Thermoelectric optimization of nanostructured graphene ribbons using Green's function method

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ABSTRACT

Using NEGF simulation, a strategy to enhance the figure of merit ZT in GNRs is proposed. The dependence of electronic and thermal transport on GNR edge orientation is explored and exploited to suggest a GNR structure with higher ZT values compared to the perfect armchair (AGNRs) and zigzag (ZGNRs) nanoribbons.

INTRODUCTION

In addition to the excellent and fascinating electronic transport properties of graphene layers [1], much attention has been recently focused on thermal [2] and thermoelectric [3] properties of graphene nanostructures. The promising results obtained for two-dimensional sheets of graphene [4] have suggested also exploring thermoelectric properties of one-dimensional structures as graphene nanoribbons (GNRs). Recently, it has been predicted that the thermoelectric figure of merit ZT can exceed unity in honeycomb chains of carbon atoms [5] and also in long rough edge GNRs [6]. However, detailed information on the potential of short GNRs to provide a high factor of merit is still missing.

MODEL

In the analyzed ribbons, the figure of merit ZT, defined by the expression $T.G_e.S^2/K$ is evaluated by solving both the electron and phonon transport equations [7]. The simulation of electron transport provides the thermopower S, the electronic conductance G_e and the electron contribution to the thermal conductance K, while the simulation of phonon transport gives access to the phonon contribution to the thermal conductance. Charge transport simulation in GNRs was performed using the non-equilibrium Green's functions (NEGF) formalism coupled with the Landauer formula. An atomistic nearest-neighbor tight-binding Hamiltonian was used to model the ribbons [6]. The NEGF formalism has been applied also to the phonon transport problem within a fifth nearest-neighbors force-constant model [7].

DISCUSSION

The electron transport properties of Mixed GNRs are strongly dependent on the fraction of armchair edges and zigzag edges. In such MGNRs, the presence of armchair edges induces a band gap opening, and the presence of zigzag edges induces edge-localized electron states. Hence, the armchair edge sections can be seen as barriers for the localized zigzag edge states. This interpretation is confirmed by the resonant oscillation of the electronic conductance and the positive values of the thermopower, which is a classical behavior of multi-barrier channels [8]. In addition to this resonant tunneling effect, MGNRs exhibit very low thermal conductance compared to perfect AGNRs or ZGNRs. The phenomenon is probably due to the mismatch of phonon modes between AGNR and ZGNR portions.

The optimized structure suggested here is built by alternating ribbons with different edge orientations and different widths as schematized in Fig. 1. For this structure, the I-V curves obtained for different temperature gradients applied to the contacts are shown in Fig. 2. At room temperature, an electronic power of about 10nW can be generated by applying a thermal gradient of 300 K.

This structure exhibits ZT values exceeding unity at room temperature, as shown in Fig. 3. It takes advantage from both electron resonant phenomenon and thermal conductance suppression. The phonon mode mismatch between the AGNR and ZGNR sections strongly reduces the thermal conductance while the electron conductance is preserved thanks to the resonant tunneling of electrons via the localized states present in this periodic structure.

CONCLUSION

The suggested structure built by alternating ribbons with different edge orientations and different width (Mixed-GNR) paves the way of promising thermoelectric applications based on graphene nanostructures.

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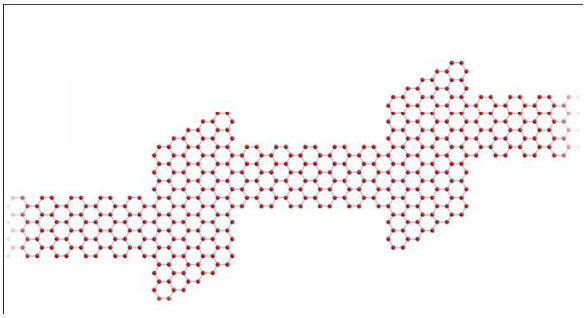

Fig. 1 Mixed GNR structure optimized to provide high ZT.

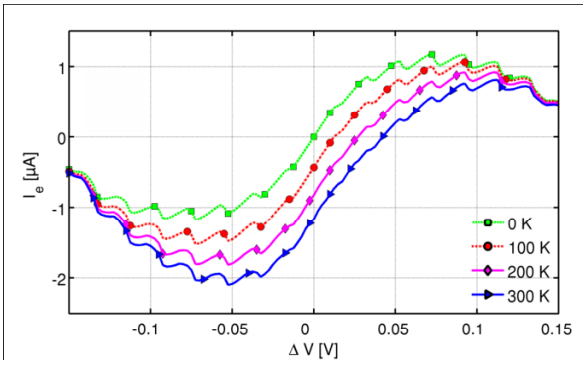

Fig. 2. Electronic current as a function of bias voltage for different temperature gradients between the contacts.

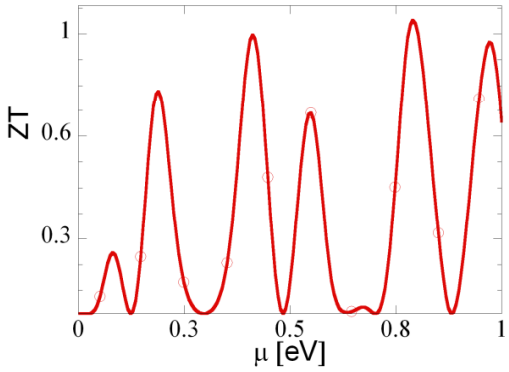

Fig. 3. Thermoelectric factor ZT as a function of the chemical potential μ at room temperature.