Atomistic effects in graphene antidot lattices: influence of lattice symmetry and hole edges on electronic structure and transport properties

Antti-Pekka Jauho[1,2], Tue Gunst[1], Rene Petersen[3], Troels Markussen[4], Mads Brandbyge[1], and Thomas Garm Pedersen[3]

[1]Dept. of Micro and Nanotechnology, DTU Nanotech, DTU, DK-2800 Lyngby, Denmark
[2]Dept. of Applied Physics, Aalto University, P.O. Box 11100, FI-00076 AALTO, Finland
[3]Dept. of Physics and Nanotechnology, Aalborg University, DK-9220 Aalborg East, Denmark
[4]Dept. of Physics, DTU Fysik, CAMD, DK-2800 Lyngby, Denmark
Antti-Pekka.Jauho@nanotech.dtu.dk

Antidot lattices defined on graphene (GAL) have been promoted as a flexible platform for creating a tunable band gap thereby possibly allowing the realization of a number of technological applications [1]. The antidot lattice can be viewed as a regular nanoperforation of the pristine graphene sheet. Theoretically the properties of triangular GALs have been examined already quite substantially (e.g., optical properties [2], excitons [3], electronic properties [4,5], electron-phonon coupling [6], detection of edge states [7], or details of band gap scaling [8]). Most importantly, the experimental techniques for fabricating GALs have evolved rapidly [9-11], presently reaching lattice constants of a few tens of nanometers, where many of the interesting quantum mechanical effects predicted by theory should become visible.

GALs may be designed in many different ways, as far as their microscopic structure is concerned. Here we report results for two specific aspects: (i) the effect of the symmetry of the antidot lattice, and (ii) the effect of the atomic arrangement at the edge of the etched holes.

(i) The block-copolymer technique for fabricating GALs [10,11] may yield many different lattice symmetries. Our calculations show, perhaps surprisingly, that only one-third of the rotated triangular or rectangular lattices lead to sizable band gaps (Figure (A), middle and bottom panels) while all triangular lattices display a gap (Figure (A), top). An explanation of these regular patterns of the gap formation can be given based on *Clar structures* [13]: structures allowing a full benzenoid structure are most stable (triangular structures belong to this class, while only one-third of rotated triangular or rectangular lattices do so), and therefore display a sizable gap. A full discussion will be given soon [12].

(ii) In view of possible thermoelectric applications, it is of interest to examine how the electronic and phonon transmission properties of graphene samples are affected by embedded GALs, and, in particular, whether the details of the hole edges have a significant effect. In Figs. (B) and (C) we report such a study; full details will be discussed soon [14]. Remarkably, the structure where the holes have a zigzag edge displays an additional splitting up of the GAL minibands (top panel in (B), inset), while a similar armchair structure does not (bottom panel in (B), inset). This can be traced to the much more pronounced structural relaxation that takes place in the structure with zigzag holes [14]. The GAL suppresses both electronic transmission and the phonon transmission ((B) and (C); respectively), however for phonons the reduction in transmission is much stronger which in turn leads to an enhancement in ZT, the thermoelectric figure of merit. In some of our simulations we have recorded ZT's approaching one-half – rather remarkable for graphene-based structures which usually have an exceedingly low ZT due to the high intrinsic heat conductivity.

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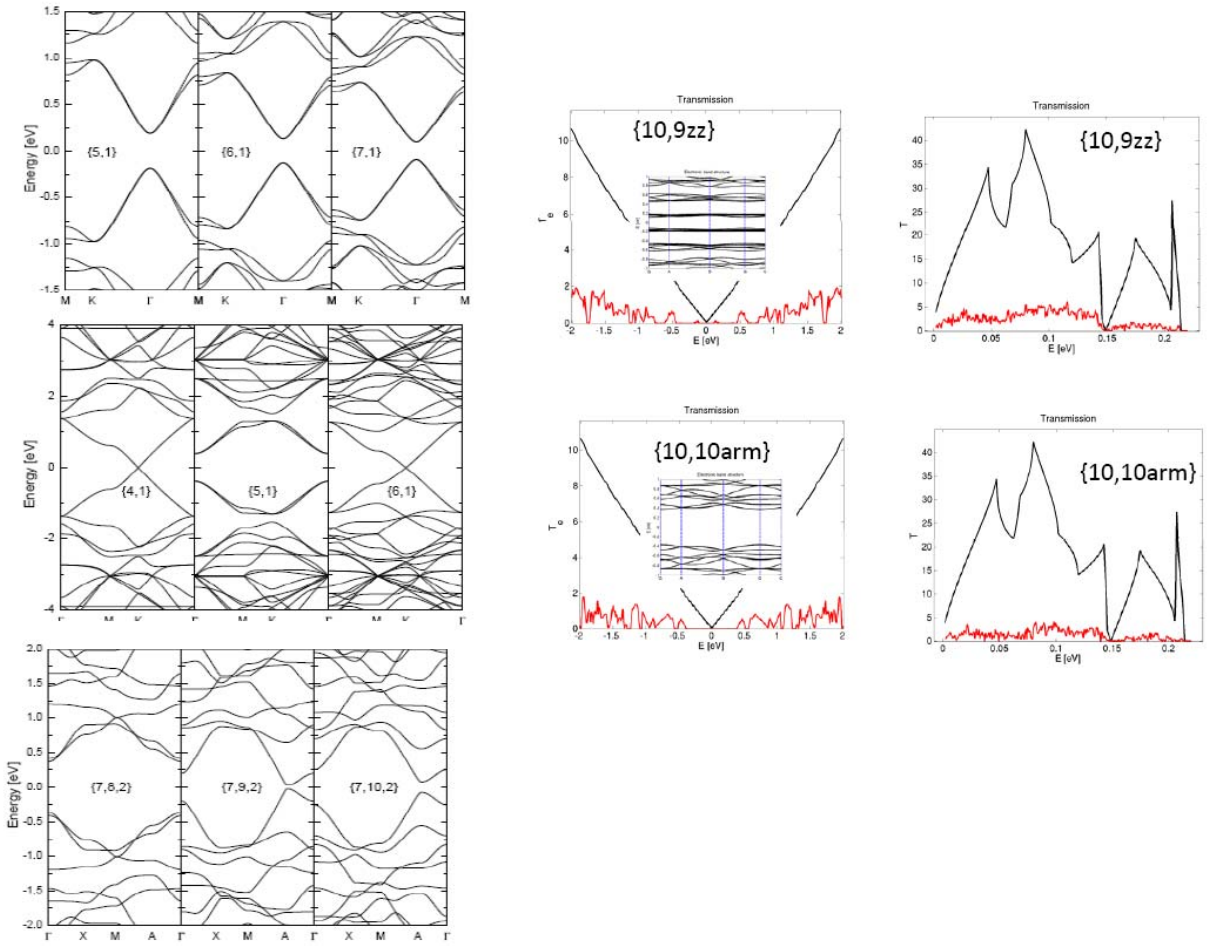
Figures



(A) (B) (C)

Figure caption. (A) Band structures for triangular (top), rotated triangular (middle), and rectangular (bottom) GALs. The insets define the details of the respective lattice structures [12]. (B) Electronic transmission for graphene samples with zigzag (top) and armchair (bottom) holes, red curve. The insets show the electronic bandstructures. (C) Phonon transmission for the geometries in (B). The black curves in (B) and (C) give the pristine electronic and phonon transmissions, respectively.