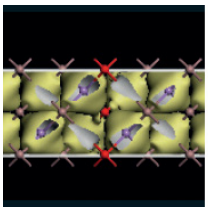

Effect of disorder on the band gap of a graphene ribbon with an antidot lattice

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The absence of an energy gap represents the main obstacle to the application of graphene for the fabrication of digital electronic devices. The introduction of a regular lattice of holes (antidots) in addition to lateral confinement is among the methods that have been proposed to introduce an energy gap in graphene. We have studied the dependence of the energy gap of a graphene ribbon with an antidot lattice on geometrical parameters [1], adopting a numerical approach based on the solution of the envelope-function (Dirac) equation, where a nonzero mass term is used to emulate the presence of the antidots. We have solved the transport problem with a scattering matrix approach and, from the resulting behavior of the conductance as a function of energy, we have obtained the transport gap, defined as the energy interval around zero where the conductance is lower than a given threshold. This simplified approach has been shown to give good results, as far as no extended zigzag edges exist at the boundaries of the antidots. We have found that, when the geometry of the structure is such that the presence of the antidots introduces a gap larger than that generated by lateral confinement, the dependence of this gap Eg is analogous to that previously observed for unconfined graphene [2], i.e. $E_g x \sqrt{N}_{rem} / N_{tot}$, where Nr_{em} and N_{tot} are the number of carbon atoms that have been removed from the unit cell of the antidot lattice to create the antidot itself, and the number of the atoms that were originally present in the unit cell, respectively. Envelope-function calculations indicate that the transport gap is preserved also when the regularity of the antidot lattice is broken by the presence of disorder, for example in the position of the antidots. Here we report the results for a ribbon with a hexagonal lattice of antidots, each with a hexagonal shape and armchair edges (Fig. 1). In Figs. 2 and 3 we show that the transport gap is enlarged by the presence of the antidots, for a 10.224 nm long and ~6 nm wide ribbon with 47 and 48 dimer lines across its width, and thus with a metallic and semiconducting behaviour, respectively. A random longitudinal and transverse shift of the antidots from their ideal position by a quantity uniformly distributed in the range [-0.25 nm, 0.25 nm] leaves the transport gap unchanged (Fig. 2). In order to verify whether an actual energy gap exists in the presence of disorder, we have performed a nearest-neighbor tight-binding calculation of the dispersion relations, considering only the $2p^z$ orbital for each carbon atom, with a transfer integral equal to -2.7 eV and disregarding edge-bond relaxation effects (in order to make this tight-binding calculation feasible, here we have considered much narrower nanoribbons with respect to Ref. [1]). Since the calculation has to be performed also for the disordered structure, we have considered a unit cell with the same length as the entire ribbon, assuming to replicate it periodically in the longitudinal direction. The results for the metallic and semiconducting ribbons without the antidots are shown in Fig. 4, while in Figs. 5 and 6 we compare (for the metallic and semiconducting ribbon, respectively) the dispersion relations obtained in the absence and in the presence of disorder. We observe that the presence of disorder strongly decreases the energy gap. We conclude that the transport gap observed for the disordered case in Figs. 2 and 3 is not always a true energy gap (i.e. an energy interval without any available state), but instead a region where strong (Anderson) localization [3] plays a major role: as a consequence of disorder in the antidot position, the states in the structure become localized and transport through the ribbon is quenched, with a corresponding suppression of the device conductance.

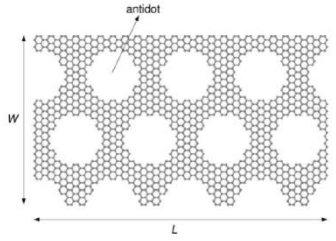

Fig. 1. Graphene ribbon with antidot lattice. The considered antidots have an hexagonal shape, with a 0.99 nm edge and a distance between the centers of neighboring antidots of 2.55 nm.

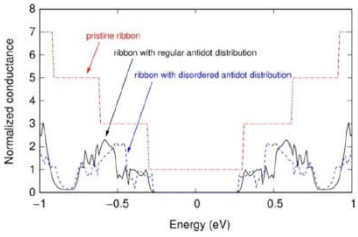

Fig. 2. Behavior of the conductance (normalized with respect to the conductance quantum) as a function of energy for the metallic ribbon, in its pristine form, with a regular antidot distribution, and with a disordered one.

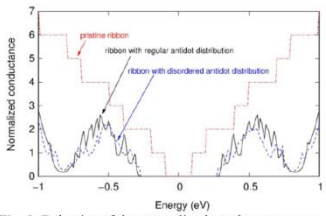

Fig. 3. Behavior of the normalized conductance as a function of energy for the semiconducting ribbon, in its pristine form, with a regular antidot distribution, and with a disordered one.

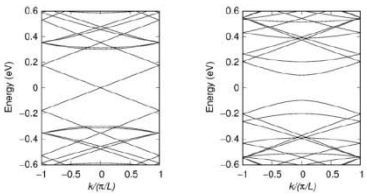

Fig. 4. Dispersion relations around zero energy for the metallic (left panel) and semiconducting (right panel) ribbon without antidots.

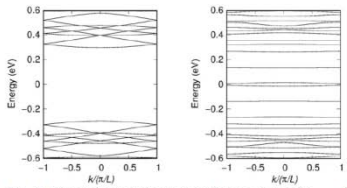

Fig. 5. Dispersion relations around zero energy for the metallic ribbon with a regular (left panel) and disordered (right panel) distribution of antidots.

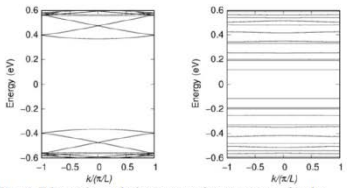

Fig. 6. Dispersion relations around zero energy for the semiconducting ribbon with a regular (left panel) and disordered (right panel) distribution of antidots.

[1] P. Marconcini et al, IEEE Trans Nanotechnol (2016),DOI: 10.1109/TNANO.2016.2645663
[2] T. G. Pedersen et al., Phys. Rev. Lett. 100, 136804 (2008)
[3] P. W. Anderson, Phys. Rev. 109, 1492 (1958)