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TOPICAL REVIEW — Thermal and thermoelectric properties of nano materials

Thermal conductivity of nanowires*

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Thermal conductivity of nanowires (NWs) is a crucial criterion to assess the operating performance of NWs-based device applications, such as in the field of heat dissipation, thermal management, and thermoelectrics. Therefore, numerous research interests have been focused on controlling and manipulating thermal conductivity of one-dimensional materials in the past decade. In this review, we summarize the state-of-the-art research status on thermal conductivity of NWs from both experimental and theoretical studies. Various NWs are included, such as Si, Ge, Bi, Ti, Cu, Ag, Bi_2Te_3, ZnO, AgTe, and their hybrids. First, several important size effects on thermal conductivity of NWs are discussed, such as the length, diameter, orientation, and cross-section. Then, we introduce diverse nanostructuring pathways to control the phonons and thermal transport in NWs, such as alloy, superlattices, core–shell structure, porous structure, resonant structure, and kinked structure. Distinct thermal transport behaviors and the associated underlying physical mechanisms are presented. Finally, we outline the important potential applications of NWs in the fields of thermoelectrics and thermal management, and provide an outlook.

Keywords: thermal conductivity, nanowires, thermal management, thermoelectrics

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1. Introduction

With the improvement of nano-fabrication and engineering technologies, one-dimensional (1D) materials, such as nanowires (NWs), nano-tubes, and quantum wires, have been designed and synthesized in the past decades.[1,2] Due to the unique properties different from bulk materials, 1D materials have attracted growing research interests,[1,3,4] and have vast applications in the fields of electronic, optoelectronic, and energy conversion devices. Among them, crystalline semiconductor NWs are very promising materials in the present miniaturization of devices towards the nanoscale. They cover a wide range of materials, from single element semiconductors (such as Si, Ge, and Bi), the compound semiconductors (such as ZnO, GaN, SiC, Bi_2Te_3, GaAs, and InP), to the composite systems (such as Si/Ge, SiO_2/SiC, and ZnS/Si), in which Si, Ge, and their composite NWs received numerous studies for the promising applications and integrability with current semiconductor electronics industry.[5–7] Moreover, the metal NWs also exhibit important applications in shape memory, heat transfer, and quantum transport.[4,8,9]

Thermal conductivity of nanoscale materials is quite different from that of bulk materials. Understanding and predicting the thermal conductivity of NWs play an important role in promoting the following two most fundamental applications: (i) thermal management, which is of fundamental and technological importance due to its broad applications in heat flow controlling,[10,11] modern phononic computations,[12,13] and novel heat dissipation solutions and materials,[14–23] and (ii) new thermoelectric materials, where the conversion efficiency is captured by the dimensionless figure of merit $ZT = S^2\sigma T/\kappa$. Here, S is the Seebeck coefficient, T is the temperature, σ is the electrical conductivity, and κ is the thermal conductivity. Thus, a low thermal conductivity together with a high thermopower factor is highly desirable for better thermoelectric performance. The thermoelectrics in NWs have attracted wide attention because of their remarkably improved thermoelectric figure of merit compared to the bulk counterparts, which is mainly caused by the significant reduction of thermal conductivity.[24–26] For example, an early experiment by Hochbaum *et al.*[24] found that ZT in Si NWs can approach to unity at room temperature, because of a remarkable 100-fold reduction in thermal conductivity over bulk values in Si NWs with rough surface, while maintaining excellent electric properties. So far, many approaches have been proposed to further reduce thermal conductivity of NWs for optimizing thermoelectric performance, such as the introduction of impu-

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rity scattering, holey structure, and surface roughness.[27–30]

On the other hand, the recent advances in nanofabrication techniques make it possible to control the geometry and dimension of NWs with atomic precision.[31,32] Consequently, various nanostructuring pathways are proposed to construct diverse NWs, such as alloy NWs,[33] superlattice NWs,[34,35] core–shell NWs,[36,37] porous NWs,[38,39] resonant structure,[40] and kinked structure.[41] Various thermal transport behaviors and reduction in thermal conductivity are discovered in these NWs. For example, the coherent phonon, found in both superlattice NWs and core–shell NWs, can be used to reduce thermal conductivity of NWs.[35,36] Moreover, various nanostructuring methods can result in remarkable reduction in thermal conductivity of NWs, while under distinct scattering mechanisms. To date, there is no systematical review on the different nanostructuring methods and thermal transport behaviors in NWs, which would be valuable for providing an overview of the existing studies and guidance to future works.

In this article, we review the recent advances in the study of thermal conductivity of NWs. First, the size effects, including the length, diameter, and orientation, on thermal conductivity of various NWs are presented. The research methods, unique phenomena, and the corresponding underlying mechanisms are also discussed. Moreover, various important impacts on manipulating thermal transport in NWs are presented in detail. Finally, we also summarize the important potential applications of NWs based on the thermal transport properties, such as thermoelectrics and thermal management. Our review would provide the basic and fundamental knowledge of thermal transport in NWs, and the key impacts on thermal conductivity of NWs.

2. Size effect

Phonons are the dominant heat carriers in semiconducting solids, and have non-negligible contribution to thermal transport in metals.[42,43] The size of the system is found to have significant impacts on the phonon scatterings and thermal transport behaviors in low dimensional materials,[23,44,45] especially for NWs. On the other hand, the continuous miniaturization of transistors and the consequent increase in power density pose severe thermal management challenges, further complicated by small characteristic device dimensions which also make thermal transport in NWs an important phenomenon to investigate.[44] In the following, the recent studies of size effects, including length effect, diameter effect, and orientation effect, on thermal conductivity of NWs are summarized.

2.1. Length effect

Lattice thermal conductivity of a material has mainly been described in terms of the average mean free path (MFP) of phonons. When the length scale becomes comparable to the MFP of those phonons which make significant contribution to thermal transport, an apparent reduction in thermal conductivity can be observed. Thus the length dependence of thermal conductivity in NWs is so interesting, meaningful, and vital to study. For Si NWs, the length dependence of thermal conductivity is controversial in literature studies. From molecular dynamics (MD) and Green–Kubo calculations, Volz and Chen found that the Si NWs possess weak length dependence.[44] Ohara *et al.* also reported the phonons MFP of Si NWs is quite short,[46] below 5 nm when the diameter of NWs is smaller than 6.5 nm. These results indicate that the phonon MFP of Si NWs is much shorter than that of bulk Si, in which more than half of thermal conductivity at room temperature is contributed by phonons with MFP longer than 1 μm.[47] Meanwhile, Yang *et al.*[48] demonstrated through non-equilibrium MD simulations that the thermal conductivity κ of Si NWs diverges with the length as $\kappa \sim L^{\beta}$, even when the length is up to 1.1 μm which is much longer than the phonon MFP, indicating a breakdown of Fourier's law in low-dimensional materials, as shown in Fig. 1(a). The diverged length dependence found in theoretical study is originated from the fact that the phonon–phonon interaction alone is not sufficient to induce a diffusive process, causing a super-diffusive phonon transport. In experimental measurement, however, because of the strong phonon scattering effect by the rough surface and defects in experimental samples, this diverged length dependence is difficult to observe. Recently, both the experimental and theoretical works have confirmed this result.[49,50] Moreover, Zhou and Hu[51] found another type of Si NWs with thermal conductivity insensitive to length, due to the suppression of propagative phonons. By performing non-equilibrium and Green–Kubo MD simulations, they reported that thermal conductivity of Si NWs in polycrystalline form can reach a record low value substantially below the Casimir limit. The strong localization in polycrystalline NWs results in a prominent decrease of effective MFP for the heat carriers, including both propagons and diffusons, and thus the breaking of Casimir limit and weak length dependence.[51,52]

There are also a number of studies that witness the strong length dependence of thermal conductivity and ballistic thermal transport in NWs. Hsiao *et al.*[53] found that ballistic thermal conduction can persist over 8.3 μm in SiGe alloy NWs, with low thermal conductivity, for a wide range of structural variations and alloy concentrations. There is an unexpectedly low percentage ($\sim 0.04\%$) of low frequency (below 0.3 THz) phonons carrying out the heat conduction process in SiGe NW, which results in an extremely long ballistic transport distance. Their subsequent work also reported a micron-scale ballistic thermal conduction in Si/Ge heterogeneously interfaced NWs, showing low thermal conductivities at small scales.[54] The in-

terfaces in the heterogeneous NWs elongate the MFPs over 5 μm at room temperature. Such MFP is not only more than 25 times longer than that of Si or Ge, but also longer than those of the best thermal conductors like diamond or graphene.[23,55]

Polyethylene chain is another type of extra-thin NWs and exhibits some intriguing thermal transport behaviors. Bulk polymer materials are generally regarded as thermal insulators for their low thermal conductivities of the order of 0.1 $W\cdot m^{-1}\cdot K^{-1}$. Interestingly, the theoretical work by Henry and Chen[56] showed that the thermal conductivity of an individual polymer chain can exceed 100 $W\cdot m^{-1}\cdot K^{-1}$, and is even divergent in some cases. Their following experimental work also verified this finding.[57] It is found that the cross correlations for the mid-frequency longitudinal-acoustic phonons are responsible for the divergent thermal conductivity.[58] Moreover, the competition between ballistic phonon transport and diffusive phonon transport in a polymer chain leads to a diverging length-dependent thermal conductivity.[59]

2.2. Diameter effect

In 1D NWs structures, the effective thermal conductivity is a function of both surface (boundary) and internal phonon–phonon scattering, as reported in Si NWs,[50,60] diamond NWs,[61] GaAs NW,[62] and Cu NW.[63] As a consequence of the unique surface scattering in NWs determined by the nature of NWs structure, the thermal conductivity values can be reduced by one order of magnitude, even below the Casimir limit.[52,64,65] The small cross section in NWs implies a more significant reduction of the thermal conductivity due to the surface scattering, compared to that in thin films because of a higher surface to volume ratio (SVR) in NWs.[66,67] For example, early experiments and simulations on Si or Si/Ge NWs verified that the room temperature thermal conductivity is strongly dependent on diameters, exhibiting a decreasing tendency with the increase of surface scatterings.[45,68] Recently, Lee *et al.*[69] experimentally demonstrated that this dependence is still valid at high temperature up to 700 K. At high temperature, the thermal conductivity of smooth Si NWs also shows the classical diameter dependence from 40 to 120 nm, and there is an increasing contribution of high-frequency phonons (optical phonons) as the diameter decreases and the temperature increases.[69]

On the other hand, other scattering mechanisms, such as phonon–surface scattering and phonon–impurity scattering, would also affect the degree of the diameter dependence. For instance, Hochbaum *et al.*[24] found in experiment that after surface etching, thermal conductivity of the rough Si NWs not only has lower value but also exhibits weaker diameter dependence. Furthermore, Martin *et al.*[60] computed the frequency-dependent phonon scattering rate from perturbation theory, and found that thermal conductivity of rough Si NWs shows a quadratic dependence on diameter D and roughness Δ as $(D/\Delta)^2$.

For other kinds of NWs, similar diameter-dependent thermal conductivity of NWs has also been reported, such as ZnO NWs,[70] PbTe NWs,[71] Bi_2Te_3 NWs,[72] and Bi NWs.[73] In most NWs, the thermal conductivity usually shows a dramatic reduction by at least an order of magnitude compared to the bulk values, due to the enhanced phonon–surface scattering. Meanwhile, there are also some unique diameter-dependent thermal transport phenomena and phonon activities observed in NWs. Bui *et al.*[70] experimentally found that in individual ZnO NW thermal conductivity approximately shows a linear dependence on the cross-sectional area of the NWs in the measured diameter range, $\sim$ 50–210 nm. In addition, through MD simulations, Chen *et al.*[67] found a simple universal linear dependence of thermal conductivity on SVR for Si NWs with small diameter, regardless of the cross sectional geometry. We will discuss in detail in the following section. As a high-performance thermoelectric material, the thermal conductivity of Bi_2Te_3 NWs is experimentally studied by Rojo *et al.*[72] Basically speaking, a remarkable reduction of thermal conductivity was observed, more than 70% when the diameter of the NW was reduced by one order of magnitude (from 300 nm to 25 nm). More interestingly, the analysis based on kinetic–collective model reveals that the surface scattering has significant impacts on acoustic phonons and largely altered the MFP of the low-frequency phonons.

Moreover, some studies[74,75] reported an abnormal diameter-dependent thermal conductivity in ultrathin NWs, that is, thermal conductivity increases with the decrease of diameter, which is different from or even contradictory to our conventional understanding. For example, Ponomareva *et al.*[75] found in MD simulations that the thermal conductivity increases with the decrease of diameter at very small diameter (< 1.5 nm). They attributed this phenomenon to the phonon confinement effect in ultrathin NWs. A similar increasing tendency has also been reported by Donadio *et al.*[74] from Green–Kubo MD simulations in thin Si NWs. Recently, Zhou *et al.*[76] carried out a systematical study on this abnormal increasing tendency of thermal conductivity in extremely thin Si NWs, by using MD simulations with various potentials. As shown in Fig. 1(b), the thermal conductivity of NWs exhibits a non-monotonic dependence on diameter, and thermal conductivity of the thinnest possible Si NW reaches an ultrahigh level that is more than one order of magnitude higher than that of bulk materials. The competing mechanism between hydrodynamic phonon flow and boundary scattering is responsible for this abnormal dependence. In the ultrathin NWs, the normal (N) process (energy and momentum conservation) of low-frequency acoustic phonons dominates the thermal transport, which induces the hydrodynamic phonon

flow in the Si NWs without being scattered.[77] With diameter increasing, the downward shift of optical phonons triggers strong Umklapp (U) scatterings with acoustic phonons, leading to the regime of phonon boundary scattering. The two competing mechanisms result in the non-monotonic diameter dependence of thermal conductivity, showing minimum thermal conductivity at a critical diameter around 2–3 nm.

2.3. Orientation effect

The crystals with different orientations have been synthesized in experiments, and the corresponding thermal transport properties would be varied.[78] For instance, the experimentally synthesized Si NWs are typically oriented in the ⟨100⟩, ⟨110⟩, ⟨111⟩, or ⟨112⟩ directions.[79] Previous studies found that the room-temperature thermal transport in Si NWs is highly anisotropic,[80,81] and the crystal orientation effects should be an important design parameter for NW devices. Based on atomistic calculations, it was shown that Si NWs oriented along the ⟨110⟩ direction have about 50%–70% higher thermal conductance than that oriented along the ⟨100⟩ and ⟨111⟩ directions.[81] The underlying physics is that the phonons in the ⟨110⟩ Si NWs generally have a larger group velocity than that in other orientations, leading to a higher thermal conductance.[81] Similarly, by using MD simulations, Zhou *et al.*[82] also found a remarkable anisotropy for the thermal conductivity of InAs NW, in which the thermal conductivity along ⟨110⟩ growth direction is about three times larger than that along ⟨100⟩ or ⟨111⟩ direction. Therefore, the anisotropy of thermal conductivity is a common nature for NWs with zinc blende structures.[81]

Moreover, thermal conductivity of NWs can also be modulated by selecting orientation direction.[83,84] Recently, the anisotropic thermal conductivity of single-crystal Bi NWs was also experimentally observed by HR-TEM and SAED investigations.[83] The thermal conductivity of Bi NWs is strongly orientation-dependent, in which the ⟨110⟩ Bi NWs is about 4-fold lower than that of the ⟨102⟩ Bi NWs, as shown in Fig. 1(c). Moreover, for both growth directions, the thermal conductivity still scales down with diameter, verifying the presence of strong boundary scattering. The strongly anisotropic thermal conductivity has also been found in tilted NWs. By using MD simulations, Li *et al.*[85] found that the thermal conductivity of tilted Bi_2Te_3 NW with the infinite size is 0.34 $W{\cdot}m^{-1}{\cdot}K^{-1}$, which is significantly reduced compared to that of NW along the ⟨010⟩ direction (0.59 $W{\cdot}m^{-1}{\cdot}K^{-1}$). Interestingly, orientation of shell atoms in core–shell NWs can also greatly reduce thermal conductivity of NWs. Zhou *et al.*[86] reported that the different surface orientations of Si atoms can alter the thermal conductivity of Si NWs by as large as 2.7–4.2 times, in which the variation in the distribution of atoms on the surface determines the degree of phonon coupling between the core and the surface.

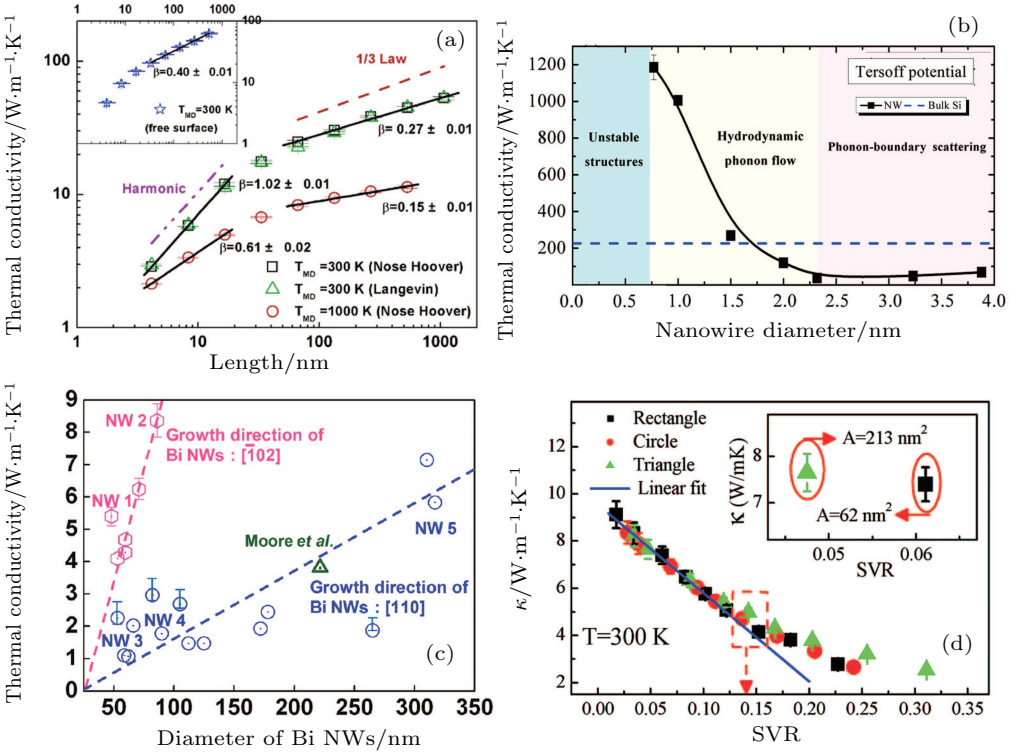


Fig. 1. (color online) Size effect on thermal conductivity of NWs. (a) Room temperature thermal conductivity of Si NWs (with fixed transverse boundary condition) versus longitudinal length with different heat baths. The inset is free (transverse) boundary condition case. (b) Diameter-dependent thermal conductivity of Si NWs calculated by Green–Kubo calculations with Tersoff potential. (c) Diameter-dependent thermal conductivity of Bi NWs with growth directions of [102] (pink hexagon) and [110] (blue circle) at 300 K. (d) Thermal conductivity of [100] Si NWs versus surface-to-volume ratio (SVR) for different geometries at 300 K. Panels adapted with permission from (a) Ref. [48], ©2010 Elsevier; (b) Ref. [76], ©2017 ACS; (c) Ref. [83], ©2011 ACS; (d) Ref. [67], ©2011 AIP.

2.4. Cross-section effect

To manipulate the surface scatterings and thermal transport in NWs, different cross-section is designed. By using MD simulations, Chen *et al.*[67] revealed that thermal conductivity of Si NWs varies with different cross sectional geometries (Fig. 1(d)), and the NWs with triangular cross section possess the lowest thermal conductivity under the same cross sectional area. Interestingly, thermal conductivity also decreases monotonically with the increase of SVR, and a simple universal linear dependence of thermal conductivity on SVR is observed within modest cross sectional area (larger than 20 nm^2).[67]

In addition to the external surface, the phonon–surface scattering can also be induced to internal of NWs. Chen *et al.*[87] proposed an idea to reduce the thermal conductivity of Si NWs by introducing a small hole at the center of NW cross-section to construct a Si nanotube (Si NT) structure. A very small hole (only 1% reduction in cross-section area) can induce a 35% reduction in room temperature thermal conductivity. Moreover, with the same cross sectional area, thermal conductivity of Si NT is only about 33% of that of Si NW at room temperature. This is because more localization modes are concentrated on the inner and outer surfaces of Si NTs. By using a highly sensitive measurement system, Wingert *et al.*[88] found in experiment the sub-amorphous thermal conductivity in ultrathin crystalline Si NTs. The crystalline Si NTs with shell thickness as thin as ~ 5 nm have a low thermal conductivity of $\sim 1.1\ \mathrm{W\cdot m^{-1}\cdot K^{-1}}$. Apparently, this value is lower than the boundary scattering limit and is even about 30% lower than the measured value for amorphous Si NTs with similar geometries.

3. Alloy and superlattices

Compared to bulk materials, NWs exhibit 100-fold reduction in thermal conductivity because of the strong phonon–boundary scattering. However, as one of the promising applications, thermoelectric performance of NWs is still far from the requirement for industry use. Therefore, it is indispensable to further reduce the thermal conductivity of NWs to optimize thermoelectric performance. Previous studies have shown that one effective way is the construction of alloy or superlattices.[89,90] For example, Si_xGe_{1-x} NWs is a promising candidate, because both Si and Ge belong to the same group, have the same crystal structure, and display total solubility.

By using MD simulations, Chen *et al.*[91] demonstrated that the thermal conductivity of Si_xGe_{1-x} NW depends on the composition remarkably, as shown in Fig. 2(a). When Ge content is 50%, the thermal conductivity reaches the minimum, which is only about 18% of that of pure Si NW. The reduction of thermal conductivity mainly comes from the localization of phonon modes due to impurity scattering, which is reflected by the variation of phonon participation ratio. This suppression effect on thermal conductivity of Si_xGe_{1-x} NW has also been experimentally observed by Kim *et al.*[92] Moreover, by performing Boltzmann transport equation (BTE) approach, Li and Mingo[33] found that the alloy could enhance anisotropic thermal conductivity of Si_xGe_{1-x} NWs. As shown in Fig. 2(b), the room temperature thermal conductivity of a 100-nm-thick $Si_{0.6}Ge_{0.4}$ NW in the $\langle 001 \rangle$ direction is 16% higher than that in the $\langle 111 \rangle$ direction. At the low-temperature limit, the anisotropy of thermal conductivity can reach 87% at any alloy concentration. This anisotropy is caused by the phonon focusing effect for the long MFP phonons, in which low-frequency phonons focus in the $\langle 001 \rangle$ direction, while the intermediate-frequency phonons focus in the $\langle 111 \rangle$ direction.[33]

Constructing superlattice NWs is another way that can effectively reduce the thermal conductivity of pure NWs. With non-equilibrium MD simulations, Hu and Poulikakos[35] found ultralow values of thermal conductivity in Si/Ge superlattice NWs, taking advantage of the combination of surface and interfacial phonon scattering. As shown in Fig. 2(c), the thermal conductivity of Si/Ge superlattice NW varies non-monotonically with both the Si/Ge lattice periodic length and the NW cross sectional area. The optimal reduction of room temperature thermal conductivity is about an order of magnitude (92%), compared to the pristine single-crystalline Si NWs. There are two competing mechanisms governing the thermal transport in superlattice NWs: interface modulation hinders heat conduction,[34,35] while coherent phonons can counteract the interface effect and facilitate thermal transport at extremely short periodic lengths.[35,93,94] However, the coherent phonon/waves cannot be easily observed in most of superlattice NWs, such as in Kr/Ar superlattice NWs.[34] This is because short-wavelength phonons are easily scattered and long-wavelength phonons are very few in number.

In order to further reduce the thermal conductivity of superlattice NWs, other approaches are proposed to destroy the coherent phonon. For instance, Mu *et al.*[95] demonstrated through MD simulations that the already low thermal conductivity of Si/Ge superlattice NWs can be further reduced by introducing hierarchical structure, as shown in Fig. 2(d). The structural hierarchy introduces defects to disrupt the periodicity of regular superlattice and scatters coherent phonons, which are the key contributors to thermal transport in regular superlattice NWs. Compared to pure Si NW, they found that the reduction of thermal conductivity in Si/Ge hierarchical superlattice NWs can be as large as $\sim 95\%$.

Thermal transport in another novel superlattice NW, the crystalline/amorphous Si superlattice NWs,[96,97] has also been studied.[98] The cross-plane thermal conductivity of the crystalline/amorphous Si superlattices NW is very low, which is close to that of amorphous bulk Si even for amorphous layer as thin as ~ 6 Å. Interestingly, the cross-plane thermal conductivity increases weakly with temperature, which is associated with a decrease of the Kapitza resistance at the crystalline/amorphous interface with temperature.[98]

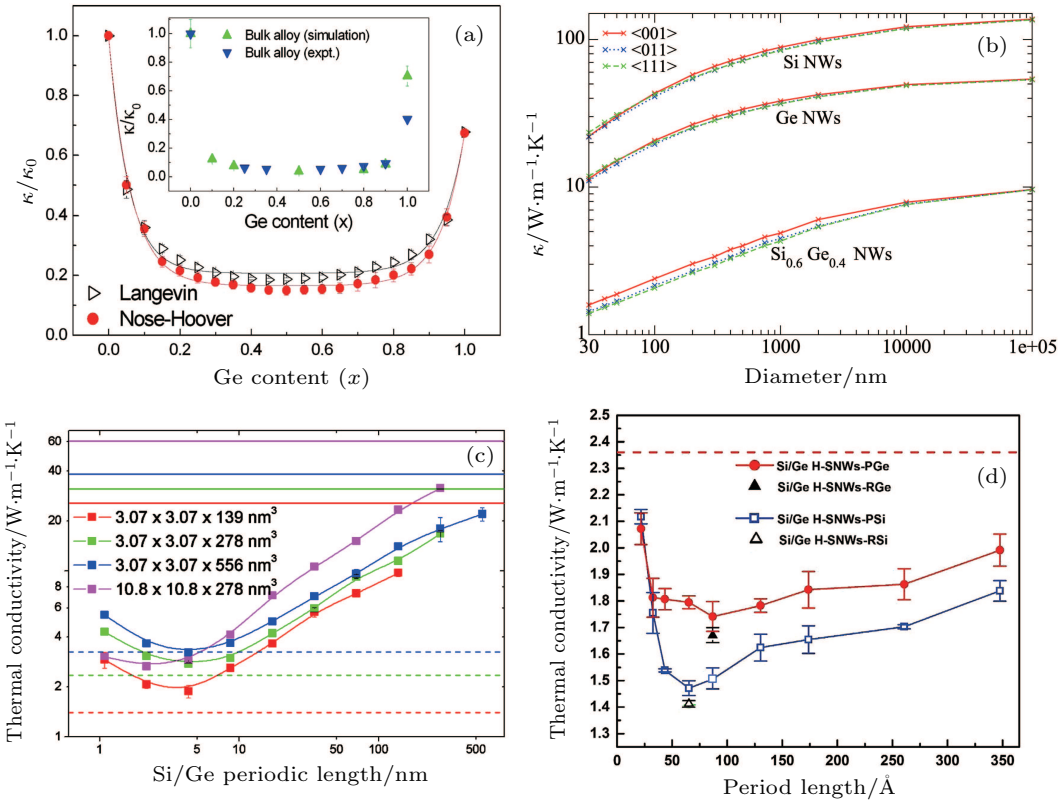


Fig. 2. (color online) Thermal conductivity of alloy and superlattice NWs. (a) Room temperature thermal conductivity versus concentration of Ge in $Si_{1-x}Ge_x$ alloy NWs. (b) Room temperature thermal conductivity of Si NWs, Ge NWs, and $Si_{0.6}Ge_{0.4}$ alloy NWs, as a function of the diameter for ⟨001⟩, ⟨011⟩, and ⟨111⟩ growth directions. (c) Periodic length dependence of the thermal conductivity of Si/Ge superlattice NWs for different total lengths. The solid and dashed lines represent the thermal conductivity of pure smooth Si NWs and $Si_{0.5}Ge_{0.5}$ alloy nanowires with same length and cross-section width, respectively. (d) Room temperature thermal conductivities of Si/Ge H-SNW (hierarchical superlattice nanowires) as a function of their period lengths. Two kinds of Si/Ge H-SNWs: periodically Si- or Ge-defected SNW (denoted as H-SNW-Psi or H-SNW-PGe), and randomly Si- or Ge-defected SNW (denoted as H-SNW-RSi or H-SNW-RGe). The red dashed line represents the thermal conductivity of regular Si/Ge SNW with the period of "AB". Panels adapted with permission from (a) Ref. [91], © 2009 AIP; (b) Ref. [33], ©2013 AIP; (c) Ref. [35], ©2012 ACS; (d) Ref. [95], ©2015, Macmillan Publishers Limited.

4. Structure engineering

The most innovative way to further modulate the thermal conductivity of NWs is via the structure engineering, such as core–shell structure, porous structure, resonant structure, and kinked structure. The structure engineering not only induces additional surface scattering, defect scattering, and phonon localization, but also controls the coherent wave-like transport behaviors, and consequently alters the thermal transport properties of NWs.

4.1. Core–shell structure

Core–shell NW is another type of heterostructures with additional interfaces, such as in Si–Ge[99] and III–V core–shell materials, which becomes an important class of nanomaterials because of their remarkable electronic, optical, and thermal properties as well as potential applications in nanoelectronics, nanophotonics, photovoltaics, and thermoelectrics.[100–102] The thermal transport in core–shell NWs also attracted lots of research interests, especially for Si–Ge NWs, due to the fundamental importance and applications in heat dissipation and thermoelectrics.[100,103,104] By using non-equilibrium MD simulations, Hu *et al.*[105] found that a simple deposition of a very thick Ge shell on a crystalline Si NW can lead to a dramatic 75% decrease of room temperature thermal conductivity compared to an uncoated Si NW, as shown in Fig. 3(a). They demonstrated that the reduction of thermal conductivity originates from the suppression and localization of long-wavelength phonon modes at the Si–Ge interface and high-frequency, non-propagating, diffusive modes. In addition, they also found that the phonon confinement of the core in Si–Ge NWs results in the thermal conductivity variation with NW length much weaker than in pure NWs,[106] and is almost independent of temperature in a wide region between 50 and 600 K.

Moreover, Chen *et al.*[36] found a remarkable oscillation effect in heat current autocorrelation function in core–shell NWs from equilibrium MD simulations, while the same effect is absent in pure Si NWs. This intriguing oscillation is caused by the coherent resonance effect (Fig. 3(b)), which results in the localization of the longitudinal modes and the reduction of thermal conductivity. Their following theoretical study[107] on the Si shell coated Ge NW also found a more than 25% reduction in thermal conductivity. They found that there is a critical coating thickness beyond which thermal conductivity of the

coated NW is larger than that of the host NW. Furthermore, interface roughness can induce further reduction of thermal conductivity, which causes localization of the high-frequency phonons. These findings are nicely consistent with experimental results from Wingert *et al.*[37] The core–shell effects on the reduction in thermal conductivity has also been reported in experimental study on Bi/Ti NW by Kang *et al.*[108]

4.2. Porous structure

Porous structures, such as porous bulk materials, thin films, and even single crystalline porous NWs, nowadays can be fabricated and have been proposed for different applications, ranging from lithium ion batteries to solar cells. The previous studies have shown that the porosity would induce large reduction in thermal conductivity due to the large reduction in phonon group velocities caused by coherent phononic effects,[109] and strong phonon localizations.[110] Inspired by these suppression phenomena, there are also some attempts to realize porous structures in NWs. Experimentally, Weisse *et al.*[38] found that in Si NWs with diameters larger than the phonon MFP, as shown in Fig. 3(c), the porosity substantially reduces the thermal conductivity. In highly porous Si NWs, thermal conductivities can be as low as 1 $W{\cdot}m^{-1}{\cdot}K^{-1}$. The theoretical work by Cartoixa *et al.*[111] revealed the underlying nature that the presence of pores suppressed the long MFP phonons, leading to the greatly reduced thermal conductivity in porous Si NWs. Moreover, they illustrated the failure of Matthiessen's rule to describe the coupling between boundary and pore scattering, which they accounted for by the inclusion of an additional empirical term. For the metal NWs, the excellent performance of heat exchange in porous Cu NW is experimentally observed by Jung *et al.*[39]

More interestingly, recent experimental work by Zhao *et al.*[112] demonstrates that with high spatial resolution through selective helium ion irradiation with a well-controlled dose, the structure porosity or defects in Si NWs can be optionally tuned. As shown in Fig. 3(d), they found that the local thermal conductivity along a single Si NW can be tuned to a desired value (between crystalline and amorphous limits), which makes it possible to control the flow of heat and derive novel functionalities, such as thermal rectification, thermal switching, and thermal cloaking.

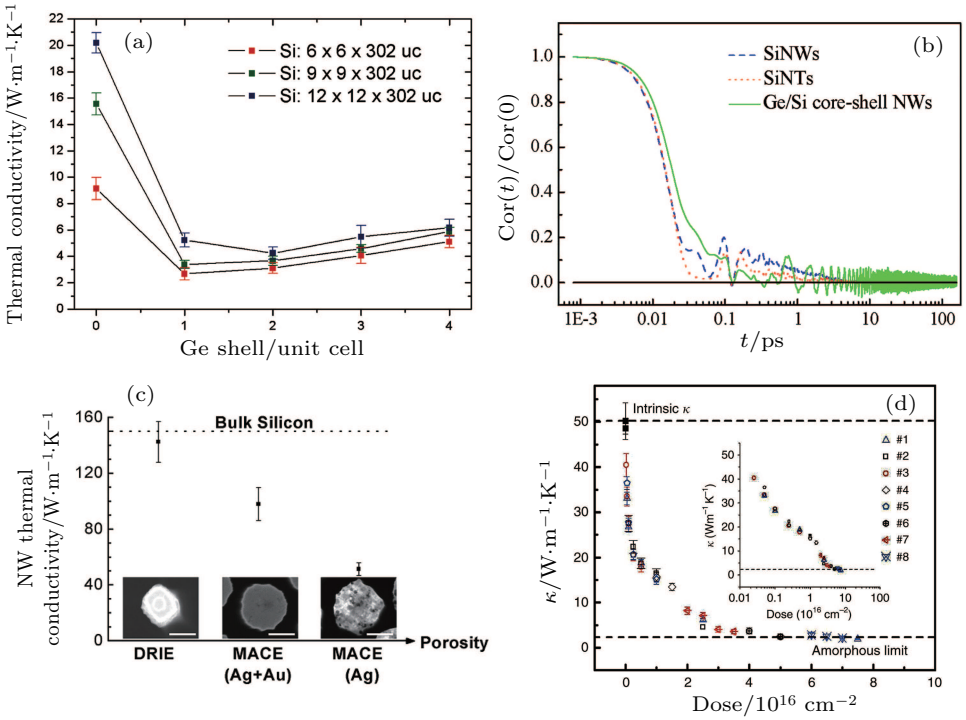


Fig. 3. (color online) Thermal conductivity of core–shell and porous NWs. (a) Overall thermal conductivity of the Si–Ge core–shell NW as a function of the number of layers in the Ge shell for different cross-sectional areas of the Si core. (b) Time dependence of normalized heat current autocorrelation function for Si NWs, Si NTs, and Ge/Si core–shell NWs. (c) Thermal conductivity with three levels of porosity corresponding to different etching conditions. (d) Measured thermal conductivity of Samples #1 to #8 versus dose. The inset is the same data plotted on a logarithmic scale. Panels adapted with permission from (a) Ref. [105], ©2011 ACS; (b) Ref. [36], ©2011 AIP; (c) Ref. [38], ©2012 Springer; (d) Ref. [112], ©2017 NPG.

4.3. Resonant structure

The concept of a locally resonant phonon mode is widely used to optimize the thermoelectric energy conversion efficiency, such as in clathrates, perovskites, and skutterudites,[113–115] leading to a large reduction of lattice thermal conductivity. The resonant/hybridized mode is also a basic concept to construct electron-crystal phonon-glass materials, which have great potential application in thermoelectric field due to the ultra-low thermal conductivity and excellent electric properties. Under this concept, Davis and Hussein[116]

proposed a Si resonant configuration, a silicon thin film with a periodic array of pillars on the free surfaces, which can qualitatively alter the phonon spectrum due to a hybridization mechanism between the pillar local resonances and the underlying atomic lattice dispersion. Similarly, for NWs Markussen *et al.*[117] demonstrated through atomistic calculations that the surface-decorated Si NWs, nanotrees and alkyl functionalized silicon NWs, can have a high ZT value ~ 1 due to the significantly reduced phonon conductance. The resonant transmission dips are observed in the nanotrees (Fig. 4(a)). They found that two quasi-localized vibrational modes, the rotational and flexural mode, lead to the phonon backscattering resonances, which are responsible for the dip in the thermal conductance around $T = 10$ K.

As a recent advance, Xiong *et al.*[40] proposed a novel NW structure, the branched alloy NWs. Using atomistic simulations, they found that this structure can combine designed resonant structures with the alloying effect, leading to the extremely low thermal conductivity in such Si NWs. The hybridization between resonant phonons and propagating modes greatly reduces the group velocities and the phonon mean free paths. As shown in Fig. 4(b), the branched resonators can produce numerous resonant frequencies in almost the acoustic range below 4 THz, and the resonant frequency can be tuned by the variation of the branch size and material. Meanwhile, alloy Si–Ge scattering hinders the propagation of high-frequency thermal phonons. Finally, the combination of two mechanisms yields a low thermal conductivity of 0.9 $\mathrm{W{\cdot}m^{-1}{\cdot}K^{-1}}$, which is only 53% of the corresponding amorphous thermal conductivity limit of Si NWs and 4.5% of the value for the pristine Si NWs.[40]

4.4. Kinked structure

Structure wrinkling or kinking is another effective way to manipulate thermal conductivity in NWs as the phonon transport channel is distorted. Based on MD simulations, Jiang *et al.*[41] found that thermal conductivity of kinked Si NW is 70% lower than that of pure NW at room temperature (Fig. 4(c)). They revealed that two mechanisms are responsible for this reduction: (i) the interchanging effect between the longitudinal and transverse phonon modes and (ii) the pinched localization for the twisting and transverse phonon modes in the kinked position. Recently, Zhang *et al.*[118] experimentally

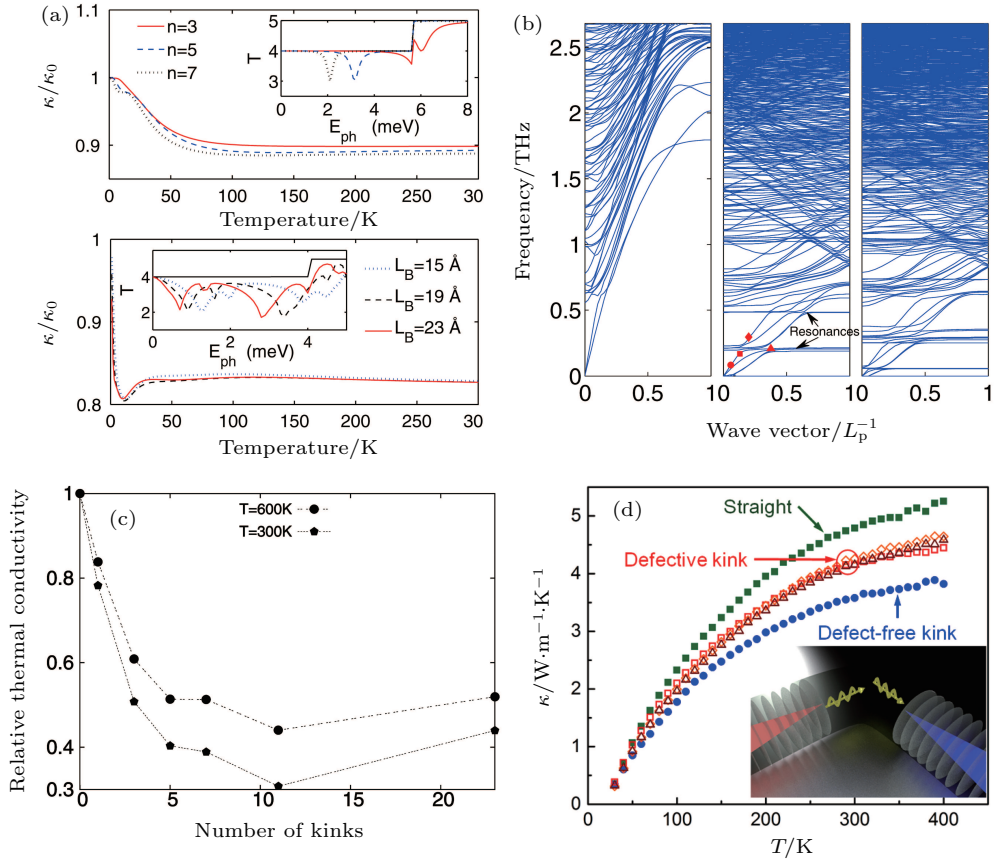


Fig. 4. (color online) Thermal conductivity of resonant and kinked NWs. (a) Thermal conductance ratio for alkyl functionalized Si NWs with different branch lengths n (top panel) and for nanotrees with different branch lengths L_B (bottom panel). The insets show the phonon transmission function at low energies, and Fano-like resonant scattering is observed. (b) Phonon dispersion for pristine Si NWs, and two-side branched Si NWs with branch length 1.63 nm and 3.26 nm. (c) Relative thermal conductivity versus number of kinks in kinked Si NWs of 11.0 Å in diameter and 190.0 Å in length along the axial direction. (d) Thermal conductivity of boron carbide nanowires which are straight, with defect-free kinks, and with defective kinks, respectively. Panels adapted with permission from (a) Ref. [117], ©2009 APS; (b) Ref. [40], ©2016 APS; (c) Ref. [41], ©2013 ACS; (d) Ref. [118], ©2017 ACS.

found an unusual phenomenon in kinked boron carbide NWs. Firstly, the defect-free kinked NW has thermal resistance up to ~ 30 times larger than that of a straight NW, which is attributed to the combined effects of backscattering of highly focused phonons and required mode conversion at the kink. Interestingly, the structural defects in the kink can anomalously assist phonon transport through the kink and reduce its thermal resistance, leading to the enhanced thermal conductivity,[118] as shown in Fig. 4(d).

There are other structural engineering methods in NWs very similar to the structural kinking, such as sawtooth NWs[119] and twinning superlattice NWs,[120] and interesting thermal transport behaviors are observed in these structures. For example, by using Monte Carlo simulations, Moore *et al.*[119] found that the sawtooth roughness on a NW can also cause phonon backscattering and suppress the thermal conductivity below the diffuse surface limit. The backscattering effect can be accounted for only by a negative specularity parameter if the detail of the surface roughness is ignored. The phonon localization phenomenon in twinning superlattice NWs is studied by Xiong *et al.*[120] by using non-equilibrium MD simulations, in which they found the disappearance of favored atom polarization directions and large reduction in thermal conductivity.

5. Applications

5.1. Thermoelectric properties

Because of the important potential applications in the thermoelectric field, there have been tremendous efforts to optimize thermoelectric properties of NWs by reducing the lattice thermal conductivity. As reported in an early experiment in 2008, Hochbaum *et al.*[24] reported that the rough Si NWs exhibit 100-fold reduction in thermal conductivity compared to bulk counterpart, without much affected Seebeck coefficient and electrical resistivity, thus yielding $ZT = 0.6$ at room temperature. These findings encouraged the further studies on reducing thermal conductivity of NWs with various mechanisms.[7,26,27,121] For Si NWs, Markussen *et al.*[117] proposed surface-decorated silicon NWs, nanotrees and alkyl functionalized silicon NWs, to improve thermoelectric performance, showing larger ZT than that in ultrathin Si NWs.[30] Benefitting from the large suppression of thermal transport in porous silicon NW arrays, Zhang *et al.*[29] experimentally found that the large-area porous silicon NW arrays exhibit a high Seebeck coefficient up to 513 $\mu V \cdot K^{-1}$ and a thermal conductivity down to 1.68 $W \cdot m^{-1} \cdot K^{-1}$, resulting in a high ZT value of 0.493 at 300 K, which is 77 times higher than that of the bulk silicon and other reported NW arrays.

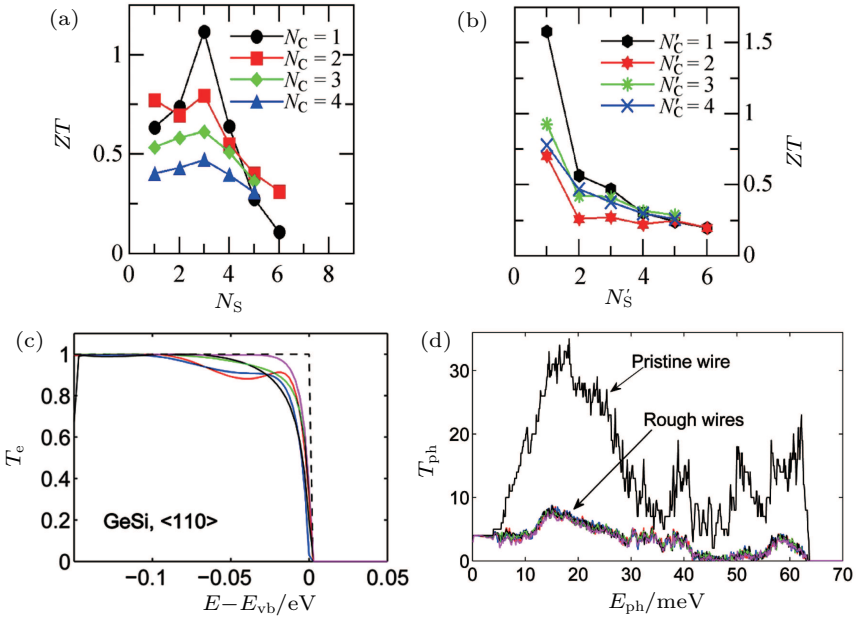


Fig. 5. (color online) Thermoelectric properties of NWs. Thermoelectric figure of merit as a function of the number of atomic layers in the shell, N_S for (a) clean Si/Ge and N'_S for (b) clean Ge/Si NWs with different core sizes N_C and N'_C. Electronic (c) and phononic (d) transmission functions through wires with different surface roughness disorder. In panel (c) the transmission of the pristine wires are shown by dashed lines. Panels adapted with permission from (a) and (b) Ref. [100], ©2015 Springer; (c) and (d) Ref. [122], ©2012 ACS.

As mentioned above, the core–shell NWs possess low thermal conductivity, which should result in optimal thermoelectric properties in NWs. As shown in Fig. 5(a), Yang *et al.*[100] demonstrated that the presence of a thin Ge shell on a Si core NW increases the overall figure of merit, and there is an optimal thickness of the Ge shell to provide the largest figure of merit in Si–Ge core–shell NW. For the Ge-core/Si-shell NWs, the figure of merit monotonically decreases with the radius of NWs (Fig. 5(b)). Interestingly, by using atomistic calculations, Markussen[122] found the decoupling of the

electronic and phonon transport in surface disordered Ge–Si core–shell NWs. The surface roughness should significantly suppress the phonon thermal conductance (Fig. 5(d)), while maintain large electronic conductance values even with surface disorder (Fig. 5(c)), because the hole states are confined to the Ge core shielded from the surface disorder. This decoupling method makes the Ge–Si core–shell NWs a very promising candidate for thermoelectric applications.

Because of the adjustable low lattice thermal conductivity of NWs, there are also other types of NWs which have been investigated in the thermoelectric field, such as SnTe,[123] GaSb,[124] Ag_2Te,[125] PbTe,[126] and Bi.[73] For the single crystalline NWs, the diameter-dependent thermoelectric properties of individual Bi NWs and SnTe NWs were recently investigated in experiments by Kim *et al.*[73] and Xu *et al.*,[123] respectively. Moreover, the heterostructure NWs for the hybrid materials also show enhanced thermoelectric performance due to the further reduced lattice thermal conductivity in NWs, such as GaSb/InAs core–shell NWs,[124] Bi/Te core–shell NWs,[28] and PbTe/Ag_2Te heterostructure.[127]

5.2. Thermal management

The controllable thermal conductivity of NWs also provides the ideal platform and materials for thermal management in nanomaterials, not only for heat dissipation application but also for exploring unique thermal transport phenomenon.[128,129] Most importantly, the different scattering mechanisms can only dominate the thermal transport in a certain range of frequency. For example, high frequency phonons are sensitive to impurity/doping[130] and defect/porous scattering[131] in various NWs. In addition, low frequency phonons can be scattered by the interface in superlattices NW,[45] the amorphous disorder in polycrystalline NW,[51] and coherent resonance in core–shell structures.[36] Therefore, in a NW, the thermal conductivity or phonons transport can be managed in a well-controlled fashion. For example, by using atomic simulations, thermal rectification phenomena in NWs are reported by Zhang *et al.*[128] In a graded Si NW (Fig. 6(a)), they found that the thermal rectification ratio increases non-monotonically with the geometric asymmetry, as shown in Fig. 6(b). The ratio exhibits a sharp reverse when the vertex angle of the graded NW is approximately 90°. This abnormal behavior is originated from the match/mismatch between the vibrational spectra in two ends, as shown by the S_+/S_- ratio. Cartoixa *et al.*[132] also reported the thermal rectification in asymmetric two-segment Si NWs. Their results show that the diameter dependent thermal conductivity and surface scattering in the pure NWs lead to the thermal rectification. In addition, Liu *et al.*[133] proposed a graded NW with a core–shell cross-section, in which an apparent thermal rectification is revealed. They claimed that this phenomenon is originated from standing waves that hinders the propagation of phonon waves, which is similar to the phonon coherent resonances in Si–Ge core–shell NW.[36]

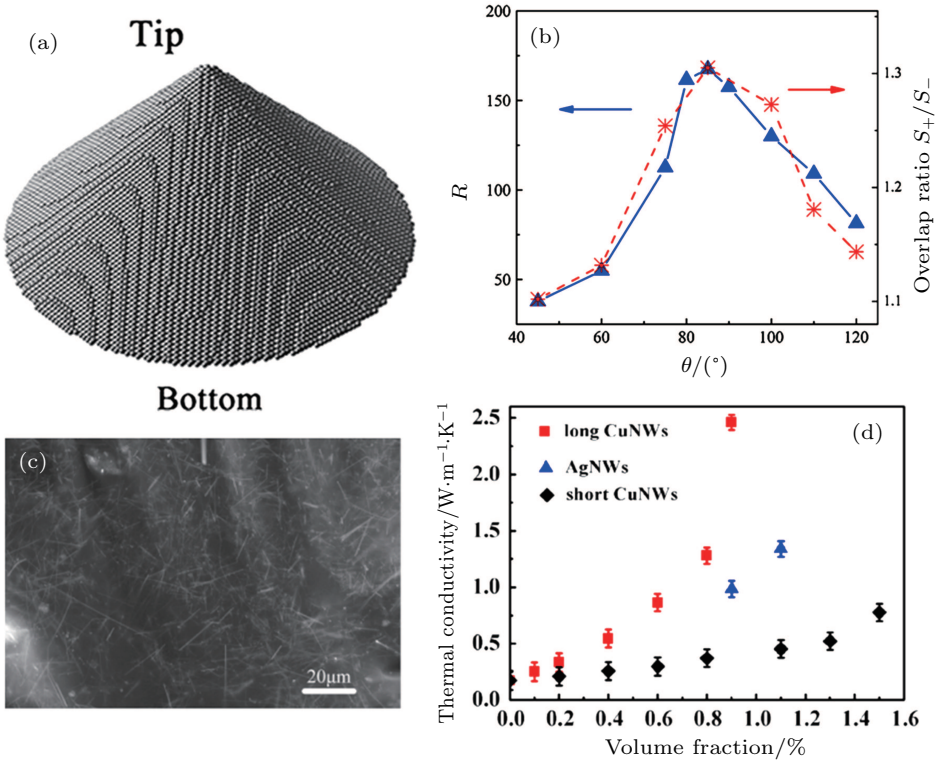


Fig. 6. (color online) Thermal management of NWs. (a) Schematic drawing of the graded Si NWs. (b) Rectification ratio (left vertical axis) and normalized S_+/S_- of phonon density of states overlap ratio (right vertical axis) as function of angle. (c) SEM images of short-CuNW–polyacrylate composites. (d) Experimental thermal conductivity of metal NW–polyacrylate composites with different volume fractions at 298 K. Panels (a) and (b) adapted with permission from Ref. [128], ©2016 Elsevier; (c) and (d) from Ref. [137], ©2014 ACS.

Moreover, recently some works engaged in using NWs to improve the heat-transfer performance and stability of flow boiling system, which is used for the cooling of high-thermal-load systems, such as power plants and integrated electrical devices. For example, Li *et al.*[134] successfully synthesized Si NWs *in situ* in parallel silicon micro-channel arrays, and integrated NWs into micro-channel heat sinks. Finally, they found that such setup can significantly enhance the flow boiling heat transfer and suppress the flow boiling instability in the NW which acts as the coatings for the flow boiling system. In addition, Shim *et al.*[135] found that the aligned silicon NWs exhibit improved heat dissipation properties compared to the conventional random silicon NWs. The alignment can increase the critical heat flux significantly with efficient coolant supply, and ensure high stability in extremely high thermal load systems.

Meanwhile, the metal NWs coatings for the flow boiling system have also been experimentally investigated. Morshed *et al.*[136] found that the Cu NWs coatings can enhance the single-phase heat transfer rate by up to $\sim 25\%$, whereas in the flow boiling regime, the enhancement was up to $\sim 56\%$ with a pressure drop increased by $\sim 20\%$ in the single-phase regime. Moreover, Wang *et al.*[137] found that Cu NWs as filling materials can enhance the interfacial thermal transport. The high-aspect-ratio is beneficial to achieve low percolation threshold for nano-composites, and thermal conductivity value of 2.46 $\mathrm{W{\cdot}m^{-1}{\cdot}K^{-1}}$ was obtained at an ultralow loading fraction, which was enhanced by 1350% compared with plain matrix (see Figs. 6(c) and 6(d)). Hsu *et al.*[138] proposed a system for personal thermal management using metallic NW-embedded cloth that can reduce the heat waste. The metallic NWs form a conductive network that not only is highly thermally insulating because it reflects human body infrared radiation, but also allows Joule heating to complement the passive insulation.

6. Conclusion

In this review, we present the state-of-the-art studies on the topics of manipulation and fundamental understanding of the thermal conductivity of NWs, including Si, Ge, Bi, Ti, Cu, Ag, Bi_2Te_3, ZnO, AgTe, and their hybrids. Various important size effects on thermal transport in NWs are discussed, such as length, diameter, orientation, and cross-section effects. We also review the diverse influencing factors and effective pathways to engineer the thermal transport in NWs, such as alloy, superlattices, core–shell structure, porous structure, resonant structure, and kinked structure. Correspondingly, several important thermal transport behaviors and unique underlying physical mechanisms are presented. Based on the understanding and effective manipulation of thermal transport in NWs, we also summarize the important potential applications of NWs from the aspects of thermal conductivity of NWs, including thermoelectric field and thermal management. It should be noted that although this review mainly focuses on thermal transport related fields, NWs also possess exotic properties and many applications in other fields, such as optics and electronics.

7. Outlook

In this review, we have clearly presented that there has been significant progress in the understanding and manipulation of the thermal conductivity in various NWs in the past decade. Yet further systematical investigations from both experimental and theoretical efforts are still needed in this research direction. For example, although various methods and pathways are proposed to reduce the thermal conductivity for optimizing thermoelectric properties in NWs, the explored figure of merit in NWs is still behind the requirement for practical industry use. Therefore, further improvements on these materials are expected by combining experimental and theoretical efforts together.

Generally speaking, only a limited portion of phonons, particularly high-frequency phonons, is efficiently suppressed or scattered in NWs. However, long wavelength or low-frequency phonons still possess a significant contribution to thermal conductivities. Therefore, novel strategies that can alter phonons in a wide or full range of frequency, especially for the low-frequency spectrum, are highly desirable to obtain an even lower thermal conductivity. Besides, it is important to incorporate different mechanisms together to achieve optimized ZT, as a single scattering mechanism alone only affects phonons with certain frequencies.

Finally, there are some unique phonon transport behaviors where a comprehensive understanding is still lacking, such as the coherent phonon/wave effect on the thermal transport in NWs. In the superlattice NWs, the coherent scattering and interference of thermal phonons could happen at the atomically smooth interfaces with perfect periodicity. This phenomenon is related to many practical applications, such as waveguides or cloaking. To conclude, we believe that thermal transport in NWs is still an active research topic worth exploring for future study.

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