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TOPIC REVIEW — Thermal and thermoelectric properties of nano materials

Surface effects on the thermal conductivity of silicon nanowires*

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Thermal transport in silicon nanowires (SiNWs) has recently attracted considerable attention due to their potential applications in energy harvesting and generation and thermal management. The adjustment of the thermal conductivity of SiNWs through surface effects is a topic worthy of focus. In this paper, we briefly review the recent progress made in this field through theoretical calculations and experiments. We come to the conclusion that surface engineering methods are feasible and effective methods for adjusting nanoscale thermal transport and may foster further advancements in this field.

Keywords: silicon nanowires, thermal conductivity, phonon transport, surface effect

PACS: 68.65.–k, 44.10.+i, 63.22.–m , 65.80.–g **DOI:** 10.1088/1674-1056/27/3/036801

1. Introduction

The utilization of nanostructures for controlling thermal properties is a fast-growing research area.[1] Thermal transport in low-dimensional nanomaterials has recently become a research hotspot because it is a fundamental issue in solid-state physics and has significant practical applications in nanotechnology.[2–5] Specifically, the manipulation of heat-carrying phonons, or elastic waves that propagate and scatter, in nanoscale materials can provide beneficial thermal properties that are different from those of macroscopic bulk samples. One of the most significant applications of nanomaterials is related to thermoelectrics, that is, the conversion of heat energy into electricity and vice versa. The efficiency of thermoelectric (TE) devices (Fig. 1) is characterized by the figure of merit, $ZT = S^2\sigma T/\kappa$, of the material, where S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature, and κ is the total thermal conductivity ($\kappa = \kappa_p + \kappa_e$, where κ_p and κ_e are the phonon and electronic contributions, respectively).[6] A $ZT > 3$ is required for commercial use. Figure 2 shows the typical TE ZT in various temperature ranges of many materials that already are, or have the potential to be, used in industry. The TE ZT values of all the materials are below 2, even at increased temperature (Fig. 2).[7] The low efficiency of current TE materials limits their widespread application. Finding an effective method to improve the efficiency of TE materials has become a key issue in current TE research.

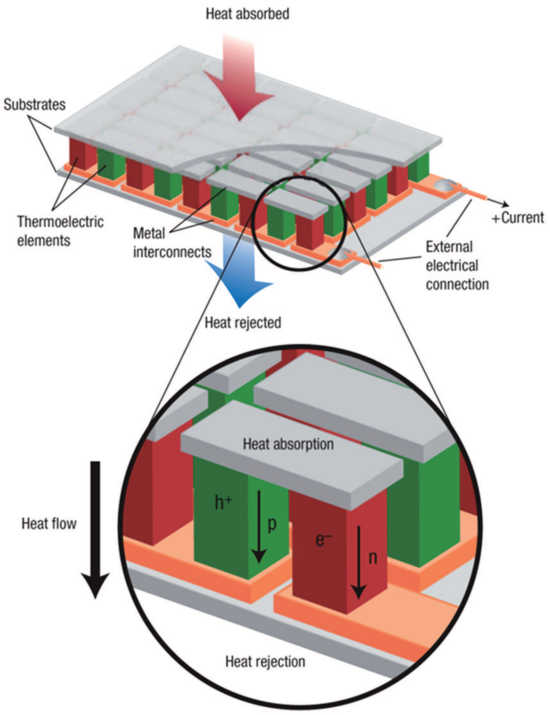


Fig. 1. (color online) Schematic of TE module showing the direction of charge flow in cooling and power generation (from Ref. [1]).

The strategies for improving the ZT of established TE materials have focused on two aspects: 1) enhancing the electric transport properties of TE materials by modifying the band structure near optimal carrier concentrations and 2) decreasing the thermal conductivity.[8] However, an increase in α normally implies a decrease in σ because of carrier density considerations, whereas an increase in σ indicates an increase in the electronic contribution to κ. Thus, independently control-

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ling these variables to increase the ZT value of bulk materials is very difficult.[1] Thankfully, when the dimensions of a material decrease, its size becomes a new variable that determines its electronic and thermal properties. Therefore, the use of low-dimensional nanostructures to decrease κ without negatively affecting the power factor $S^2\sigma$ provides a promising avenue for achieving TE energy conversion with high ZT values.[9]

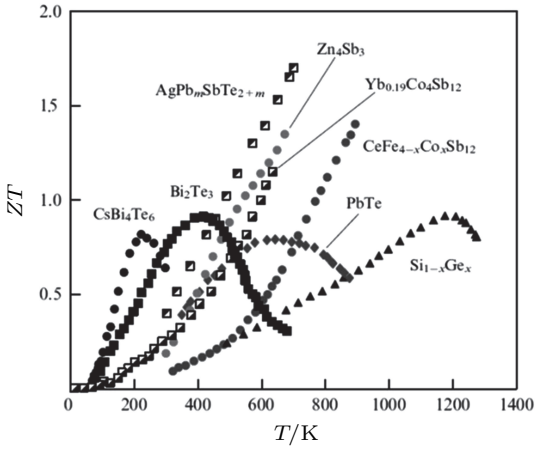


Fig. 2. (color online) Dimensionless ZT of popular or prospective TE materials (from Ref. [7]).

The development of nanotechnology has enabled the fabrication of materials with structural sizes of a few nanometers.[10] Si nanostructures are a central component of modern micro/nanoelectronics. Silicon nanowires (SiNWs), which are one-dimensional (1D) nanostructures, have stimulated a surge of research interest in TE nanomaterials given their excellent compatibility with conventional Si-based technology. Bulk Si, however, is a poor TE material ($ZT \approx 0.01$ at 300 K) because of its high κ value. Nevertheless, Hochbaum *et al.*[11] and Bukai *et al.*[12] independently developed SiNWs with significantly improved ZT values. Hochbaum *et al.* obtained a ZT value of 0.6 at 300 K for rough SiNWs. They suspected that surface roughness has a crucial role in scattering a broad spectrum of phonons, thus fundamentally altering the phonon transmission mechanisms of the SiNW structures.[11] Bukai *et al.* reported ZT values of approximately 0.4 at 300 K and 1.0 at 200 K for doped SiNWs and demonstrated that decreasing the diameter of SiNWs decreases the electrical conductivity and considerably increases the Seebeck coefficient.[12] Such findings have inspired the research community to reconsider the applications of Si in TE and provide a new strategy for increasing ZT values by decreasing the thermal conductivity.

The effects of size, cross-section, interface, defect, and surface roughness on the thermal conductivity of SiNWs have been studied.[13–24] These aforementioned studies propose the principles behind various strategies that decrease the thermal conductivity of SiNWs and provide guidance for the experimental realization of these strategies.[15] We direct readers interested in these topics to recent review papers.[2,7,25–29] This paper provides a review of the recent advances in the research on thermal transport in SiNWs, with particular emphasis on the surface effects of tunable phonon thermal conductivity. Studies on the thermal conductivity of pristine SiNWs are briefly reviewed in Section 2. Studies on the adjustment of the thermal conductivity of SiNWs by surface effects are reviewed in Section 3. Finally, concluding remarks are provided in Section 4.

2. Phonon thermal transport in SiNWs

The thermal conductivity of high-purity bulk Si has been experimentally measured.[30,31] Si is not often used to insulate hot objects given that it conducts heat well, with a relatively high thermal conductivity of approximately 150 W/mK at room temperature. The electronic contribution to thermal energy transport in Si is negligible because electrons are tightly bound to the atomic nuclei. In fact, this electronic contribution has been experimentally determined as approximately 0.65 W/mK at 1000 K (approximately 2% of the total value of 31.0 W/mK) and can be negligible below 1000 K.[32]

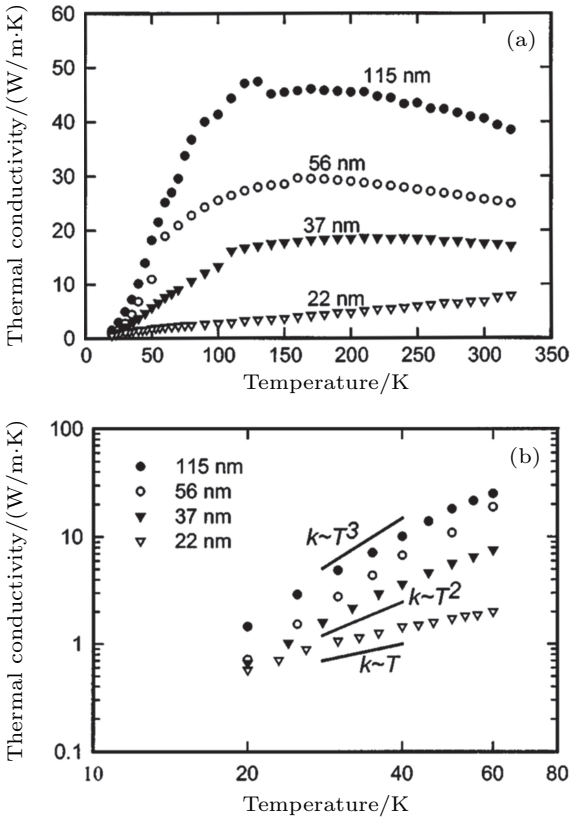


Fig. 3. (a) Measured thermal conductivity of SiNWs with different diameters. The number beside each curve denotes the corresponding wire diameter. (b) Low-temperature experimental data on a logarithmic scale. T^3, T^2, and T^1 curves are shown for comparison (from Ref. [46]).

The thermal conductivity of SiNWs can significantly differ from that of bulk Si because of the size effect and high

surface-to-volume ratio of SiNWs. In early studies, thermal transport in SiNWs was studied through various theory-based methods, including equilibrium and non-equilibrium molecular dynamics (MD) simulations,[33–38] Monte Carlo (MC) simulations[39,40] and lattice dynamics, the non-equilibrium Green function formalism, and the Boltzmann transport equation.[41–45] Several works have demonstrated that the thermal conductivity of pristine nanowires is strongly dependent on their diameter, shape, and surface roughness.[11–13,46,47] For example, in 1999, Volz and Chen used equilibrium MD simulations to discover a remarkable reduction in the thermal conductivity of SiNWs.[33] Two main factors are likely responsible for the low thermal conductivity of SiNWs: on one hand, long-wavelength phonons that act as the main contributors to thermal conductivity are suppressed in the nanowire because the mean free path of phonons is limited by the nanowire size; on the other hand, with the decrease in nanowire diameter, the surface-to-volume ratio increases, and phonon boundary scattering thus becomes more dominant in the nanowire, further decreasing the thermal conductivity.

Li *et al.*[46] presented the mesoscopic thermal transport measurements of individual SiNWs that were synthesized through the vapor–liquid–solid (VLS) method. As shown in Fig. 3(a), the thermal conductivity of individual SiNWs decreases with decreasing diameter. When the wire diameter decreases to below 150 nm, the thermal conductivity of the smooth VLS-grown SiNWs is significantly lower than the bulk value and can closely follow predictions based on Boltzmann transport theory, assuming that diffuse boundary scattering is the dominant phonon-scattering mechanism. The thermal conductivity at 300 K ranges from 40 W/mK to 9 W/mK for SiNWs with diameters that range from 115 nm to 22 nm, respectively. This finding provided the first experimental evidence for the importance of phonon boundary scattering in evaluating the thermal conductivity of NWs. The researchers also observed the anomalous temperature dependence of SiNWs with small diameters (Fig. 3(b)). In order to understand the physical mechanism that underlies the decreased thermal conductivity of SiNWs, different groups used theoretical models and simulations to predict the phonon thermal conductivity of NWs. For example, Mingo *et al.*[20] theoretically predicted the temperature dependence of thermal conductivity in Si and Ge nanowires and found that the traditional Callaway and Holland approaches show large disagreements with experimental data whereas the real dispersions approach yields good agreement with experiments for SiNWs between 37 nm and 115 nm wide. Martin *et al.*[48] and Malhotra *et al.*[49] performed studies on the thermal conductivity of SiNWs, accurately considering the effect of surface roughness and phonon confinement. Xie *et al.*[50] theoretically showed that phonon surface scattering controlled the length dependence of the thermal conductivity of SiNWs. In addition, various MC simulations were performed to simulate phonon interactions in SiNWs and the thermal conductivity at different temperatures was calculated.[39,51,52]

3. Surface effects of phonon thermal transport in SiNWs

SiNWs exhibit a large surface-to-volume ratio, which increases with decreasing size. The electronic and thermal properties of SiNWs differ significantly from those of bulk silicon owing to the surface effect.[48,53–57] Consequently, the surface effects and characteristics have received extensive research attention given their key role in SiNWs. Surface atoms may play an important role in the overall thermal transport properties of SiNWs, particularly in those of thin SiNWs.[15] Therefore, the effect of surface treatments on phonon transport to further decrease the thermal conductivity of SiNWs remains the focus of researchers' interest. A parallel and simultaneous investigation of phonon transport is clearly needed in light of the extreme sensitivity of electron transport in nanostructures to the surface condition.[48,58] The thermal conductivity of SiNWs has been tuned through various theoretical and experimental surface engineering methodologies based on surface roughness, surface chemical functionalization, surface disorder, and surface doping.[28]

3.1. Surface roughness

Li *et al.* observed that smooth VLS-grown SiNWs have low thermal conductivity.[46] The thermal conductivity of electroless-etched (EE) SiNWs is five- to eight-fold lower than that of smooth VLS-grown SiNWs.[11] The surprising reduction in thermal conductivity to a value below the Casimir limit cannot be explained by phonon boundary scattering alone.[59] Hochbaum *et al.* concluded that this unusually large reduction may be due to the surface roughness of the EE SiNWs.[11] Different groups have analyzed the effect of surface roughness, although the exact mechanism of phonon roughness scattering remains unclear. Through MC simulations, Moore *et al.* proposed a backscattering mechanism in SiNWs with sawtooth structures.[60] Wang *et al.* investigated the effect of surface roughness on thermal conductivity using an indirect MC method that accounts for the multiple scattering of phonons at a rough surface.[61] Martin *et al.* studied the effect of NW surface roughness through a perturbation theory and suggested that thermal conductivity is limited by surface asperities.[48,62] Recently, Malhotra *et al.* investigated the impact of phonon surface scattering on the distribution of thermal energy across phonon wavelengths and mean free paths in Si and SiGe nanowires. They presented a rigorous and accurate description of surface phonon scattering and predicted

heat transport in nanowires with different diameters and surface conditions.[63] Xie *et al.* utilized a kinetic model to investigate the anomalous thermal conductivity of SiNWs by focusing on the mechanism of phonon boundary scattering.[50] Carrete *et al.*[64] found that surface roughness along with deep defects in the nanowire may decrease the thermal conductivity of SiNWs. They reported that the theoretical thermal conductivity of SiNWs could be lower than Casimir's classical limit for deep surface degradation. However, the Casimir formula provides a good approximation of the phonon mean free paths and conductivity of SiNWs with shallow surface roughness.[64]

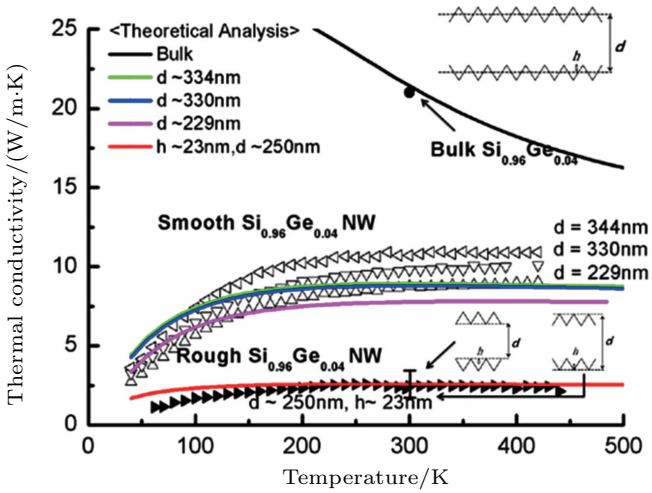


Fig. 4. (color online) Temperature-dependent thermal conductivities of bulk, smooth, and rough $Si_{0.96}Ge_{0.04}$ nanowires (from Ref. [65]).

Although current theoretical works have shed some light on the dependence of thermal conductivity on surface roughness, an experimental determination of the dependence of the thermal conductivity on the surface roughness of SiNWs remains lacking. Kim *et al.* synthesized VLS-grown rough $Si_{1-x}Ge_x$ nanowires and measured their thermal conductivities.[65] As shown in Fig. 4, the thermal conductivity of smooth $Si_{0.96}Ge_{0.04}$ nanowire is approximately four times higher than that of rough $Si_{0.96}Ge_{0.04}$ nanowire. Theoretical analysis demonstrated that mid-wavelength phonons are scattered by rough surfaces. In fact, the effect of roughness parameters on the thermal conductivity of SiNWs is remarkable.[66,67] As expected, the thermal conductivity decreases with increasing the root-mean-square height Δ of the surface and increases with increasing correlation length ξ (the surface "looks" smoother with a higher ξ).[67] Lim *et al.* experimentally studied the dependence of the thermal conductivity on the surface roughness of SiNWs.[59] Experimental observations showed that the surface of VLS-grown SiNWs is rough, with root-mean-square values that range from 0.3 nm to 5 nm. As shown in Fig. 5, the thermal conductivity significantly decreases with increasing surface roughness. The coefficient of the surface roughness of single-phase crystalline SiNWs is well correlated with the reduction in thermal conductivity.[59]

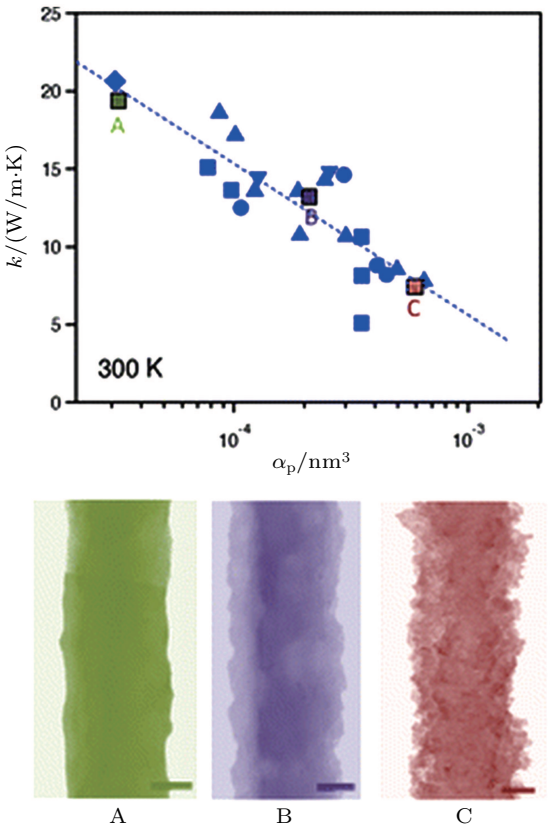


Fig. 5. (color online) Measured thermal conductivity as a function of roughness factor α_p at 300 K (from Ref. [59]).

3.2. Surface chemical functionalization

SiNWs are easily oxidized in air given the numerous dangling bonds distributed on their surfaces. Hydrogen termination on the surface is a natural consequence of the hydrogen fluoride treatment of synthesized SiNWs.[56] In addition, the large surface-to-volume ratio of SiNWs provides an extensive area for surface functionalization.[53] Park *et al.* proposed the selective surface functionalization of SiNWs through a nanoscale Joule-heating method.[68] Surface chemical functionalization is crucial for electronic and thermal transport in SiNWs. Earlier theoretical studies have shown that passivating atoms, such as hydrogen and nitrogen, on the surfaces of Si nanostructures provide structurally stable structures and clean gap states.[54,69] The electrical and thermal conductivities of SiNW arrays and silicon membranes can be tuned through surface chemical modification.[58,70] Liu *et al.* experimentally studied the effect of surface chemistry on thermal transport in colloidal nanocrystals and demonstrated that the thermal conductivity of colloidal nanocrystal solids can be varied by an overall factor of 4 from $\sim$ 0.1 W/mK to 0.4 W/mK.[71] Notably, the thermal conductivity of hydrogenated SiNWs is slightly higher than that of naked SiNWs.[16,41] However, the thermal conductivity of nitrogenated SiNWs is remarkably

lower than that of fully hydrogenated SiNWs. As shown in Fig. 6, the functionalization of 14% of the surface Si atoms by nitrogen atoms decreases the thermal conductivity of SiNWs by $\sim 43\%$, and the functionalization of 29% and 43% of surface Si atoms further decreases the thermal conductivity by $\sim 60\%$ and $\sim 75\%$, respectively.[15] Markussen *et al.* utilized atomic calculations for electron and phonon transport to investigate the properties of alkyl-functionalized SiNWs.[72] Their results showed that phonon conductance significantly decreases relative to electronic conductance, thus providing SiNWs with a high thermoelectric figure of merit.

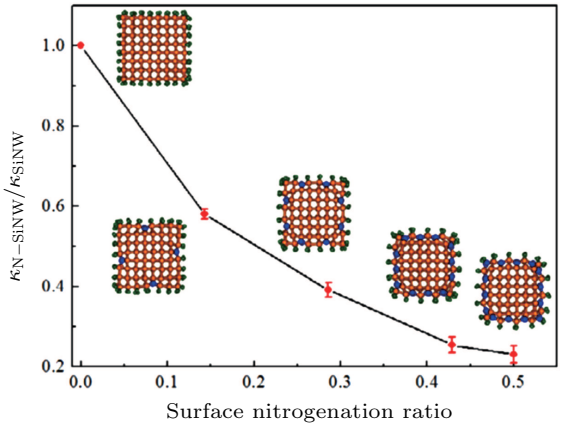


Fig. 6. (color online) Variation in the calculated longitudinal thermal conductivity of nitrogenated SiNWs (κ_{N-SiNW}) as a function of the surface nitrogenation ratio compared with that of pure SiNW (κ_{SiNW}) (from Ref. [15]).

3.3. Surface disorder

In addition to surface roughness mentioned above, the surface structure of SiNWs can be tailored by inducing surface disorder. An amorphous surface/shell layer can often form during the growth of NWs. Phonon scattering by surface roughness is different from that by an amorphous shell.[28] In general, the amorphous phase has low thermal conductivity; thus, crystalline core and amorphous shell nanostructures may be used to modulate thermal conductivity to enhance the ZT value of NWs.[73–75] For example, under a very low temperature limit, the thermal conductivity of core–shell (CS) NWs with a thick amorphous surface shell is lower than that of rough crystalline NWs[73] because of interface scattering and phonon-coherent resonance.

Sansoz[76] performed direct MD simulations to investigate the dependence of thermal transport on surface faceting in SiNWs and found that crystalline [111] SiNWs with periodic sawtooth faceting have significantly lower thermal conductivity than nanowires of the same size with smooth sidewalls (Fig. 7). The thermal conductivities of crystalline SiNWs and SiNWs with amorphous shells were also calculated through MD.[77,78] As shown in Fig. 8, the thermal conductivity of amorphous SiNWs decreases by 80% relative to that of pure crystalline SiNW with the same size due to strong phonon scattering at the interface, as well as the non-propagating diffusion of phonons in the amorphous region.[78] The behavior of thermal conductivity in crystalline SiNWs also displays an unusual temperature dependence: the thermal conductivity of crystalline SiNW monotonically decreases with temperature following $1/T$. However, the thermal conductivity of amorphous SiNW remains nearly constant in the temperature range considered in the study and is analogous to that of its bulk counterpart. The temperature dependence of crystalline core–amorphous shell SiNW is considerably weaker than that of crystalline SiNW. These different temperature trends reflect the different natures of the dominant scattering mechanisms in the materials. The thermal conductivity of crystalline SiNWs is proportional to $1/T$ because of the dominance of normal and Umklapp phonon scattering processes. The κ of amorphous SiNWs (a-SiNWs) is constant because structural disorder mainly contributes to scattering.

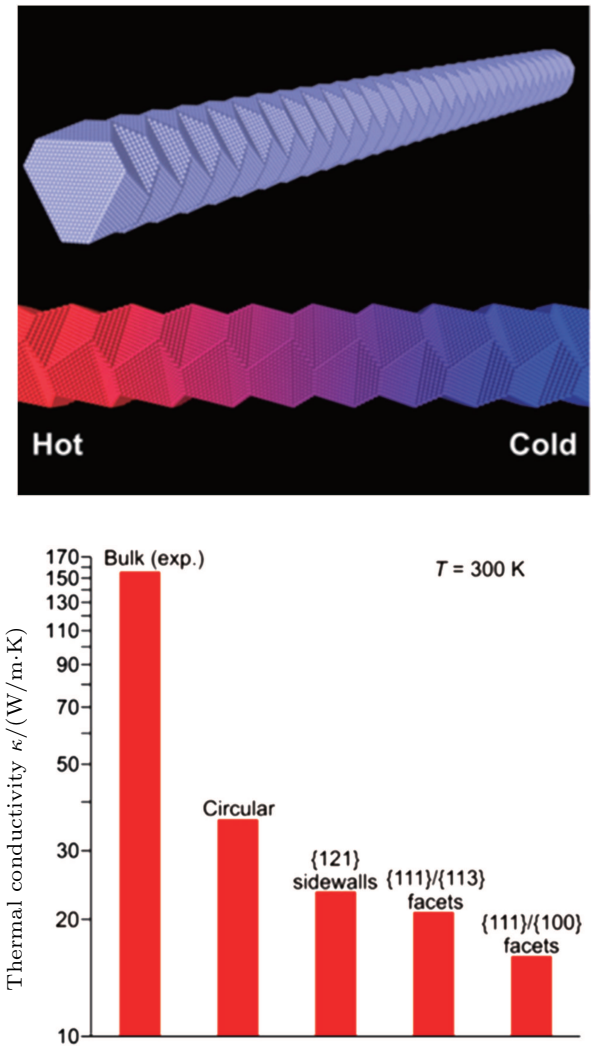


Fig. 7. (color online) Effects of surface structure on the lattice thermal conductivity of [111] SiNWs at 300 K (from Ref. [76]).

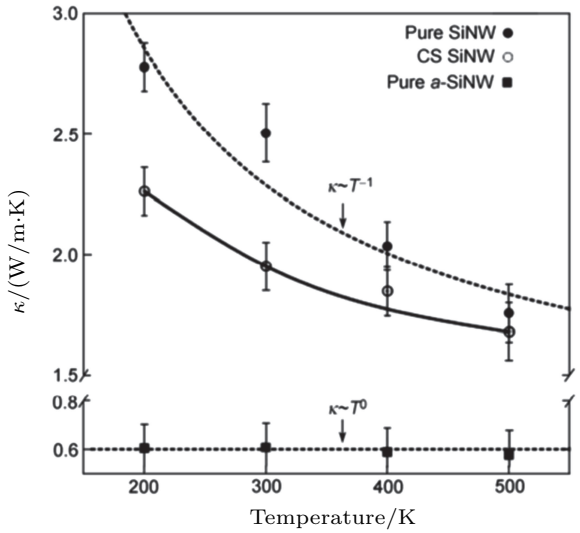


Fig. 8. Temperature dependence of the thermal conductivity of pure SiNW, CS SiNW, and a-SiNW (from Ref. [78]).

3.4. Surface doping

Many studies have shown that doping is an effective and feasible approach for decreasing thermal conductivity. Introducing dopant defects to the whole SiNWs can weaken electronic conductivity;[79] by contrast, surface/shell doping can improve thermoelectric performance. In contrast to traditional doping, in which dopant atoms are uniformly distributed inside nanowires, shell doping spatially confines dopant atoms within a few atomic layers in the shell region of a nanowire. Given their low thermal conductance and high electrical conductance, shell-doped SiNWs containing high amounts of dopants have potential applications in the thermoelectric field.[80]

The thermoelectric figure of merit of SiNWs can be increased by decreasing their thermal conductivity. Using a non-equilibrium MD simulation, Wang *et al.*[81] and Hu *et al.*[82] demonstrated that shell-doped SiNWs coated with Ge have remarkably low thermal conductivity due to the impurity and interface scattering associated with their unique structure. Pan *et al.* investigated surface Ge-doped SiNWs with diameters of approximately 100 nm.[83] Figure 9 shows that the thermal conductivity of Ge-coated SiNW arrays decreases by 23% at room temperature relative to that of uncoated SiNWs. Subjecting the Ge-doped SiNW arrays to thermal annealing decreased thermal conductivity by 44% because the surface-doped Ge interacts strongly with Si, thus enhancing phonon scattering at the Si–Ge interface.

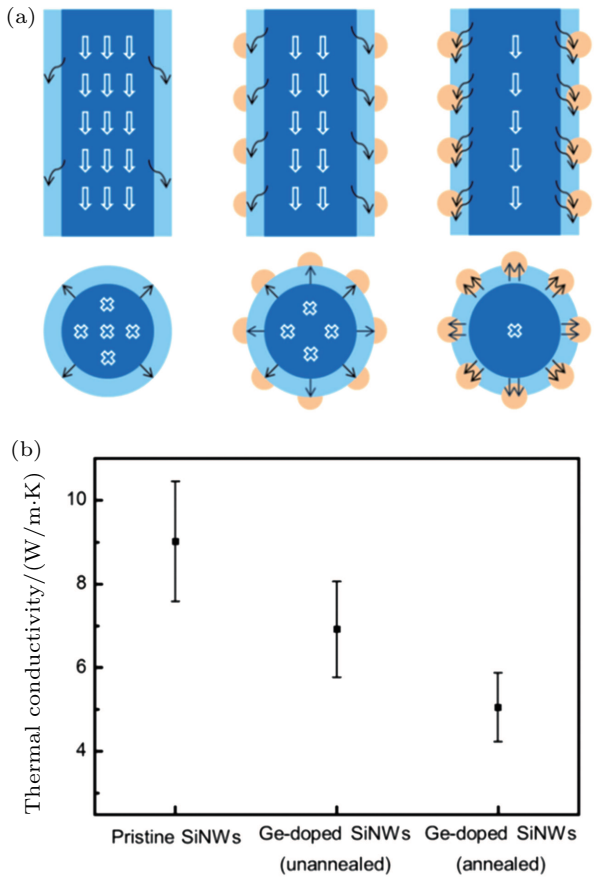


Fig. 9. (color online) (a) Schematic of the proposed phonon scattering mechanism in pristine SiNW, unannealed Ge-doped SiNW, and annealed Ge-doped SiNW. (b) Thermal conductivity of pristine SiNWs, unannealed Ge-doped SiNW, and annealed Ge-doped SiNW (from Ref. [83]).

3.5. Surface softening

Recently, it was discovered that the phonon softening effect also plays an important role in the thermal conductivity of solid solutions[84] and nanomaterials.[85–88] For example, by solving the full Boltzmann equation, the significantly reduced phonon thermal conductivity due to the observed acoustic phonon softening was quantitatively examined in $Mg_2Si_{1-x}Sn_x$.[84] Wingert *et al.*[85] experimentally found that crystalline Si (c-Si) nanotubes (NTs) with shell thickness as thin as ~ 5 nm exhibit a low thermal conductivity of ~ 1.1 W/mK, which is lower than the apparent boundary scattering limit and is even about 30% lower than the measured value for amorphous Si (a-Si) NTs with similar geometries. By using MD simulations, they also found a close link

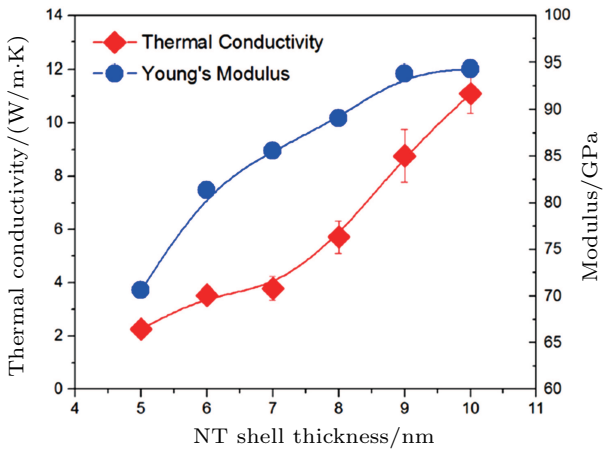


Fig. 10. (color online) Thermal conductivity and elastic modulus with different nanotube thickness (from Ref. [85]).

between thermal and elastic properties for the ultrathin c-Si nanotubes (Fig. 10). It was revealed that one can engineer the thermal transport properties of crystalline nanostructures beyond the phonon boundary scattering limit via the surface phonon softening effect due to the drastically reduced mechanical stiffness. This finding paves the way for new approaches to reduce thermal conductivity in nanostructures.[86–88]

4. Conclusion and perspectives

Thermal transport in low-dimensional nanomaterials such as SiNWs has attracted extensive research interest in the last decade. Understanding thermal transport in Si-based nanomaterials has practical and academic importance given the modern electronic and thermoelectric applications of these materials. Therefore, we briefly reviewed the recent advances in the study of surface effects on the thermal conductivity of one-dimensional SiNWs. The presented review clearly shows that phonon transport is significantly affected by the surface effects of SiNWs. Thermal conductivity is decreased by the surface effects in other nanostructures, including graphene,[89,90] carbon nanotubes,[91,92] and ZnO nanowires.[93] Thus, surface engineering methods are feasible and effective methods for adjusting thermal transport in nanomaterials.

Nonetheless, many questions and challenges remain in this field. For example, given the limited accuracy of the treatment of phonon surface scattering phenomena, the precise mechanisms that underlie the surface-induced reduction of thermal conductivity remain unknown. In particular, the synergistic effects of the material surface and other factors on the thermal transport in SiNWs remain unclear.[94] Measuring thermal conductivity at the nanoscale continues to face many difficulties,[2] such as thermal contact resistance between the nanowire and substrate. Conventional density functional theory theoretically offers high accuracy but cannot handle a large system, whereas the empirical potentials used in classical MD often lack transferability or accuracy as a result of ignoring electronic contributions.[95] Developing an improved theory and method to rapidly and accurately calculate the thermal conductivity of nanostructures is necessary. Therefore, surface effects on thermal conductivity still deserve further systematic experimental and theoretical investigations in the future.

References

[1] Snyder G J and Toberer E S 2008 *Nat. Mater.* **7** 105
[2] Yang N, Xu X, Zhang G and Li B 2012 *AIP Adv.* **2** 041410
[3] Ni X, Leek M L, Wang J S, Feng Y P and Li B 2011 *Phys. Rev. B* **83** 045408
[4] Sales B C 2002 *Science* **295** 1248
[5] Miao T T, Song M X, Ma W G and Zhang X 2011 *Chin. Phys. B* **20** 056501
[6] Dresselhaus M S, Chen G, Tang M Y, Yang R G, Lee H, Wang D Z, Ren Z F, Fleurial J P and Gogna P 2007 *Adv. Mater.* **19** 1043
[7] Dmitriev A V and Zvyagin I P 2010 *Phys. Usp.* **53** 789
[8] Ying P J, Li X, Wang Y C, Yang J, Fu C G, Zhang W Q, Zhao X B and Zhu T J 2017 *Adv. Funct. Mater.* **27** 1604145
[9] Davis B L and Hussein M I 2014 *Phys. Rev. Lett.* **112** 055505
[10] Teo B K and Sun X H 2007 *Chem. Rev.* **107** 1454
[11] Hochbaum A I, Chen R, Delgado R D, Liang W, Garnett E C, Najarian M, Majumdar A and Yang P 2008 *Nature* **451** 163
[12] Boukai A I, Bunimovich Y, Tahir-Kheli J, Yu J K, Goddard W A III and Heath J R 2008 *Nature* **451** 168
[13] Chen J, Zhang G and Li B 2011 *J. Chem. Phys.* **135** 204705
[14] Chen J, Zhang G and Li B 2010 *Nano Lett.* **10** 3978
[15] Li H P, Sarkar A D and Zhang R Q 2011 *Europhys. Lett.* **96** 56007
[16] Li H P and Zhang R Q 2014 *Europhys. Lett.* **105** 56003
[17] Zhang Y, Bi K, Chen W, Chen M and Chen Y 2014 *ECS Trans.* **60** 1159
[18] Yang N, Zhang G and Li B 2008 *Nano Lett.* **8** 276
[19] Liu L and Chen X 2010 *J. Appl. Phys.* **107** 033501
[20] Mingo N, Yang L, Li D and Majumdar A 2003 *Nano Lett.* **3** 1713
[21] Murphy K F, Piccione B, Zanjani M B, Lukes J R and Gianola D S 2014 *Nano Lett.* **14** 3785
[22] Ponomareva I, Srivastava D and Menon M 2007 *Nano Lett.* **7** 1155
[23] Kwon S, Wingert M C, Zheng J, Xiang J and Chen R 2016 *Nanoscale* **8** 13155
[24] Markussen T, Jauho A P and Brandbyge M 2009 *Phys. Rev. Lett.* **103** 055502
[25] Ali A, Chen Y, Vasirajuand V and Vaddiraju S 2017 *Nanotechnology* **28** 282001
[26] Kim W 2011 *Mater. Res. Innov.* **15** 375
[27] Schierning G 2014 *Phys. Status Solidi A* **211** 1235
[28] Zhang G and Zhang Y W 2013 *Phys. Status Solidi RRL* **7** 754
[29] Zhang G and Li B 2010 *Nanoscale* **2** 1058
[30] Glassbrenner C J and Slack G A 1964 *Phys. Rev.* **134** A1058
[31] Inyushkin A V, Taldenkov A N, Gibin A M, Gusev A V and Pohl H J 2004 *Phys. Stat. Sol.* **1** 2995
[32] Tiwari M D and Agrawal B K 1971 *Phys. Rev. B* **4** 3527
[33] Volz S G and Chen G 1999 *Appl. Phys. Lett.* **75** 2056
[34] Schelling P K, Phillpot S R and Keblinski P 2002 *Phys. Rev. B* **65** 144306
[35] Sellan D P, Landry E S, Turney J E, McGaughey A J H and Amon C H 2010 *Phys. Rev. B* **81** 214305
[36] Li X, Maute K, Dunn M L and Yang R 2010 *Phys. Rev. B* **81** 245318
[37] Donadio D and Galli G 2010 *Nano Lett.* **10** 847
[38] Abs da Cruz C, Termentzidis K, Hantrenne P and Kleber X 2011 *J. Appl. Phys.* **110** 034309
[39] Chen Y, Li D, Lukes J R and Majumdar A 2005 *J. Heat Transfer* **127** 1129
[40] Bong V N S and Wong B T 2015 *AIP Conference Proceedings* **1674** 020017
[41] Markussen T, Jauho A P and Brandbyge M 2008 *Nano Lett.* **8** 3771
[42] Markussen T, Jauho A P and Brandbyge M 2009 *Phys. Rev. B* **79** 035415
[43] Liangruksa M and Puri I K 2011 *J. Appl. Phys.* **109** 113501
[44] Mingo N 2003 *Phys. Rev. B* **68** 113308
[45] Mingo N and Broido D A 2004 *Phys. Rev. Lett.* **93** 246106
[46] Li DY, Wu Y Y, Kim P, Shi L, Yang P D and Majumdar A 2003 *Appl. Phys. Lett.* **83** 2934
[47] Li DY, Wu Y, Fan R, Yang P D and Majumdar A 2003 *Appl. Phys. Lett.* **83** 3186
[48] Martin P N, Aksamija Z, Popand E and Ravaioli U 2010 *Nano Lett.* **10** 1120
[49] Malhotra A and Maldovan M 2016 *Sci. Rep.* **6** 25818
[50] Xie G F, Guo Y, Li B H, Yang L W, Zhang K W, Tang M H and Zhang G 2013 *Phys. Chem. Chem. Phys.* **15** 14647
[51] Kukita K and Kamakura Y 2013 *J. Appl. Phys.* **114** 154312
[52] Lacroix D, Joulain K, Terris D and Lemonnier D 2006 *Appl. Phys. Lett.* **89** 103104
[53] Zhang R Q, Lifshitz Y, Ma D D D, Zhao Y L, Frauenheim T, Lee S T and Tong S Y 2005 *J. Chem.Phys.* **123** 144703
[54] Zhang R Q, Costa J and Bertran E 1996 *Phys. Rev. B* **53** 7847
[55] Yang X B and Zhang R Q 2009 *Appl. Phys. Lett.* **94** 113101
[56] Guo C S, Luo L B, Yuan G D, Yang X B, Zhang R Q, Zhang W J and Lee S T 2009 *Angew. Chem., Int. Ed.* **48** 9896
[57] Xu H, Yang X B, Zhang C, Lu A J and Zhang R Q 2011 *Appl. Phys. Lett.* **98** 073115
[58] Pan Y, Tao Y, Qin G Z, Fedoryshyn Y, Raja S N, Hu M, Degen C L and Poulikakos D 2016 *Nano Lett.* **16** 6364

[59] Lim J, Hippalgaonkar K, Andrews S C, Majumdar A and Yang P 2012 *Nano Lett.* **12** 2475
[60] Moore A L, Saha S K, Prasher R S and Li S 2008 *Appl. Phys. Lett.* **93** 083112
[61] Wang Z, Nin Z H, Zhao R J, Chen M H, Bi K D and Chen Y F 2011 *Physica B* **406** 2515
[62] Martin P, Aksamija Z, Pop E and Ravaioli U 2009 *Phys. Rev. Lett.* **102** 125503
[63] Malhotra A and Maldovan M 2016 *Sci. Rep.* **6** 25818
[64] Carrete J, Gallego L J and Varela L M 2011 *Phys. Rev. B* **84** 075403
[65] Kim H, Park Y H, Kim I, Kim J, Choi H J and Kim W 2011 *Appl. Phys. A* **104** 23
[66] Sadhu J and Sinha S 2011 *Phys. Rev. B* **84** 115450
[67] Maurer L N, Aksamija Z, Ramayya E B, Davoody A H and Knezevic I 2015 *Appl. Phys. Lett.* **106** 133108
[68] Park I, Li Z, Pisano A P and Williams R S 2007 *Nano Lett.* **7** 3106
[69] Lu A J, Zhang R Q and Lee S T 2008 *Appl. Phys. Lett.* **92** 203109
[70] Scott S A, Peng W, Kiefer A M, Jiang H, Knezevic I, Savage D E, Eriksson M A and Lagally M G 2009 *ACS Nano* **3** 1683
[71] Liu M, Ma Y and Wang R Y 2015 *ACS Nano* **9** 12079
[72] Markussen T, Jauho A P and Brandbyge M 2009 *Phys. Rev. Lett.* **103** 055502
[73] Hu M, Giapis K P, Goicochea J V, Zhang X L and Poulikakos D 2011 *Nano Lett.* **11** 618
[74] Blandre E, Chaput L, Merabia S, Lacroix D and Termentzidis K 2015 *Phys. Rev. B* **91** 115404
[75] Kandemir A, Ay F, Perkgöz N K and Sevik C 2016 *J. Electron. Mater.* **45** 1594
[76] Sansoz F 2011 *Nano Lett.* **11** 5378
[77] Donadio D and Galli G 2009 *Phys. Rev. Lett.* **102** 195901
[78] Liu X J, Zhang G, Pei Q X and Zhang Y W 2014 *Sci. China Tech. Sci.* **57** 699
[79] Chen J, Zhang G and Li B 2009 *Appl. Phys. Lett.* **95** 073117
[80] Zhong J X and Stocks G M 2006 *Nano Lett.* **6** 128
[81] Wang Y, Li B and Xie G 2013 *RSC Adv.* **3** 26074
[82] Hu M, Giapis K P, Goicochea J V, Zhang X L and Poulikakos D 2011 *Nano Lett.* **11** 618
[83] Pan Y, Hong G, Raja S N, Zimmermann S, Tiwari M K and Poulikakos D 2015 *Appl. Phys. Lett.* **106** 093102
[84] Tan X J, Liu G Q, Shao H Z, Xu J T, Yu B, Jiang H C and Jiang J 2017 *Appl. Phys. Lett.* **110** 143903
[85] Wingert M C, Kwon S, Hu M, Poulikakos D, Xiang J and Chen R K 2015 *Nano Lett.* **15** 2605
[86] Yang L, Yang Y, Zhang Q, Zhang Y, Jiang Y F, Guan Z, Gerboth M, Yang J K, Chen Y F, Walker D G, Xu T T and Li D Y 2016 *Nanoscale* **8** 17895
[87] Neogi S, Reparaz J S, Pereira L F C, Graczykowski B, Wagner M R, Sledzinska M, Shchepetov A, Prunnila M, Ahopelto J, Sotomayor-Torres C M and Donadio D 2015 *ACS Nano* **9** 3820
[88] Massoud A M, Bluet J M, Lacatena V, Haras M, Robillard J F and Chapuis P O 2017 *Appl. Phys. Lett.* **111** 063106
[89] Chien S K, Yang Y T and Chen C K 2011 *Appl. Phys. Lett.* **98** 033107
[90] Pei Q X, Sha Z D and Zhang Y W 2011 *Carbon* **49** 4752
[91] Padgett C W and Brenner D W 2004 *Nano Lett.* **4** 1051
[92] Padgett C W, Shenderova O and Brenner D W 2006 *Nano Lett.* **6** 1827
[93] Jiang J W, Park H S and Rabczuk T 2013 *Nanoscale* **5** 11035
[94] Liu X J, Zhang G, Pei Q X and Zhang Y W 2016 *Materials Today: Proceedings* **3** 2759
[95] Wang Q, Wang X, Guo R and Huang B 2017 *J. Phys. Chem. C* **121** 15472