Effect of zigzag and armchair edges on the electronic transport in single-layer and bilayer graphene nanoribbons

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We have studied the transmission properties of mono- and bilayer grapheme nanoribbons with defects focusing on the role of the edge termination (zigzag vs armchair). Using the standard tight-binding model of p-orbital electrons on a hexagonal lattice we have developed an analytical approach based on the Green's function technique and the Dyson equation for calculation of the transmission coefficient of monolayer grapheme nanoribbons with a single short-range defect. Calculation of the conductance in monolayer graphene nanoribbons with many defects and calculations for bilayer graphene nanoribbons are performed numerically on the basis of the tight-binding recursive Green's function technique. The principal conclusions of our work (see [1]) can be summarized as follows:

1. For the case of the zigzag edge termination, both monolayer and bilayer nanoribbons in a single- and a few-mode regime remain practically insensitive to defects situated close to the edges (fig.1 (a), (c), fig.2 (a), (c)). This remarkable behavior is related to the effective boundary condition at the zigzag edges which do not couple valleys, thus prohibiting the intervalley scattering due to short-range defects situated close to the edges. In contrast, the armchair edges mixes the valleys; as a result, the conductance of both monolayer and bilayer nanoribbons is strongly affected by even a small defect concentration at the edges (fig.1 (b), (d), fig.2 (b), (d)).

2. For higher electron energies in the many-mode regime, the difference of the transmission between the armchair and zigzag ribbons diminishes and for sufficiently high defect concentration they become equally sensitive to the edge disorder (fig. 2).

3. Both monolayer and bilayer nanoribbons with a short-range defect show resonant features in the lowest energy mode (fig.1). Resonances are identified to be of Fano type and emerge from the interference between the quasi-bound localized state around the defect and the extended state in the ribbon. We consider four different cases of a defect in (a) zGNR, (b) zBGN, (c) aGNR, and (d) aBGN. We discuss in detail how the interplay between the defects position at different sublattices in the ribbons, defect distance to the edge and the structure of the extended states in ribbons with different edge termination influence the width and the energy of Fano resonances.

References

[1] A. Orlof, J. Ruseckas, I. V. Zozoulenko, Phys. Rev. B, **88** (2013) 125409.

Figures

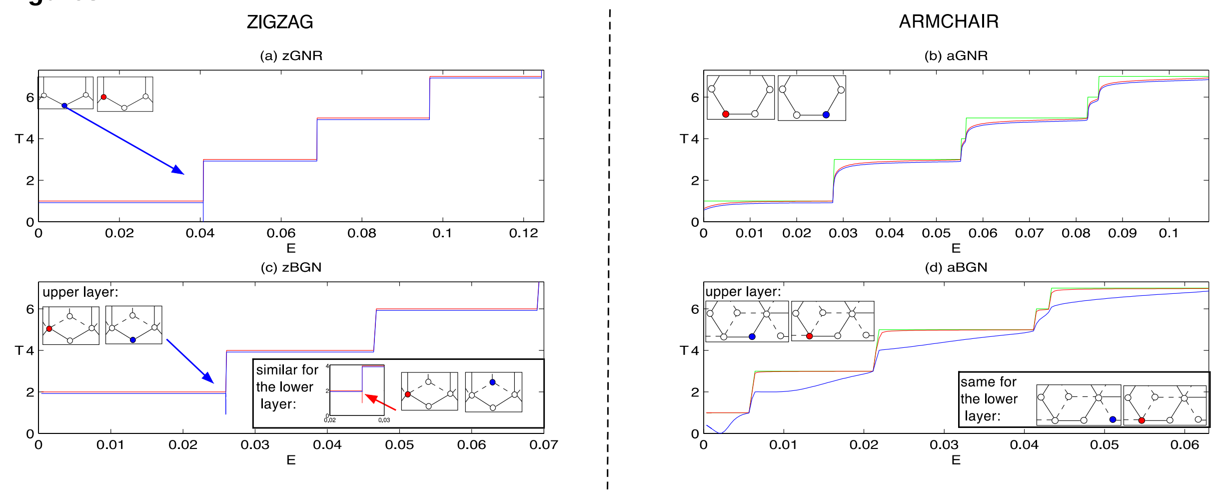

Figure 1. Transmission of the monolayer (a),(b) and bilayer (c), (d) nanoribbons with a single defect at the edge as a function of the energy. Insets indicate defect positions and correspond to the curve color. Green curves indicate the transmission probability for ideal nanoribbons (without defects).

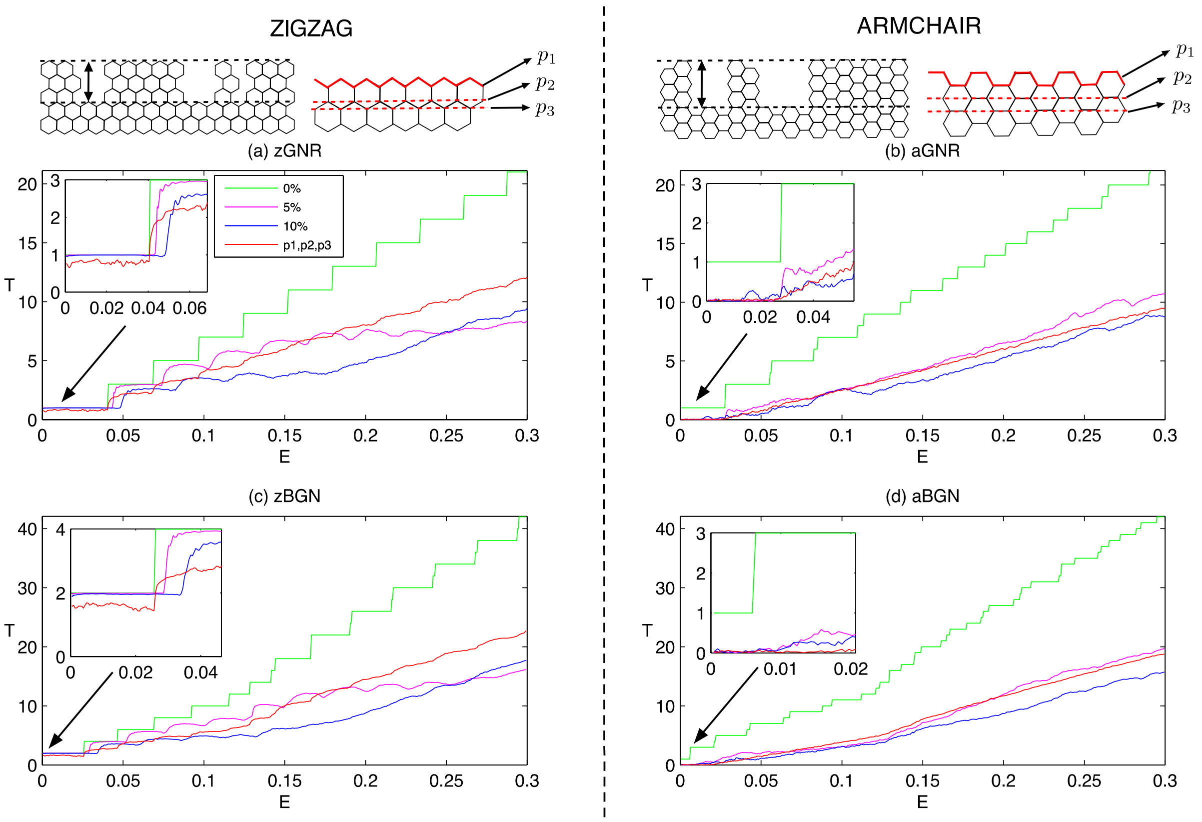

Figure 2. Transmission of monolayer (a), (b) and bilayer (c), (d) nanoribbons with disordered edges. Top insets illustrate two disorder models. Green curves indicate the transmission probability for ideal nanoribbons, red for nanoribbons with edge disorder of model p_1, p_2, p_3, the remaining curves are the result of the rectangular edge disorder sketched in the inset.