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Ballistic thermoelectric properties in double-bend graphene nanoribbons

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ABSTRACT

Ballistic thermoelectric properties in double-bend graphene nanoribbons (GNRs) are investigated by using the nonequilibrium Green's function. We find that due to the elastic scattering caused by the interface mismatching, the thermal conductance contributed by phonons is greatly reduced, while ballistic transport behaviors for electrons are dramatically demolished, and even some gaps can be opened at antiresonance energies. Near these antiresonance gaps, the maximum value of ZT (ZT_{max}) can be observed, much larger than that for straight GNRs. Moreover, this ZT_{max} can be effectively tuned by modulating the length or width of double-bend GNRs.

1. Introduction

The thermoelectric (TE) materials as one key for sustainable and clean energy solution have attracted an increasing interest since the world's demand for energy rapidly increases while fossil fuel supplies decrease [1]. The energy-conversion efficiency of TE devices is determined by the dimensionless figure of merit $ZT = GS^2T/(\kappa_{el} + \kappa_{ph})$ [2–4], in which G is the electronic conductance, S is the Seebeck coefficient, T is the absolute temperature, $\kappa_{el(ph)}$ is the electronic (phonon) thermal conductance, and GS^2 is usually defined as the power factor. The larger ZT is, the better is the performance of a TE material. So a promising TE material should simultaneously have the high power factor and low thermal conductance. In order for TE materials to become competitive with conventional refrigerators and generators, a large increase of ZT is imperative. For conventional bulk materials, however, it is found that optimizing ZT is a big challenge due to the strong interdependence among G, S, κ_{el}, and κ_{ph}: changing one often adversely alters the others [2]. Fortunately, recent progresses in nanofabrication technology have provided the possibilities to this important problem [5–7]. It has been demonstrated that nanomaterials or low-dimensional structures can dramatically enhance the ZT due to the suppressive thermal conductance caused by boundary scattering and increased power factor caused by the quantum confinement. Enhanced TE performance has been observed in these systems such as Bi_2Te_3/Sb_2Te_3 superlattices [5], PbSeTe/PbTe-based quantum dot superlattice [6], silicon nanowires [7–10], and so on.

Graphene, a recently discovered form of carbon, has drawn extensive attention due to its intriguing physical properties such as high intrinsic mobility [11], ballistic transport [12], and width-dependent band gap [13]. As the quasi-one-dimensional graphene nanostructures, graphene nanoribbons (GNRs) exhibit unique electronic and thermal transport properties [14–17], which can be tuned by modulating the edge shapes and geometric sizes. Recently, the TE properties in GNRs become a new focus due to the potential applications in the TE conversion [18–21]. Ouyang et al. report that the Seebeck coefficient in semiconductor GNRs is much higher than that in 2D graphene, indicating quasi-1D geometry can improve the TE performance of GNRs [21]. On the other hand, recent studies also show that GNRs have high thermal conductance dominated by phonons [22], which is detrimental to increase ZT. The natural question is whether it is possible to suppress high thermal conductances so that GNRs may be good candidates for TE performances. To this question, several ways have already been examined in order to increase ZT including the interface mismatching [23], structural defects [24], isotope modulation [25–27]. Recently, Sevincli et al. presented a study of the TE properties in edge-disordered GNRs, and found ZT can exceed 3 in the diffusive limit [28]. Mazzamuto et al. found the strongly enhanced TE properties exist in mixed GNRs consisting of alternate zigzag and armchair sections [29]. More recently, we also reported the enhancement of TE properties in GNRs modulated with stub structures due to the elastic scattering of stub structures [20]. In spite of these advancements above, a more comprehensive study

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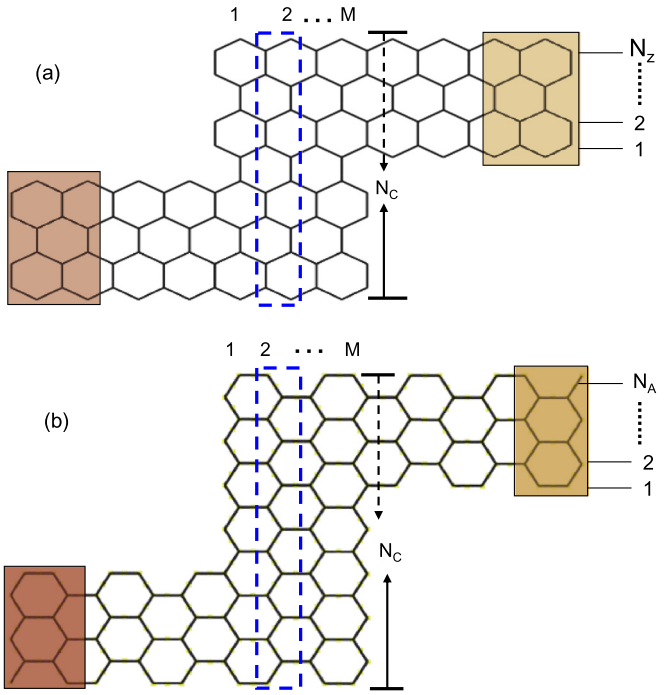

Fig. 1. Schematic diagram of the double-bend GNRs with the width N_C and length M (namely the number of the unit cell indicating by the rectangular frame). (a) and (b) correspond to double-bend ZGNRs with two leads' width N_Z and double-bend AGNRs with two leads' width N_A, respectively.

of understanding the electronic and phonon transport properties is still needed to well implement GNRs-based nanostructures in TE applications. Recently, Huang et al. presented a theoretical study of the acoustic phonon transmission and thermal conductance in double-bend nanowires, and found the thermal conductance is suppressed in such structures [30]. Furthermore, ballistic thermoelectricity in double-bend nanowires has been also explored, and a large Seebeck coefficient was obtained due to the quantum interference effect [31]. These two favorable aspects indicate that the TE performance can be improved in double-bend nanowires compared to straight nanowires. In the present work, we investigate the ballistic TE properties in double-bend GNRs. Such these structures can be easily realized by cutting mechanically exfoliated graphene, and are expected to exhibit many outstanding TE properties.

2. Model and formalism

We consider two typical structures shown in Fig. 1: (a) and (b) are double-bend zigzag GNRs (ZGNRs) and double-bend armchair GNRs (AGNRs) according to their edge shapes, respectively. Each structure consists of two semi-infinite leads with the width $N_Z(N_A)$ and the central double-bend junctions with the width N_C and the length M. It is assumed that the contacts between the two leads and reservoirs are perfect without any reflection, and the elastic scattering only occurs at mismatching interfaces in double-bend structures. Since it has been proven that both phonon–phonon and electron–phonon interactions are very weak in GNRs [32], we can assume that the electron and phonon transmissions travel ballistically and independently. For the electronic transport, in the linear-response limit, using the Landauer formalism we can introduce an intermediate function [8,9,19–21]

$$\mathcal{L}^{(m)} = \frac{2}{h}\int (E-\mu)^m\big[-\partial f(E,\mu,T)/\partial E\big]\tau_{el}(E)\,dE, \tag{1}$$

where $f(E,\mu,T)$ is the Fermi–Dirac distribution function, μ is the chemical potential, h is the Planck's constant, $\tau_{el}(E)$ is the electronic transmission coefficient. Then, the electronic conductance G, Seebeck coefficient S, and the electronic contribution to the thermal conductance κ_{el} can be conveniently expressed as [8,9,19–21]

$$G = e^2\mathcal{L}^{(0)}, \tag{2}$$

$$S = \frac{1}{qT}\frac{\mathcal{L}^{(1)}}{\mathcal{L}^{(0)}}, \tag{3}$$

$$\kappa_{el} = \frac{1}{T}\left[\mathcal{L}^{(2)} - \frac{(\mathcal{L}^{(1)})^2}{\mathcal{L}^{(0)}}\right], \tag{4}$$

where q is the electric charge of carriers, which is positive for holes and negative for electrons. Similarly within the Landauer formalism, the phonon contributions to the thermal conductance κ_{ph} can be given as [8,9,19–21]

$$\kappa_{ph} = \frac{1}{2\pi}\int_0^\infty \hbar\omega\big[\partial n(\omega,T)/\partial T\big]\tau_{ph}(\omega)\,d\omega \tag{5}$$

with $n(\omega,T)$ being the Bose–Einstein distribution function, $\tau_{ph}(\omega)$ being the phonon transmission coefficient. Apparently in the calculation of the ZT, a central issue is then to obtain both transmission coefficients $\tau_{el}(E)$ and $\tau_{ph}(\omega)$. Following the atomistic approach, in this work we apply the nonequilibrium Green's function to handle these two transmission coefficients in a parallel way. For the case of the electronic transport, the retarded Green's function of double-bend structures is given by [33,34]

$$\boldsymbol{G}^r = \big(E\boldsymbol{I} - \boldsymbol{H} - \boldsymbol{\Sigma}_L^r - \boldsymbol{\Sigma}_R^r\big)^{-1}, \tag{6}$$

where $\boldsymbol{\Sigma}_{L(R)}^r$ is the retarded self-energy coupling with the left (right) electrode, which can be calculated by using the Sancho–Rubio iterative method [35], and the Hamiltonian $\boldsymbol{H}$ is describe by a simple nearest-neighbor tight binding model [36]. Following the conventional procedure, the electronic transmission coefficient can be expressed as

$$\tau_{el}(E) = \mathrm{Trace}\big(\boldsymbol{G}^r\boldsymbol{\Gamma}_L\boldsymbol{G}^a\boldsymbol{\Gamma}_R\big) \tag{7}$$

with the broadening function $\boldsymbol{\Gamma}_{L(R)} = i[\boldsymbol{\Sigma}_{L(R)}^r - \boldsymbol{\Sigma}_{L(R)}^a]$ and $\boldsymbol{G}^a = (\boldsymbol{G}^r)^\dagger$. Similar equations hold for the phonon transmission only with the substitutions $\boldsymbol{H}\to\boldsymbol{K}$ and $E\boldsymbol{I}\to\boldsymbol{M}\omega^2$, where $\boldsymbol{M}$ is the diagonal mass matrix, ω is the phonon frequency, and $\boldsymbol{K}$ is the dynamical matrix constructed using the fourth nearest-neighbor force constant model [37].

3. Results and discussion

Figs. 2(a) and 2(b) describe the electronic transmission coefficient $\tau_{el}(E)$ as a function of the energy E for double-bend ZGNRs and double-bend AGNRs, respectively. Similarly, we also give the corresponding results for straight GNRs (namely pristine GNRs). Note that the on-site Coulomb interaction will affect the energy bands of electrons and the electronic transmission in GNRs [38,39]. However, in our calculations, we only consider the case without the Coulomb interactions to give a comparison with the previous works. Due to electron–hole symmetry of the Hamiltonian, all the curves are symmetric with respect to the charge neutrality point (CNP), which is different from that with the Coulomb interaction. Apparently for straight GNRs, some smooth staircase-like transmission platforms corresponding to the number of available transport channels of electrons, can be observed. However, for double-bend GNRs, these transmission platforms are observed to resolve into a number of peak-dip structures stemming from the interface elastic scattering. With increasing the width N_C or the length M, such peak-dip structures become more and more intricate. These results