Thermoelectric properties of finite graphene antidot lattices

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GRAPHENE ANTIDOT LATTICES

Graphene antidot lattices (GALs) have been proposed as a flexible platform for creating a semiconducting material with a tunable band gap controlled by the hole dimension. The regular nanoperforation of a graphene layer may therefore be a promising system in future electronic applications [1]. A selection of different fabrication techniques exists for creating this nanostructured system [2], [3].

It is interesting to examine how the electron and phonon transport properties are affected by an embedded GAL [6], e.g. in terms of thermoelectric applications. Thermoelectric materials conduct electricity very well while the heat conduction is poor. They can be used for applications including power generation and refrigeration among others. Promising candidates for future thermoelectric devices within nanotechnology include passivated silicium nanowires [4] and edge disordered graphene nanoribbons [5]. Graphene cannot by itself be used for thermoelectric applications. Its efficiency in transforming heat into charge current is limited by its very high ability to conduct heat, exceeding that of copper. The device efficiency is quantified by the dimensionless figure of merit $ZT = S^2 G_e T/\kappa$, where high ZT implies a good thermoelectric. We thus seek a high electronic power factor, $S^2 G_e$, and minimal both electron and phonon thermal conductance $\kappa = \kappa_{ph} + \kappa_e$, to maximize the thermoelectric efficiency at an average temperature T and chemical potential μ.

THERMOELECTRIC PROPERTIES

We consider a GAL of finite length between two graphene leads, Fig. 1,2. Both the electronic and thermal properties converge fast toward that of the corresponding infinite GAL within only ≈ 6 repetitions of the device unitcell. This is illustrated in Fig. 3 for the electron transmission where M is the number of unitcell repetitions between the leads. The present calculations indicate that drilling a periodic lattice of nanosized holes in graphene could modify the thermal conductance substantially such that thermoelectric applications in principle could be possible (Fig. 4). It is indeed surprising that an almost ideal thermal conductor can be used as a basis for thermoelectric components (Fig. 5). Our simulations predict that not only does the nanoperforated graphene provide flexible control of the electronic transport gab, it is also a platform for thermal management and thereby reveals several routes to increased thermoelectric efficiency. These promising findings calls for further investigations of GALs as thermoelectric devices, perhaps as an integrated element in future graphene nanoelectronics.

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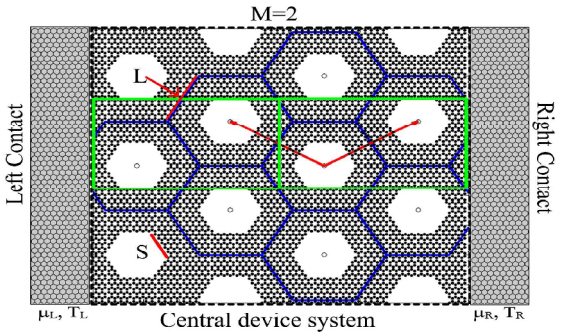

Fig. 1. System setup showing a finite GAL between two graphene leads. The number M of rectangular device unit cells (green rectangle) is varied in the simulations. The depicted system is a $\{L,S\}$=$\{10,5zz\}$ GAL with a length of 2 ($M = 2$) corresponding to 4 holes in the direction of transport. The label zz here indicates that the holes have zigzag edges and not armchair (arm) or mixed circular (cir) edges.

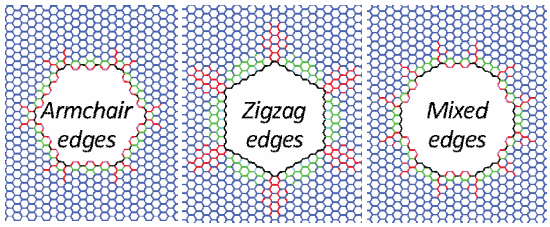

Fig. 2. Different edgetypes considered in the transport simulations. We find that atomistic effects results in an additional splitting of the GAL electronic minibands for zigzag edges as compared to armchair edges. This is a result of the localization of electron states at zigzag edges. The colors in thefigure shows where the bond distance is changed after relaxation compared to the nearest neighbour distance in graphene (blue).

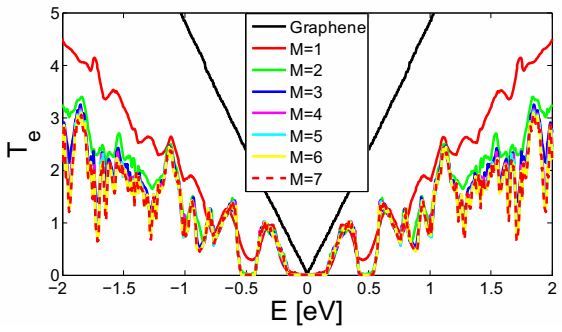

Fig. 3. Convergence with length (M, the number of unit cells with two holes along the device) of the electron transmission for a $\{10,3arm\}$ antidot lattice.

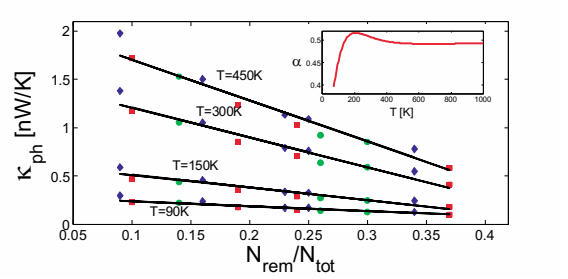

Fig. 4. Phonon thermal conductance as a function of hole dimension given as the ratio of atoms removed from the perfect graphene device cell. The red squares, blue diamonds and green circles label holes with armchair, zigzag and circular/mixed edges respectively. Four different temperatures are plotted for each system and the thermal conductance is decreasing almost linearly in the shown region. The thermal conductance at these four temperatures is for pristine graphene found to be $[8.5,6.1,2.6,1.2]\,\frac{\mathrm{nW}}{\mathrm{K}}$.

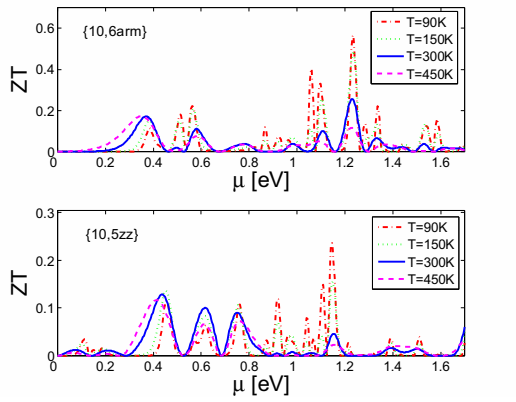

Fig. 5. ZT for $\{10,6arm\}$ and $\{10,5zz\}$ lattices at the four temperatures $[450,300,150,90]$ K. At low temperature many sharp transmission features also becomes visible inZT. Hexagonal holes with pure armchair edges lead to a larger ZT as compared to pure zigzag edges. This is a consequence of the localization of states, which predominantly occurs for zigzag edges, since the increased splitting of the electronic minibands reduces the power factor.