
\varphi(0) = \varphi'(0) \\
\varphi(\bar{W}) = e^{2ikW} \varphi'(W),
\end{array} \right.
\end{align*}
\]

where \( \sigma_x, \sigma_y \) and \( \sigma_z \) are the Pauli matrices, \( \sigma = d/dy \), \( f(y) = U(y) - E/\gamma \) (\( U \) is the potential energy, assumed to be zero in the present simulation, \( E \) is the injection energy, \( \gamma = v_F \hbar \) with \( h \) the reduced Planck constant), \( q(y) = m(y)v_F^2/\gamma \). If we define the following function over the domain \([0, \bar{W}]\):

\[
\varphi(y) = \begin{cases} 
\varphi(y), & y \in [0, \bar{W}] \\
 e^{2ikW} \varphi'(2\bar{W} - y), & y \in [\bar{W}, 2\bar{W}],
\end{cases}
\]

the system can be rewritten in this form:

\[
\begin{align*}
\left\{ \begin{array}{l}
\left( \partial_y \sigma_z + \tilde{f}(y) \sigma_y \right) \varphi \varphi(y) = -k_y \varphi(y) \\
e^{-2ikW} \varphi(2\bar{W}) = \varphi(0),
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where \( \tilde{f}(y) = f(\bar{W} - W - y) \) and \( \tilde{q}(y) = q(\bar{W} - W - y) \).

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Fig. 2. Behavior of the conductance \( G \) of the normalized conductance of the ribbon with the antidot lattice represented in Fig. 1 (with \( d = 200 \) nm and \( r = 50 \) nm). Inset: behavior of the energy gap (identified here as the region around the zero energy where \( G/G_0 < 0.02 \)) as a function of the radius of the antidots for a square antidot lattice with \( d = 200 \) nm.

Fig. 3. Behavior, as a function of the injection energy \( E \), of the normalized conductance of the ribbon with the antidot lattice represented in Fig. 1 (with \( d = 200 \) nm and \( r = 50 \) nm), reported for a wider range of positive energies.

III. NUMERICAL RESULTS

We have focused on the transport properties of a regular square lattice of circular antidots (with radius \( r \) and a distance \( d \) between the centers of the antidots) in a 600 nm wide and 800 nm long graphene ribbon, with 4878 dimer lines across its width (see Fig. 1).

We have first studied the behavior of the conductance of the ribbon as a function of the injection energy with and without an antidot lattice with \( d = 200 \) nm and \( r = 50 \) nm (see Fig. 1). In the absence of the antidot lattice the ribbon has an energy gap \( E_g = 2g \pi/(3W) \approx 2 \) meV. We observe that, as expected, the antidot lattice leads to a suppression of the conductance, in particular increasing the band gap \( E_g \) around zero energy (see Fig. 2).

In Fig. 3 we report, with less resolution, the behavior of the conductance over a wider range of positive energies.

In the inset of Fig. 2 we show, for the square antidot lattice with \( d = 200 \) nm, the energy gap as a function of the antidot radius. In the regions in which the gap differs from that of the pristine ribbon, this behavior is approximately linear, as
long as the antidots are sufficiently small.

In Fig. 4 we report the results of a more extensive analysis of the behavior of the energy gap as a function of the main geometric parameters of the antidot lattice. In Fig. 4(a) we show the dependence on the radius of the antidots for a square antidot lattice with \( d = 100 \) nm. In Fig. 4(b)-(d), instead, we keep the radius of the antidots constant at 15 nm and we analyze the dependence of the gap on the distance between the antidot centers. In detail, in Fig. 4(b) we consider a square lattice of antidots and we report the behavior of the gap as a function of the distance \( d \) between the antidot centers. Instead, in Fig. 4(c) and (d) we consider rectangular lattices with distances between the antidot centers equal to \( d_x \) and \( d_y \) along the transport and transverse direction, respectively (Fig. 1). In Fig. 4(c) we consider a constant \( d_y = 100 \) nm and we study the dependence of the gap on \( d_x \), while in Fig. 4(d) we consider a constant \( d_x = 100 \) nm and we study the dependence of the gap on \( d_y \). In the regions in which the gap differs from the value of the pristine ribbon, its value is compatible with the dependence on \( \sqrt{N_{rem}/N_{tot}} \) (where \( N_{tot} \) is the total number of atoms of the pristine graphene ribbon, while \( N_{rem} \) is the number of atoms that have been removed introducing the antidot lattice) that has been reported in the literature for unconfined graphene [14], [15].

In Fig. 5 we show, for the antidot lattice with \( d = 200 \) nm and \( r = 50 \) nm, the value of conductance obtained as a function of the orientation \( \alpha \) (represented in the left inset of the figure) of the antidot lattice with respect to the longitudinal direction \( x \). We observe that, at least for the considered antidot lattice, the variation of the conductance (and also of the energy gap, as shown in the right inset of the figure) as a function of \( \alpha \) is rather small.

In Fig. 6 we report, for a fixed distance \( d = 100 \) nm between the antidot centers (see the inset of the figure), the value of the conductance of the ribbon as a function of the antidot radius \( r \): starting from the value characteristic of the pristine ribbon (for \( r = 0 \)), the conductance decreases towards zero (value which is obtained when the antidots coalesce and physically isolate the input and output leads).

Finally, in Fig. 7 we simulate the effect on the conductance of an antidot lattice of finite extension. In particular, we consider a rectangular lattice of circular antidots with \( d = 100 \) nm and \( r = 25 \) nm and we examine how the
Conductance varies as a function of the number of antidot columns. We find that for a single column the conductance is approximately half of that for the pristine ribbon (because, for the values of \(d\) and \(r\) that we are considering, the antidots make about one half of the ribbon cross section inaccessible to charge carriers). Increasing the number of antidot columns, the value of the conductance is further decreased, until an asymptotic value is reached for about 6 columns.

IV. CONCLUSIONS

We have simulated transport in graphene antidot lattices, with a code based on the solution in the reciprocal space of the envelope function equation (with a sufficiently large mass term mimicking the effect of antidots) and on a scattering matrix approach for the evaluation of the overall transmission. This model, although approximate, is numerically very efficient and allows the simulation of large graphene samples, for which atomistic methods are impractical. The presence of antidots widens the energy gap and suppresses the conductance of the ribbon, which depends strongly on the antidot density, but weakly on the angular orientation of the antidot lattice.

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