Enhanced thermoelectric properties of in-plane 90°-bent graphene nanoribbons with nanopores

Alessandro Cresti[1]
Van-Truong Tran[2]
[1] *Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, IMEP-LAHC, F-38000 Grenoble, France*
[2] *IMPMC, Université Pierre et Marie Curie (UPMC), Sorbonne Universités, F-75252 Paris Cedex 05, France*
alessandro.cresti@grenoble-inp.fr

Thermoelectric generators allow the harvesting of heat and its conversion into electric power. They are thus of central importance for emerging technologies such as autonomous sensors and internet of things. Graphene is interesting for this kind of applications thanks to its high electric conductivity, its high melting point and the possibility to be nanostructured.
In particular, graphene nanoribbons are promising because of their reduced thermal conductance, in addition to be basic elements of the graphene-based nanoelectronics.
In this contribution, we focus on planar graphene nanoribbons with a 90°-bent section where nanopores have been included, see figure 1. By numerical simulations based on atomistic models and the Green's function method, we show that the thermal conductance is significantly decreased (more than one order of magnitude) by the pores and the bending, while the presence of a transport gap allows a large Seebeck coefficient [1]. As a consequence, at a temperature of 500 K, the figure of merit *ZT* can reach the value of 0.88, with an improvement of about 200% compared to straight nanoribbons without nanopores. For temperatures above 1000 K and in the presence of a large number of nanopores (up to 24 in our simulations), *ZT* can reach the unit value and above, see figure 2.
Physical analyses of electron conductivity, Seebeck coefficient and phonon and electron thermal conductance are performed for different nanoribbon geometries, numbers of nanopores and symmetry of the contacts.

References

[1] Van-Truong Tran and Alessandro Cresti, Nanotechnology, 32 (2021) 395401

Figures

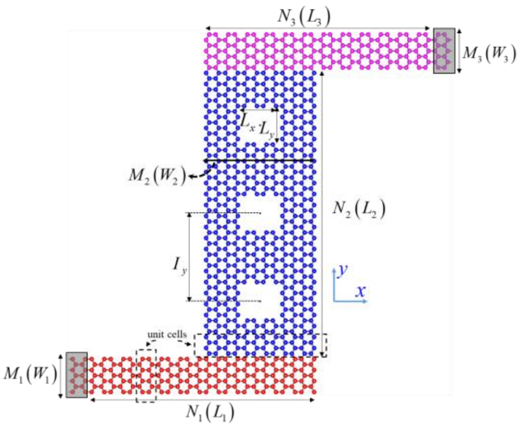

Figure 1: Sketch of a 90⁰-bent graphene nanoribbon composed of two horizontal armchair-edge sections and a vertical zigzag-edge section with nanopores.

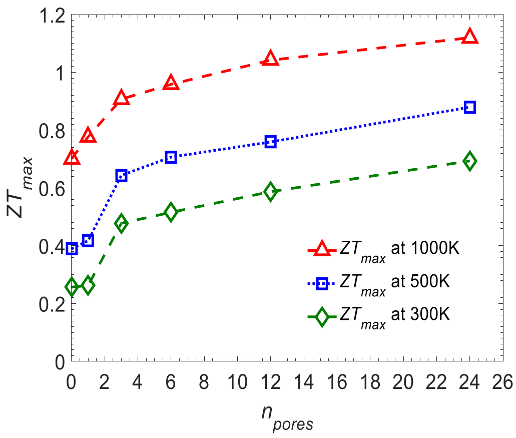

Figure 2: Maximum *ZT* as a function of the number of nanopores at different temperatures. The size of the nanopores is $L_x = L_y \approx 0.71$ nm. Other dimensions: $W_1 = W_3 \approx 0.74$ nm, $W_2 \approx 2.41$ nm, L_2 varies with the number of nanopores.