Manipulating Thermal Conductivity via Targeted Phonon Excitation

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Abstract

Thermal conductivity appears as a critical material property in numerous applications, such as those related to thermoelectric devices and to heat dissipation. It has become an issue of great concern to effectively manipulate thermal conductivity. Here, it is proposed that a quantum strategy to manipulate heat conduction, that is, to manipulate heat conduction via exciting the targeted phonons. It show that the thermal conductivity of graphene can be tailored in the range of 1559 W/m-K (49%) to 4093 W/m-K (128%), compared with the intrinsic value as 3207 W/m-K. A similar trend is also observed for graphene nanoribbons. The results are obtained by both ab initio calculations and molecular dynamics simulations. This brand new quantum strategy to manipulate heat conduction paves a way for quantum heat conduction.
Introduction

The manipulation of thermal conductivity holds great importance in applications, such as thermal managements [1-3], and energy devices [4-6]. A deep understanding of phonon scattering mechanisms in different heat transfer regimes is critical for modulating the thermal conductivity of materials to achieve desirable performances [7-16]. However, manipulating thermal conductivity remains a long-standing challenge in physics and material science, owing to the complex nature of phonon transport.

Recently, the developments in heat conduction led to a better understanding of the scattering dynamics of heat carriers at nanoscale. Heat conduction in dielectrics can be understood as the propagation of phonons and their scatterings such as phonon-phonon [17-20], impurity [21-23] and boundary scattering [9,24,25]. Phonon-phonon scattering has been exploited to produce less and weak couplings [26-28] and also to highlight hydrodynamic phonon transport [11,29] in nanostructures. Impurity scattering is highly frequency dependent and also closely related to normal processes [30], which can redistribute phonon frequencies and control phonon transport by nano-engineering [1,15,21,31,32]. Due to size confinement, phonon transport is largely affected by the boundary scattering [9], resulting in the size dependence of thermal conductivity and in an invalid Fourier’s law [33-35].

These progresses have led to new strategies to modulate phonon scattering and thermal conductivities, motivated by the widely demand for thermal management. An enhanced thermal conductivity can be achieved by minimizing phonon–phonon scattering phase space and phonon–impurity scattering in bulk materials [2,14,18-20,36-42]. On the other hand, a reduced thermal conductivity, can be achieved through strategies increasing phonon scattering [43,44], such as intrinsically increasing anharmonicity or crystal complexity, or extrinsically introducing disorder, defects, boundaries, interfaces and nanoparticles. Besides, the wave nature of phonon [45] can also be utilized to
modulate the thermal conductivity, such as in nanophononic crystals [46-48], or by tuning phonon coherence [49,50] and localization [51-53]. In recent works, the external fields have been implemented to change the morphology of structures, thereby regulating thermal conductivity [37,41,54-56]. Nevertheless, the strategies mentioned above cannot manipulate the thermal conductivity with quantal precision or controllability.

Recently, targeted phonon mode excitation by the THz optical pulses or tensile strain has been studied in manipulating optical and electrical properties, whose advantages are in-situ, flexible, quick response and directness, without modifying the original structure. For instance, optical phonons in MAPbI$_3$ can be directly excited by terahertz excitation pulses and can significantly perturb the electron relaxation dynamics [57]. It was also experimentally demonstrated that the performance of an organic optoelectronic system can be modulated by selectively exciting vibrational modes of the molecules [58]. Moreover, the non-equilibrium carrier-phonon dynamics in photovoltaic systems have been discussed in details for a few perovskites. When injecting abundant carriers, the quantal emission of longitudinal optical (LO) phonons, the optical phonon decay to acoustic phonons and other relaxation processes have been uncovered in experiments [59-61]. Additionally, non-equilibrium between optical and acoustic phonons has been observed in photoexcited graphene and MoS$_2$ [62,63]. In black phosphorene, the excitation of out-of-plane acoustic phonons induced by tensile strain can provide a strong modulation of the electronic band structures, carrier lifetime and carrier mobility [64]. The excitation of targeted phonons is also used to enhance ion diffusion [65] and induce structural phase transitions [66,67]. Above results provide feasibility for targeted phonon excitation. However, less studies on manipulating thermal conductivity have been performed by mode excitations.

Here, the strategy of quantal excitation of phonons is proposed to manipulate the thermal conductivity of dielectric materials, where phonons dominate in the heat conduction. This strategy consists in exciting targeted phonons with the aim to
increase/decrease phonon scattering for desired thermal conductivities. Ab initio density functional theory (DFT) calculations [68] and molecular dynamical simulations [69] are utilized to demonstrate the effectiveness and capability of this strategy. The graphene and graphene nanoribbon are chosen as the model systems because the thermal conductivities of graphene and its derivatives are well-studied. The results indicate that the thermal conductivity can be manipulated by quantal exciting phonons instead of modifying the structure.

### Strategy for Controlling Thermal Conductivity

![Fig. 1. Manipulating thermal conductivity via targeted phonon excitation. (a) Schematic of manipulation strategy. (b) Density of states (DOS) and intrinsic scattering rates $\gamma_{Gr}^0$ of graphene by ab initio calculations used for choosing targeted phonons. The superscript “0” represents the intrinsic value.](image)

The strategy is to manipulate the overall thermal conductivity via quantal excitation of targeted phonon modes, as depicted in Fig. 1(a). Firstly, the dominant modes for transport are identified utilizing first principles and molecular dynamics. And then, the energy of these modes is increased artificially. Dominant phonons with larger thermal conductivity contribution and weak coupling with others are excited. Due to the excitation of these carriers, the thermal conductivity can be significantly enhanced. Conversely, when phonons with a high scattering rate and a relatively low thermal
conductivity contribution are excited, scattering processes are promoted resulting in a
decrease of the thermal conductivity. Phonon DOS determines the number of excited
modes around a specific frequency, thus indicates the effectiveness of activating those
modes. It is worth noting that thermal conductivity can be modulated in a wide range
by exciting only a few of the dominant phonons, without introducing other scattering
mechanisms.

The method is basically relying on the nature of phonon scattering. Heat conduction in
solids is directly related to phonon scattering, where an individual mode can participate
in various scattering processes. By identifying the characteristic time of phonon
relaxation time or lifetime, \( \tau \), the thermal conductivity can be generally written as an
integration as \([9,10,24]\):

\[
\kappa = \frac{1}{3} \int C(\omega) v^2(\omega) \tau(\omega) d\omega
\]

(1)

where parameter \( 1/3 \) is related to the dimension of the system, \( C(\omega) \) refers to the
spectral volumetric specific heat, \( v \) to the phonon group velocity and \( \omega \) is the
frequency. In general, the diverse scatterings can be incorporated into the Matthiessen’s
rule \([9,24]\):

\[
\frac{1}{\tau} = \frac{1}{\tau_{ph-ph}} + \frac{1}{\tau_{im}} + \frac{1}{\tau_b}
\]

(2)

where \( \tau_{ph-ph}, \tau_{im}, \) and \( \tau_b \) are the relaxation times due to phonon-phonon, impurity,
and boundary scattering processes, respectively. The phonon-phonon relaxation time is
computed based on the Fermi’s golden rule \([70]\). The impurity scattering can be
obtained on the basis of Klemens’ derivation \([9]\). Besides, the crystal boundary
scattering is based on diffuse boundary absorption/emission, which depends on the
Casimir length. To be emphasized, the impurity and boundary scattering aren’t included
in the calculation of this work.

By increasing the energy of targeted phonons, the scattering rate can be changed
significantly, leading to the modulation on the thermal conductivity. To change the
energy of mode \( n \), the phonon occupation numbers are modified in ab initio
calculations according to the following formulation:

\[ E_n' = \hbar \omega_n \frac{N}{\frac{\hbar \omega_n}{e^{k_BT} - 1}} \]  

(3)

where \( E_n' \) corresponds to the energy of mode \( n \) after the modification, \( \hbar \) denotes the reduced Planck constant, \( k_B \) the Boltzmann’s constant, \( T \) is the absolute lattice temperature and \( N \) represents the multiple of energy increase. To rescale the mode kinetic energy \( E_{n,K} \) in molecular dynamic (MD) simulations, the atomic velocities are rescaled according to the formulation (The derivation is presented in Appendix C):

\[ v_j' = v_j + \frac{1}{\sqrt{m_j}} (\sqrt{M} - 1) \dot{Q}_n(t) e_{j,n} \]  

(4)

where \( v_j' \) and \( v_j \) are the velocity of atom \( j \) after and before the modification, respectively. The rescale factor \( M \) is set to 10 in MD simulations. In addition, \( m_j \) indicate the atomic mass, \( \dot{Q}_n \) the normal mode velocity coordinate and \( e_{j,n} \) the eigenvector. Considering the time evolution of mode kinetic energy in the MD simulation (Fig. S4), the actual multiple of kinetic energy increase \( N \) is much lower than \( M \), and it can be defined as the relative time-averaged mode kinetic energy after and before the excitation \( \langle E_{n,K}' \rangle / \langle E_{n,K} \rangle \). The effectiveness of the strategy is validated in graphene and graphene nanoribbon but the proposed strategy could be applicable to other weak-coupling systems [26-28]. Ab initio calculations (Details in Appendix A) for graphene are performed with the Vienna ab initio simulation package (VASP) [71]. The phonon transport properties are obtained by solving the phonon Boltzmann transport equation using ShengBTE packages [72] with the aid of the PHONOPY package [73]. Additionally, nonequilibrium molecular dynamic (NEMD, Details in Appendix B) simulations for graphene nanoribbon are conducted using the LAMMPS package [74].
**Results and Discussions**

Firstly, the spectral contribution to intrinsic thermal conductivity of graphene $\kappa_{Gr}^0$ is calculated as a guidance to highlight the effectiveness of the manipulation strategy, as shown in Fig. 2(a). An iterative solving method is utilized to solve the Boltzmann transport equation accurately [72]. The obtained value for $\kappa_{Gr}^0$ is 3207 W m$^{-1}$ K$^{-1}$ at 300 K, which is comparable with the one of previous works (1500–4000 W m$^{-1}$ K$^{-1}$) [75-79]. Fig. 2(a) suggests that the modes in the low frequency range dominate the heat conduction in graphene, especially the modes below 5 THz and around 10 THz. The spectral $\kappa_{Gr}^0$ drops drastically in the higher frequency range, implying a negligible contribution of these modes to heat conduction. This observation provides a prominent information for the choice of modes to be corrected in energy.

Then, the energy is injected to excite more heat carriers into those dominant modes. However, it can be found from Fig. 2(b) that the results do not correspond perfectly to the tendency shown in Fig. 2(a), since the DOS and scattering rates are also essential factors to implement the modification, as illustrated in Fig. 1(b). DOS indicates the density of modes in a certain frequency interval. Hence, it determines how many modes can be affected during the excitation. Besides, a high scattering rate means that the modes are strongly scattered, which often leads to smaller contribution to heat conduction and a larger resistance of other modes. For graphene, ZA modes play a much more important role in the heat conduction due to the symmetry-based selection rule [78]. The reflection symmetry of its 2D structure excludes all the 3-phonon scatterings that involve odd numbers of flexural phonons, causing a profound reduction in the scattering rates of flexural modes, especially ZA modes. Thus, the excitation those modes can generate more obvious effects. As a result, the peak of $\kappa_{Gr}/\kappa_{Gr}^0$ located at around 1.7 THz, ensures a high enough DOS, a low scattering rate as well as a high spectral thermal conductivity. Whereas the trough is situated around 13.9 THz, near the maximum frequency of the ZA phonon branch, ensuring high enough DOS, a relatively
high scattering rate and small spectral thermal conductivity compared to other ZA modes. The scattering rates’ changes after and before the excitation are also presented in Appendix A.

Fig. 2. Thermal conductivity manipulation for graphene via targeted phonon excitation. (a) Spectral contributions to $\kappa_{Gr}^0$ as a function of frequency. (b, c) The relative overall thermal conductivity of graphene after and before the excitation $\kappa_{Gr}/\kappa_{Gr}^0$ as a function of the center frequency for targeted phonons. For instance, the first center frequency is 0.05 THz, and a few modes in 0−0.1 THz are excited with a twenty-five- or five-times larger energy. The energy needed for the excitation is at most 20.8 mJ m$^{-2}$ ($N=25$) or 3.5 mJ m$^{-2}$ ($N=5$).

Molecular dynamics simulations are performed to validate the feasibility of the modulation strategy, especially considering high-order scatterings. As shown in Fig. 3(a), the thermal conductivity contribution spectrum of graphene nanoribbon (24.9×21.6 Å$^2$) are extracted employing NEMD simulations [80,81]. The intrinsic thermal conductivity of graphene nanoribbon $\kappa_{GNR}^0$ is 59.0 W m$^{-1}$ K$^{-1}$ at 300 K, which is consistent with a previous study [47]. Due to the limitation in size of the simulation cell, the possible excited phonons have smaller wavelengths and higher frequencies (above 3 THz). In the simulations, the intermediate region where the temperature difference remains small (<0.3 K in all the cases), is chosen for deriving the thermal conductivity contribution spectrum to ensure that the lattice dynamic method is valid. Except for the heat sink and fixed region, other parts are set as the excitation regions.
Hence, there is the additional heat flux produced by the excitation, which is relatively small (2–5%) compared to the heat flux generated by Langevin thermostat (Fig. S5 in Appendix B). The equivalent input energy density of the excitation is around 0.21–0.48 mJ m\(^{-2}\). And the excitation is conducted every 100 fs. The thermal conductivity refers to an effective quantity measuring the heat flux. It should also be noted that there are only a few modes in each 1 THz frequency range, which accounts for 2–7% of all modes of the Brillouin Zone. Moreover, modes around 10 THz highly contribute to the overall thermal conductivity in Fig. 3(a). Specially, when two modes between 9 and 10 THz are chosen as targeted phonons (excited-A), the overall thermal conductivity of graphene nanoribbon \(\kappa_{\text{GNR}}\) increases by 97.8% (from 59.0 to 116.7 W m\(^{-1}\) K\(^{-1}\)) when those modes are excited with \(N=3.34\) (3.34 times larger kinetic energy). Fig. 3(a) also shows the thermal conductivity contribution after the excitation. It can be concluded that the increase of \(\kappa_{\text{GNR}}\) is mainly contributed from modes below 10 THz and modes in 24–26 THz, yet the contribution of those modes has not changed greatly compared to the original one. Furthermore, targeted phonons in other frequency range are excited similarly, as shown in Fig. 3(b). The excitation of these modes regulates the overall thermal conductivity by different ratios. The modes between 9 and 10 THz show the highest modulation ratio due to high contribution to \(\kappa_{\text{GNR}}\), with which the modes in 25–26 THz is similar. In general, the enhancement of \(\kappa_{\text{GNR}}\) decreases with an increased frequency (below 15 THz). It can be attributed to higher phonon DOS in the high frequency range.
Fig. 3. Thermal conductivity manipulation for graphene nanoribbon via targeted excitation of phonons. (a) Thermal conductivity contribution spectrum by molecular dynamics simulations, “A” refers to the case where two modes, 9.84 THz, \( \mathbf{k} = (-0.64,0.96,0) \) and 9.84 THz, \( \mathbf{k} = (0.64,-0.96,0) \), are excited with a 3.34 times larger kinetic energy \( (N=3.34) \), and “B” represents the case where four modes, 23.59 THz, \( \mathbf{k} = (-0.64,0.37,0) \); 23.41 THz, \( \mathbf{k} = (-0.64,0.66,0) \); 23.41 THz, \( \mathbf{k} = (0.64,-0.66,0) \); and 23.59 THz, \( \mathbf{k} = (0.64,-0.37,0) \), are excited with \( N=2.71 \). (b) Relative thermal conductivity of graphene nanoribbon after and before the excitation \( \kappa_{GNR}/\kappa_{GNR}^0 \) by exciting a few modes in each 1 THz frequency range utilizing molecular dynamics simulations.

The manipulation results of NEMD simulations for to decreasing \( \kappa_{GNR} \) show a similar tendency, compared with ab initio calculations. As shown in Fig. 3(a), modes in 15–24 THz exhibit low contribution to \( \kappa_{GNR} \). When four modes between 23 and 24 THz are excited with a 2.71 times larger kinetic energy (excited-B, \( N=2.71 \)), \( \kappa_{GNR} \) is decreased by 59.6% (from 59.0 to 23.8 W m\(^{-1}\) K\(^{-1}\)). The comparison before and after the excitation is plotted in Fig. 3(a). The contribution of modes to \( \kappa_{GNR} \) decreases over a wide frequency range. More specifically, the reduction below 10 THz dominates owing to large original contribution values. Besides, by exciting the modes in the frequencies between 20 and 24 THz, \( \kappa_{GNR} \) exhibits a reduction (from 85.1% to 40.4%), as illustrated in Fig. 3(b). The reduction of \( \kappa_{GNR} \) is also significant and has a trend that falls as the frequency of targeted phonons increases (below 24 THz). This trend can be related to high intrinsic scattering rates and low phonon DOS of modes around 23 THz compared to other modes.

**Conclusions**

In this work, a new strategy for the thermal conductivity modulation is presented, which is realized by quantal exciting phonons. The results for the sample structures of
graphene and graphene nanoribbon show that the overall thermal conductivity can be modulated in a wide range in comparison to the intrinsic value via exciting targeted mode energies. Ab initio calculations and NEMD simulations provide a detailed verification for the modulation. Firstly, the modes with top-contribution or strong-scattering are identified; then, the energy of some of these modes is artificially increased.

It should be emphasized that the feasibility of this strategy has a high possibility to be confirmed experimentally [57,58,67]. Because the quantal excitation of vibrational mode has already been used to manipulate transport properties and induce structural phase transitions [58,64,65,67]. Furthermore, these findings provide a promising quantum way to manipulate the thermal conductivity in the scale of phonon modes.
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Declaration of Competing Interest

There are no conflicts of interest to declare.
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