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Highly efficient thermal rectification in carbon/boron nitride heteronanotubes

Xue-Kun Chen [a,*], Zhong-Xiang Xie [b], Yong Zhang [b], Yuan-Xiang Deng [b], Tong-Hua Zou [b], Jun Liu [c,**], Ke-Qiu Chen [d,***]

[a] School of Mathematics and Physics, University of South China, Hengyang, 421001, China
[b] Department of Mathematics and Physics, Hunan Institute of Technology, Hengyang, 421002, China
[c] College of Chemistry and Chemical Engineering, Central South University, Changsha, 410083, China
[d] Department of Applied Physics, School of Physics and Electronics, Hunan University, Changsha, 410082, China

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ABSTRACT

Carbon/boron nitride heteronanotubes (CBNNTs) have attracted considerable attention owing to their unique properties and functions for practical applications in many fields. However, interfacial thermal transport in such heterostructures, which plays a pivotal role in determining their functional properties, is still unknown. In this work, we use non-equilibrium molecular dynamics (NEMD) simulations to study the thermal transport across CBNNTs interface. It is found that the heat flows preferentially from the BNNTs to the CNTs region, demonstrating pronounced thermal rectification (TR) effect. In addition, the TR ratio of zigzag CBNNTs is much more than that of armchair ones, especially under lager temperature bias. With the help of wave packet dynamics simulation and power spectrum calculation, the underlying mechanism of TR in CBNNTs is identified. Furthermore, the influence of system size, ambient temperature and defect density is studied to obtain the optimum conditions for TR. More importantly, we also found that the TR ratio of CBNNTs apparently decreases when taking account of the substrate interaction or tensile strain in practical design for thermal rectifier. Our results provide a certain guidance for designing high-efficiency thermal rectifier based CBNNTs.

1. Introduction

Thermal rectification (TR), a phenomenon where heat transports preferentially in one direction than in the reverse direction, is the key for heat flow control. Due to its great potential in thermal storage and thermal logic circuits [1], much attention has been given to this field in the past decade. For instance, the experimental evidence of TR was reported in unevenly mass-loaded nanotubes [2] and vanadium dioxide beams [3], making the design of thermal devices possible. After that, some graphene-based thermal rectifiers have been experimentally realized [4–6], and specific thermal devices like thermal memory [7] and thermal cloak [8] analogous to the electronic counterparts have also been prepared. Meanwhile, numerous theoretical works were made to propose nanoscale thermal rectifiers like triangular-pyramid diamond [9], silicon nanocones [10], graded core–shell nanowires [11], asymmetric graphene nanoribbons (GNRs) [12–14], nanoheterojunctions [15–17] and phase change materials [18,19]. It is worth noting that the fabrication of most of the above nanostructures might need complicated synthetic procedures that prevents their practical application; on the other hand, the TR ratio achieved was comparatively small. Moreover, a fundamental understanding of this asymmetric thermal transport is still under debate. Normally, the observed TR phenomenon can be ascribed to the mismatch of vibrational spectrum [9,10,16,17], phonon lateral confinement [14], phonon local resonance [20] and standing wave effect [11], indicating that the origin of TR should not be considered as uniqueness.

Carbon nanotubes (CNTs) exhibit many unique properties and hold great promise for use in next-generation nanoelectronic devices. The encouraging performance of CNTs has also triggered intense research interest in their analogs like boron-nitride nanotubes (BNNTs) and carbon/boron nitride heteronanotubes

* Corresponding author.
** Corresponding author.
*** Corresponding author.
E-mail addresses: 813112490@qq.com (X.-K. Chen), lj332125065@163.com (J. Liu), keqiuchen@hnu.edu.cn (K.-Q. Chen).

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A local resonance mechanism for thermal rectification in pristine/branched graphene nanoribbon junctions

Xue-Kun Chen,[1,a)] Jun Liu,[2] Zhong-Xiang Xie,[3] Yong Zhang,[3] Yuan-Xiang Deng,[3] and Ke-Qiu Chen[4,a)]

[1]School of Mathematics and Physics, University of South China, Hengyang 421001, China
[2]College of Chemistry and Chemical engineering, Central South University, Changsha 410083, China
[3]Department of Mathematics and Physics, Hunan Institute of Technology, Hengyang 421002, China
[4]Department of Applied Physics, School of Physics and Electronics, Hunan University, Changsha 410082, China

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Using non-equilibrium molecular dynamics simulations, we investigate thermal rectification (TR) in pristine/branched graphene nanoribbon (GNR) junctions. The results indicate that the TR ratio of such junctions can reach 470% under small temperature bias, which has distinct superiority over asymmetric GNR and many other junctions. Moreover, the TR ratio decreases rapidly as the applied temperature bias increases. It seems to be against common sense that the TR ratio generally increases with temperature bias. Phonon spectra analyses reveal that the observed phenomena stem from the local resonance of longitudinal phonons in branched GNR region under negative temperature bias. Furthermore, the influence of ambient temperature, system length, branch number, and defect density is studied to obtain the optimum conditions for TR. This work extends local resonance mechanism to GNR for thermal signal manipulation. *Published by AIP Publishing.*
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Thermal rectification (TR) is a special heat transfer phenomenon in which heat transports preferentially in one direction than in the opposite one. Because of its great potential for application in thermal management and thermal signal manipulation,[1–3] it has been attracting significant attention in seeking nanostructures with high TR ratio and studying new TR mechanisms. In 2006, the experimental evidence of TR was reported in unevenly mass-loaded carbon and boron nitride nanotubes, which shaded light on the possibility of designing thermal devices.[4] Since then, extensive theoretical studies have been devoted to propose nanoscale thermal rectifiers such as asymmetric nanoribbons,[5–8] nanojunctions,[9–12] graded nanowires,[13] and phase change materials.[14,15] Up to now, some of the above-mentioned models have been realized in experiment.[16–18] However, the underlying mechanism for TR is under debate and it probably should not be considered as one-fold. According to the previous studies, the observed TR could be attributed to the mismatch of the power spectra,[1,8,9,12,14] asymmetric coupling with thermal contacts,[19] phonon localization,[7,20] and standing wave effect.[11,13] In fact, most proposed thermal rectifiers are based on the asymmetry of phonon scattering. Under this principle, high TR ratio commonly needs large temperature bias. For instance, Yang *et al.*[5] reported a large TR ratio of 350% in asymmetric graphene nanoribbon (GNR) at 300 K and with a temperature bias of 300 K. Under the same conditions, Cao *et al.*[11] found that the TR ratio of the carbon nanotube-graphene junction can reach 800%. For all this, the need of huge temperature bias prevents the practical applications of these rectifiers, so it is necessary to find high-efficiency TR scheme under small temperature bias.

a)Authors to whom correspondence should be addressed: 813112490@qq.com and keqiuchen@hnu.edu.cn

Graphene, a single layer of carbon atoms arranged in a honeycomb lattice, has excellent electronic, mechanical, and thermal properties.[21–24] Since pristine graphene has no band-gap, tailoring planar graphene into one-dimensional GNR is used to the band-gap opening.[25,26] For the application of GNR in different fields, the modulation of its thermal property will be particularly important. In contrast to heat-conducting application that requires GNR with high thermal conductivity, thermoelectric application needs it to have low thermal conductivity. Currently, the most common route to control thermal property of GNR is to enhance phonon scattering (particle-like) by introducing defects,[27–29] functional groups,[30,31] stress field,[32,33] interfaces,[34,35] and substrates.[36,37] Normally, only a limited range of high-frequency phonons gets scattered efficiently, while low-frequency phonons is hardly affected because of their long mean free path. Recently, a special thought for manipulating thermal transport with the wave nature of phonons, particularly local resonance, is growing more and more appealing.[38–43] The great advantage of this resonant mechanism is its ability to manipulate low-frequency phonons by adding branches on main structure. A natural question comes promptly: can we extend the resonant mechanism to GNR to actualize the goal of high TR ratio under small temperature bias?

In this work, we investigate TR in pristine/branched GNR junctions using non-equilibrium molecular dynamics (NEMD) simulations. The results indicate that the TR ratio of such junctions can reach 470% under small temperature bias. As the applied temperature bias increases, the TR ratio unexpectedly decreases. The detailed analyses of phonon spectra are conducted to understand the observed phenomena. Furthermore, the influence of ambient temperature, system length, branch number, and defect density are studied to obtain the optimum conditions for TR.

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Anisotropic thermal conductivity in carbon honeycomb

Xue-Kun Chen[1], Jun Liu[2], Dan Du[1], Zhong-Xiang Xie[3] and Ke-Qiu Chen[4]

[1] School of Mathematics and Physics, University of South China, Hengyang 421001, People's Republic of China
[2] College of Chemistry and Chemical Engineering, Central South University, Changsha 410083, People's Republic of China
[3] Department of Mathematics and Physics, Hunan Institute of Technology, Hengyang 421002, People's Republic of China
[4] Department of Applied Physics, School of Physics and Electronics, Hunan University, Changsha 410082, People's Republic of China

E-mail: 813112490@qq.com (X-K Chen), xiezxhu@163.com (Z-X Xie) and keqiuchen@hnu.edu.cn (K-Q Chen)

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Abstract

Carbon honeycomb, a new kind of 3D carbon allotrope experimentally synthesized recently, has received much attention for its fascinating applications in electronic device and energy storage. In the present work, we perform equilibrium molecular dynamics (EMD) to study the thermal transport properties of carbon honeycombs with different chirality. It is found that the thermal conductivity along the honeycomb axis (κ_x) is three times larger than that normal to the axis (κ_z), which shows strong anisotropy reflecting their geometric anisotropy. Lattice dynamics calculations reveal that this anisotropy stems from the orientation-dependent phonon group velocities. Moreover, when ambient temperature (T) increases from 200 K to 800 K, the T^{-1} dependence of κ is observed due to the enhanced Umklapp scattering. The detailed phonon spectra analyses indicate phonon group velocities are insensitive to the variation of ambient temperature, and the temperature dependence of the relaxation times of low-frequency phonons (<20 THz) follows $\sim T^{-1}$ behavior. Our results have a certain guiding significance to develop carbon honeycomb for effective thermal channeling devices.

Keywords: thermal conductvity, carbon honeycomb, relaxation times, molecular dynamics

(Some figures may appear in colour only in the online journal)

1. Introduction

Graphene, a single layer of carbon atoms bonded in a hexagonal lattice, has attracted intense interest due to its excellent electronic [1], mechanical [2] and optical properties [3]. In addition, graphene possesses extremely high room-temperature thermal conductivity dominated by phonons [4–6], which makes it desirable for managing heat dissipation in integrated circuits. However, it is difficult to retain such properties when scaling the two dimensional (2D) material up to three-dimensional (3D) structure for many technological applications. Although the corresponding 3D derivatives, such as multi-layer graphene or graphene/substrate systems, could be fabricated or formed more easily, the van der Waals bonding between different layers or with substrate materials may degrade its performance on tensile strength and heat dissipation etc. For instance, single-layer graphene has a tensile strength of 130 GPa [2], while the strength of graphene membrane is generally three orders of magnitude lower than that of graphene [7]. Moreover, the room-temperature thermal conductivity of single-layer graphene was reported to be about 4000 W m^{-1} K^{-1}, by contrast, that of four-layer graphene was only about 1300 W m^{-1} K^{-1} [8]. A similar trend has been predicted for the carrier mobility

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Reduction of phonon thermal conduction in isotopic graphene nanoribbon superlattices

ZhongXiang Xie[1,2], XueKun Chen[3], Xia Yu[1], Yong Zhang[1], HaiBin Wang[1], and LiFu Zhang[2*]

[1] Department of Mathematics and Physics, Hunan Institute of Technology, Hengyang 421002, China;
[2] SZU-NUS Collaborative Innovation Center for Optoelectronic Science Technology, Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, College of Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, China;
[3] School of Mathematics and Physics, University of South China, Hengyang 421001, China

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Graphene nanoribbons (GNRs) recently have drawn much interest because of their novel electronic properties such as well-controlled electronic structures [1], high Seebeck coefficient [2], and intriguing electronic transport [3]. For the thermoelectric energy conversion, GNRs are thought to be rather poor candidates because of too high phonon thermal conductance [4], though they own good electronic conduction. Thus, the reduction of the phonon thermal conductance of GNRs is particularly important for their thermoelectric applications. Several methods such as strain [5], structural defects [6,7], etc. [8], have been proposed to reduce the phonon thermal conductance of GNRs. In these methods, however, a central difficulty is that reducing the phonon thermal conductance always brings the adverse effects to the electron transport, which limits the further improvement of the thermoelectric efficiency of GNRs.

Much effort has been devoted to studying the thermal transport of isotope-doped carbon-based nanostructures [9]. For example, Pei et al. [10] found that the random isotope-doping can reduce the thermal conductivity in graphene due to the interfacial thermal resistance. Similar results were reported in subsequent studies [11]. In addition to the random isotope-doping, there exists an increasing interest in the isotopic superlattices. Several studies have explored the effects of the period length of the isotopic superlattices on the thermal conductivity in carbon nanotubes [12] and silicon nanowires [13]. Particularly in a recent study, it has been predicted that the isotopic superlattices lead to the more reduction of thermal conductivity than the random isotope-doping [14]. More recently, Mu et al. [15] studied both coherent and incoherent phonon thermal transport in isotopic GNR superlattices.

In this work, we investigate the thermal conductance in isotopic GNR superlattices using the non-equilibrium Green's function (NEGF) method. Recently, Ouyang et al. [16] presented a study of the thermal conductance of isotopic GNR superlattices with zigzag edges. However, in their study, only the out-of-plane modes are considered. It is well known that there exist two independent modes: in-plane modes and out-of-plane modes, in graphene nanostructures. The contribution of the in-plane modes to the thermal conductance is comparable to that of the out-of-plane modes at high temperatures. Here, both the in-plane modes and the out-of-plane modes are considered. Note that the isotope-doping can dramatically reduce the phonon thermal conductance without introducing any effects on the electron transport. It has been demonstrated that the mass disorder can reduce the thermal conductance, so as to improve the thermoelectric properties of GNRs [9], in agreement with that in silicon nanowires [17]. The aim of this work is to address the effective reduction of the thermal conductance of GNRs by utilizing the isotopic superlattices.

The geometric structures of the isotopic GNR superlattices

*Corresponding author (email: zhanglifu63@hotmail.com)

initially decreases as the period length decreases. However, when the period length decreases to less than the critical period length, the phonon tunneling, which makes a contribution to the phonon transmission, will play a major role in determining the thermal conductance. Moreover, the smaller the period length is, the more evident the phonon tunneling becomes. So the thermal conductance rapidly increases after decreasing the period length less than the critical period length. Naturally, the appearance of the minimum thermal conductance at the critical period length can be understood as a result of the completion between the interfacial scattering and the phonon tunneling. These behaviors are in agreement with those reported in previous studies [12,13,16,20]. Note that molecular dynamics simulation has demonstrated that the reduction of thermal conductivity of GNRs-based superlattices with ~50% isotope concentration is up to 30% [14]. From Figure 4, it is also shown that for both $^{12}C/^{14}C$ and $^{12}C/^{24}C$ systems, the critical period length d_C for AGNR is 1.704 nm (4 unit cells), while for ZGNR it is 1.476 nm (6 unit cells), which are independent of the variation of the temperature. The difference of the critical period length d_C between AGNR and ZGNR is purely due to their different geometric structures. Further calculations show that the critical period length d_C is sensitive to the total length of central scattering region, but not to the ribbon width (not shown). However, it is worth noting that the ratio of the critical period length d_C to the total length L remains unchanged in both AGNR and ZGNR. Recently, the critical period length has also been explored in other superlattice systems. It has been revealed that the critical period length corresponds to the coherence length, which indicates the crossover from incoherent to coherent phonon transport [15,21]. A recent study shows that the coherence length shifts to lower values at higher temperatures in graphene and boron nitride superlattice [22], which is different from our result.

In conclusion, we investigated the thermal conductance in isotopic GNR superlattices by using the NEGF method. Results show that the isotopic superlattices can effectively reduce the thermal conductance of GNRs due to the interfacial scattering, and such reduction for AGNR is more evident than that for ZGNR, especially at high temperatures. In both AGNR and ZGNR, the reduction of thermal conductance strongly depends on the isotopic mass and the period length of the isotopic superlattices. At the critical period length, the minimum thermal conductance, which is only 25% (32%) of the corresponding value of pristine AGNR (ZGNR), can be obtained. We also shown that the critical period length for AGNR is 1.704 nm (4 unit cells), while for ZGNR it is 1.476 nm (6 unit cells). The critical period length is sensitive to the total length of the central scattering region, but not to the ribbon width.

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