Tuning the Kapitza resistance in pillared-graphene nanostructures

Loh, G. C.; Teo, Edwin Hang Tong; Tay, Beng Kang

2012

Loh, G. C., Teo, E. H. T., & Tay, B. K. (2012). Tuning the Kapitza resistance in pillared-graphene nanostructures. *Journal of applied physics*, 111(1), 013515.

<https://hdl.handle.net/10356/95020>

<https://doi.org/10.1063/1.3676200>

© 2012 American Institute of Physics. This paper was published in *Journal of Applied Physics* and is made available as an electronic reprint (preprint) with permission of American Institute of Physics. The paper can be found at the following official DOI: [<http://dx.doi.org/10.1063/1.3676200>]. One print or electronic copy may be made for personal use only. Systematic or multiple reproduction, distribution to multiple locations via electronic or other means, duplication of any material in this paper for a fee or for commercial purposes, or modification of the content of the paper is prohibited and is subject to penalties under law.

Downloaded on 26 Apr 2023 21:59:54 SGT

Tuning the Kapitza resistance in pillared-graphene nanostructures

G. C. Loh, E. H. T. Teo, and B. K. Tay

Citation: *J. Appl. Phys.* **111**, 013515 (2012); doi: 10.1063/1.3676200

View online: <http://dx.doi.org/10.1063/1.3676200>

View Table of Contents: <http://jap.aip.org/resource/1/JAPIAU/v111/i1>

Published by the [American Institute of Physics](#).

Related Articles

Role of ethylene on surface oxidation of TiO₂(110)

Appl. Phys. Lett. **101**, 211601 (2012)

Bidirectionally tuning Kapitza conductance through the inclusion of substitutional impurities

J. Appl. Phys. **112**, 073519 (2012)

Communication: An obligatory glass surface

J. Chem. Phys. **137**, 141102 (2012)

Pressure dependency of thermal boundary conductance of carbon nanotube/silicon interface: A molecular dynamics study

J. Appl. Phys. **112**, 053501 (2012)

Effect of nanopatterns on Kapitza resistance at a water-gold interface during boiling: A molecular dynamics study

J. Appl. Phys. **112**, 053508 (2012)

Additional information on *J. Appl. Phys.*

Journal Homepage: <http://jap.aip.org/>

Journal Information: http://jap.aip.org/about/about_the_journal

Top downloads: http://jap.aip.org/features/most_downloaded

Information for Authors: <http://jap.aip.org/authors>

ADVERTISEMENT

The advertisement for AIP Advances features a green and yellow color scheme. At the top, the text 'AIP Advances' is displayed in a large, bold, green font. To the right of the text is a circular logo with the text 'Now Indexed in Thomson Reuters Databases'. Below the main text, there is a blue banner with the text 'Explore AIP's open access journal:'. To the right of the banner, there is a list of three bullet points: 'Rapid publication', 'Article-level metrics', and 'Post-publication rating and commenting'. The background of the advertisement is a light green color with a subtle pattern of curved lines.

AIP Advances

Now Indexed in Thomson Reuters Databases

Explore AIP's open access journal:

- Rapid publication
- Article-level metrics
- Post-publication rating and commenting

Tuning the Kapitza resistance in pillared-graphene nanostructures

G. C. Loh, E. H. T. Teo, and B. K. Tay^{a)}*School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore 639798*

(Received 20 September 2011; accepted 25 November 2011; published online 9 January 2012)

The pillared-graphene architecture is a conceivable way of conjoining graphene nanoribbons and carbon nanotubes (CNTs) in nanoelectronics. Especially promising is its capability to dissipate thermal energy in thermal management applications. However, the thermal boundary resistance (Kapitza resistance) at the graphene nanoribbon-CNT interface is a phonon barricade and a bottleneck for efficacious heat extraction. Parallel to strain studies on thermal conductance, this work is a first report on the effects of mechanical strain on the interfacial phonon dynamics in the pillared-graphene nanostructure (PGN). Molecular dynamics simulations are employed to derive the changes in phononics as axial, torsional, and compound strains of various degrees are applied on the PGN. The pillar lattice structure behaves dissimilarly to the different types of strains. In-plane transverse optical mode softening as induced by torsional strain is more effective than LO softening (triggered by tension) in minimizing the thermal boundary resistance. Essentially, it is shown that there is a strong relationship between strained PGN pillar lattice structure, interfacial phononics, and thermal boundary resistance. © 2012 American Institute of Physics. [doi:10.1063/1.3676200]

I. INTRODUCTION

In recent years, the world observed a rapid downsizing of micro-/nano-electronics devices; for instance, from the 45-nm technology node in 2008, it progressed to the current (2011) 22-nm technology node.¹ This reduction in device feature size allows more of these devices to be packed in a unit substrate area but inevitably raises the total amount of thermal energy generated. This thermal energy is only a by-product of the integrated circuit. If thermal management is not efficient enough to extract waste energy away quickly, the device performance and lifetime² will deteriorate. A few questions become apparent and exigent: are the current micro-/nano-electronics materials expedient heat sinks? Can we alter the topology of these materials so as to dissipate heat more efficaciously?

Silicon is the principal material in conventional semiconductor applications, mainly because (1) its oxide (silicon dioxide) is easily grown in a furnace and forms a good semiconductor–dielectric interface, and (2) unlike its chemical group neighbor germanium, it retains its semiconducting properties even at high temperatures. The measured thermal conductivity of monocrystalline silicon ranges from 100 to 300 W/m K (Refs. 3 and 4) and is comparable with that of metals such as aluminum⁵ and gold.⁶ As a material in semiconductor devices, silicon is adequate in its secondary role to dissipate waste energy. Nevertheless, with the increased heat generation in smaller devices, thermal energy is not directed away fast enough, and hence alternative materials with a higher thermal conductance have to be explored.

Carbon allotropes such as carbon nanotubes (CNTs) and graphene could provide the apposite solution to this challenging problem: the high phonon velocities in these materials

stem from their stiff and strong carbon-carbon bonds, and their crystalline nature minimizes mode scattering and gives them a relatively large phonon mean free path. The coupling of both phonon properties allow phonons to travel fast and far before they collide. In other words, thermal energy is efficiently transported in carbon nanotubes and graphene, i.e., they have a high thermal conductivity. Experimental values fall in the range of 3000–5000 W/m K.^{7–12} Similarly, other ordered carbon allotropes, such as diamond and fullerene, have outstanding thermal properties.^{13–15} But are all of these allotropes appropriate materials in thermal management applications? Because the directional uniformity/isotropicity of heat extraction relies on the topology and intermediate and long-range structure of the material, carbon nanotubes and graphene conduct heat energy anisotropically, whereas a bulk carbon material such as diamond is isotropically conductive. In this regard, anisotropically conductive materials have fewer dimensions to remove heat than isotropically conductive ones, and they therefore will not form an efficient heat sink. A simple way to artificially “metamorphose” these materials to an isotropic three-dimensional heat extraction system is to build a multi-level structure of CNT via “pillars” between large graphene sheets.^{16–18}

The notion of a pillared-graphene nanostructure (PGN) is not novel. The first reported effort to construct this nanostructure was presented by Kondo *et al.*¹⁹ They presented a synthesis method that involved growing graphene multilayers (or graphite) on the ends of vertically aligned multiwalled carbon nanotubes via chemical vapor deposition. Notwithstanding the success of creating a three-dimensional carbon nanostructure, the presence of many layers of graphene is detrimental to its efficacy as a heat sink; out-of-plane phonon modes have much lower group velocities relative to modes of other orientations. These multilayers essentially nullify the superior thermal performance of the pillared-graphene architecture.

^{a)}Author to whom correspondence should be addressed. Electronic mail: ebktay@ntu.edu.sg.

Dimitrakakis *et al.*¹⁸ then surveyed the hydrogen storage capability of such an architecture using a multiscale theoretical approach. With lithium cation dopants, a storage capacity of 41 g H₂/l was calculated under ambient conditions, which is relatively close to the requirement of 45 g H₂/l set by the U.S. Department of Energy. Varshney and coworkers¹⁶ reproduced these nanostructures via molecular dynamics simulations and computed their thermal conductivity. It is found that the interpillar distance and pillar length are critical factors that govern the extent of phonon scattering at the interface and thus the effective thermal conductivity in the nanostructure. In the same train of thought, we have studied the effects of intertube interaction on the thermal transport in PGNs. Through rigorous analyses of the three-phonon phonon scattering selection rules, the pairwise scattering of flexural modes is cogently demonstrated.²⁰

By proposing to use the pillared-graphene architecture as a heat sink, we have effectively set up a potential solution to the second problem put forth in the first paragraph: combining two materials with high intrinsic thermal and electrical conductivities in such a stacked manner increases the rate of dissipation of thermal energy. This architecture is particularly attractive because of the similar atomic composition of CNTs and graphene. Although these two materials contrast in terms of dimensionality, curvature of the structure, and edge effects, they are constituted by the same element (carbon) and are arranged in a honeycomb lattice structure. With this hexagonal structure, the materials have the same orbital hybridization (sp², other than at edges and defect regions). Despite the multitude of possibilities for how the atoms at a nanotube tip can be bonded with graphene atoms, the similar composition reduces the mismatching of lattice vibrational spectra and phonon properties such as velocities on both sides of the interface. Theoretically this implies that the impact of the interfacial encumbrance is kept to a minimum. Phonons flowing from the nanotube into the graphene sheet/nanoribbon (or from graphene sheet to nanotube) face a low thermal barrier at the interface, and ergo a smaller thermal boundary resistance (TBR) (or Kapitza resistance) develops. Consequently, it is strongly believed that this architectural design is viable in thermal management applications.

II. OBJECTIVES

This work is a first study and account of how we can engineer interfacial vibrational properties in PGNs to reduce the thermal boundary resistance. Mechanical strain is introduced in the nanostructure in the axial, torsional, and axial-torsional orientations in order to alter the phonon dynamics at the interface and thereby modify the thermal boundary resistance. It is well understood that the intrinsic thermal conductance is dependent on the lattice strain.^{21–24} However, it is still unknown how strain will affect the interfacial phononics in PGNs. This paper aims to address this issue, as well as outline the relationship between each of the three aforementioned types of strain and thermal boundary resistance. Ultimately, we seek to find a systematic way to tune the thermal boundary resistance, which aids the advancement of thermal management and thermoelectric applications.

III. SIMULATION DETAILS

Molecular dynamics simulations were carried out in this study. We employed a 13.3 Å × 27.0 Å × 100.0 Å simulation cell that contained 1108 atoms aligned in the pillared-graphene architecture. Out of these atoms, 2 sheets of 474 atoms were arranged in the graphene honeycomb structure to represent nanoribbons, and the rest (160 atoms) were ordered in the tubular CNT structure, with 16 atoms in each circumferential unit cell. To avoid coupling of the axial and torsional strain [known as axial-strain-induced torsion (ASIT)],^{25–28} the CNT is arranged in the armchair configuration.²⁸ The carbon-carbon interactions were expressed by the Brenner potential.²⁹ The velocity Verlet algorithm was adopted to predict the next positions and velocities, with a time step of 0.5 fs. Some 200 atoms around each graphene sheet were fixated and the dynamics restricted by an adiabatic approximation. Nosé-Hoover^{30,31} thermostats were used at the extreme ends of the system to create a temperature difference. Both hot and cold baths were bound to the two graphene sheets (exclusive of the fixed graphene atoms). The cold and hot thermostat temperatures were predefined as 290 K and 310 K, respectively, as the intent of this work is to study the phonon dynamics at room temperature. The interfacial atoms are attached by covalent bonds because (1) they are strong chemical bonds and will induce the weakest perturbation to phonon transport, and (2) for simplicity of simulations. Mechanical strain is applied to the nanotube pillar of the PGN by translating graphene atoms that are approximated adiabatically. (A) To induce an axial strain, the 200 adiabatic atoms are given a small positional shift in the axial direction for a certain number of time-steps [Fig. 1(a)]. (B) For a torsional strain, these atoms are made to rotate about their nanotube axis [Fig. 1(b)]. (C) A compound strain is a combination of the axial and torsional strains, with axial strain exerted before torsional strain. To calculate the thermal boundary resistance, the local instantaneous temperatures are defined and calculated from the atomic kinetic energy as

FIG. 1. (Color online) Schematic diagram of pillared-graphene hybrid nanostructure under (a) tensile strain and (b) torsional strain.

$$T(z, t) = \frac{m}{3k_b} [v_x(z, t)^2 + v_y(z, t)^2 + v_z(z, t)^2], \quad (1)$$

where k_b is the Boltzmann constant, m is the atomic mass, and the subscripts x , y , and z refer to the 3 orientations in the simulations.

IV. RESULTS AND DISCUSSION

A. Axial strain

The uniaxial strain is applied for a range of positive (tensile) and negative (compressive) values. As discussed in the preceding section, the graphene sheets are translated in order to induce uniaxial strain in the nanotube pillar. In this regard, the graphene sheets are not strained. The uniaxial strain is defined as

$$\varepsilon = \frac{l - l_0}{l_0}, \quad (2)$$

where ε is the uniaxial strain, l is the length of the nanotube, and l_0 is the initial length of the nanotube. The velocity autocorrelation function is then computed from the time history of the velocity of the atoms. To extract vibrational information from the strained nanostructure, the local vibrational density of states (VDOS) is calculated by performing a Fourier-transform on the velocity autocorrelation function at a few atomic locations in the bulk nanotube.

We perform adjacent-averaging smoothing to superpose these features and give an approximate position of the G-peak [with both in-plane transverse optical (iTO) and longitudinal optical (LO) modes³²]. Because the PGN CNT pillar is strained axially, the longitudinal modes are predominantly affected by the perturbation. Figure 2 shows how the G^+ feature position (which corresponds to the LO mode) of the vibrational spectra at two bulk nanotube locations varies with the uniaxial strain exerted. Compressive and tensile strains have a different effect on the G^+ feature: compressive strain induces a slight amount of G^+ mode stiffening from

FIG. 2. (Color online) G^+ feature position at different uniaxial strains; inset shows the compressive regime.

$\sim 1665 \text{ cm}^{-1}$ to $\sim 1690 \text{ cm}^{-1}$ (an increase of about 2%) with a uniaxial strain of -0.2 , whereas tensile strain causes G^+ mode softening from $\sim 1665 \text{ cm}^{-1}$ to $\sim 1560 \text{ cm}^{-1}$ (a decrease of about 6%) with the same magnitude of uniaxial strain. This signifies that the G^+ feature in the PGN nanotube is more sensitive to tension than compression. A zeroed-in view of the figure in the negative range (inset) indicates that the G^+ feature position varies linearly with the magnitude of the compressive strain. On a similar note, a study on strained armchair carbon nanotubes (aCNTs) by Ren and coworkers³³ shows that the sensitivity of the G^+ modes to both tensile and compressive strain is comparable. Wei *et al.* reported a set of behaviors in zigzag graphene nanoribbons³⁴ (zGNRs) that closely parallels that of this work (i.e., compressive strain blue-shifts the G^+ feature); in contrast, the G^+ feature of armchair graphene nanoribbons (aGNRs) is impervious to compression. A comparison of these reports suggests that the G^+ features of PGN armchair CNT pillars, aCNTs, zGNRs, and aGNRs respond in different fashions to compressive strain, with the order of decreasing sensitivity to compression being aCNT, PGN armchair CNT pillar (and zGNR), and aGNR. From these results, it can be inferred that the LO mode is softened by tension and stiffened by compression.

The interfacial vibrational density of states in the graphene sheet (or nanoribbon) and nanotube is computed at a range of uniaxial strain. Three sets of the VDOS (for strains of -0.17 , 0 , and 0.17 , marked with circles in Fig. 2) are plotted in Fig. 3. The purpose of this calculation is to outline the trend of change of the interfacial VDOS in both graphene and nanotubes with uniaxial strain. Notably, with a compressive strain, the G^+ feature of the interfacial VDOS in both graphene and nanotubes blue-shifts, whereas the G^+ feature red-shifts with a tensile strain. In addition, the extent of the blue-shift is significantly less than that of the red-shift. This is consistent with the observation in Fig. 2, whereby the G^+ feature of bulk nanotube undergoes a similar shift. The coherent behavior of the G^+ feature of nanotubes in bulk and at the interface suggests that mode stiffening and softening are not spatially localized in the nanotube, i.e., the stiffening (softening) is uniform with compression (tension) in the entire nanotube.

FIG. 3. (Color online) Interfacial vibrational density of states at uniaxial strains of -0.17 , 0 , and 0.17 .

The diffuse mismatch model^{35–41} and the subsequently improved flux-mediated diffuse mismatch model⁴² postulate that the thermal boundary resistance is a function of the matching of phonon density and velocity on both sides of the interface. To quantify the matching of the interface VDOS, the statistical parameter, the Pearson product-moment correlation coefficient, is used. It measures the correlation or linear dependence between two variables X and Y and ranges from $+1$ to -1 inclusive, with $+1$ referring to an exact direct linear relationship between X and Y and -1 indicating an exact inverse linear relationship. It is defined as the ratio of the covariance of the two variables to the product of their standard deviations,

$$\rho_{X,Y} = \frac{\text{cov}(X,Y)}{\sigma_X \sigma_Y} = \frac{E[(X - \mu_X)(Y - \mu_Y)]}{\sigma_X \sigma_Y}, \quad (3)$$

where cov is the covariance, E is the mean, and σ is the standard deviation. As the uniaxial strain switches from the compressive to tensile regime, the Pearson coefficient increases and then levels off at around $+0.7$ when the strain is approximately 0.5 (Fig. 4). An increase of the strain beyond 0.5 does not improve the VDOS matching. Indubitably, the thermal boundary resistance is a determinant of both the VDOS and phonon velocity matching. Nevertheless, this statistical approach to figuring out how well the VDOSs resemble each other on both sides of the interface is a facile qualitative estimation of the thermal boundary resistance.

Indeed, the relationship of the thermal boundary resistance with strain closely mirrors the Pearson analysis (Fig. 5). Defining thermal boundary resistance as the ratio of the temperature drop at the interface to the thermal flux across it,

$$R_K = \frac{\Delta T}{J}, \quad (4)$$

where ΔT is the temperature drop and J is the thermal flux through a cross-sectional area per unit time.³⁵ As the strain changes from compressive to tensile, the thermal boundary resistance decreases under compression before easing off to a more moderate rate under tension. Interestingly, when a large

FIG. 4. (Color online) Pearson product-moment correlation coefficient of interfacial VDOS at different uniaxial strains.

FIG. 5. (Color online) Thermal boundary resistance at different uniaxial strains.

tensile strain of 0.5 is exerted on the nanotube, the TBR decreases by more than 30% . This apparently suggests that the application of axial strain is a practicable method for tuning the thermal boundary resistance in PGNs. Naturally, the effective thermal conductivity of the entire PGN is contingent on both the intrinsic thermal conductance of the nanotube and the graphene sheet and the TBR at the nanotube-graphene interface. This study on the effect of axial strain on the TBR is by no means exhaustive; it is beyond the scope of this work to report on the influence on the overall conductance. Rather, this work serves to analyze the potentiality and viability of a tuning technique of TBR.

B. Torsional strain

The graphene sheets are rotated about the nanotube axis to induce torsional strain in the nanotube. Therefore, only the nanotube is strained. Cognate to the analysis with axial strain, the vibrational density of states is calculated. Figure 6 presents the position of the G-peak as the torsional angle is varied. Due to the armchair configuration of the nanotube, axial strain is not coupled with torsion. Thus this twisting of the nanotube is purely torsional, and axial strain is absent. The slightly linear and upward trend of the G^+ feature

FIG. 6. (Color online) G^+ and G^- feature positions at different torsional angles.

position with the torsional angle shows that the LO mode stiffens a little with increasing torsion. A salient observation from the plot is the extent to which the G^+ peak shifts in position with respect to the amount of torsion applied. Compared to the shift with axial strain (Fig. 2), torsion is less effective in stiffening the LO mode. This indicates that although coupling between axial and torsional strain is absent in the armchair nanotube pillar, slight LO stiffening still occurs.

In the same figure (Fig. 6), the G^- feature position shifts leftward with increasing torsion. This iTO softening is comparatively stronger than that of the LO stiffening. As the dynamics of twisting is primarily in the circumferential direction, it is not surprising that the iTO mode is affected more than the LO mode.

Torsional strain distorts the lattice structure of the nanotube, but does it pull apart or shorten the bonds? In order to understand the nature of torsional strain and the correlation between the G-peak position and structural change, two sets of mean bond lengths (overall and circumferential) across the whole nanotube are computed (Fig. 7). The overall mean bond length refers to the average of all bond lengths in the nanotube, and the circumferential mean bond length is the average length of bonds in the circumferential direction. When the nanotube is twisted, both types of bond lengths increase, with the overall mean bond length being smaller than its counterpart. Apparently, as bonds in the circumferential direction lengthen, the bond strength weakens. As a result, the iTO mode softens (Fig. 6).

What is more remarkable is the response of the interfacial modes to the torsional strain of the nanotube. As it is twisted more, the thermal boundary resistance at the CNT-graphene interface first decreases to a minimum at a torsional angle of around 50° before increasing (Fig. 8). This suggests that 50° is approximately the optimal torsional angle, such that the interfacial modes are modified to achieve a minimal TBR. Compared to the change of TBR with axial strain (Fig. 5), the torsion-TBR plot does not have a large plateau where TBR is at a minimum. Interestingly, iTO softening induced by torsion appears to be more effectual in reducing the TBR in the PGN to less than $1 \text{ p KW}^{-1} \text{ m}^2$.

FIG. 7. (Color online) Overall and circumferential mean bond lengths at different torsional angles.

FIG. 8. (Color online) Thermal boundary resistance at different torsional angles.

C. Compound strain

Seldom is the case wherein strain is a simplistic affair. In the process of fabricating the pillared-graphene nanostructure, imperfections in the structure might cause a coupling of axial and torsional strains. This coupling is slightly different from the aforementioned ASIT effect, (1) which occurs only in chiral nanotubes,²⁸ and (2) with which either of the strains triggers the other type of strain. Therefore it is important to extend the investigation of the strain-TBR relationship beyond the scenarios presented in the two preceding sections.

Here compound strain is defined as a coupling of axial and torsional strain. If the nanotube pillar is strained both axially and torsionally, the combined effect of the mode stiffening or softening on thermal boundary resistance can be studied. Figure 9 is a comparison of the effects of axial strain (as shown in Fig. 5) and compound strain on the TBR. The compound strain is induced by first twisting the nanotube by 20° , after which the uniaxial strain is varied in order to calculate the TBR. The minimum point on the compound strain plot is approximately at zero uniaxial strain. In the compressive and tensile regime, TBR increases with uniaxial strain.

FIG. 9. (Color online) Comparison of thermal boundary resistance under different uniaxial and compound (20° torsion and variable uniaxial strain) strains.

Palpably, the additional LO stiffening/softening is detrimental to the transport of thermal energy across the interface. The inclusion of the torsion (comparing axial and compound strains in Fig. 9) changes the response of interfacial modes to the axial strain, especially in the tensile regime, and not so much in the compressive regime.

V. CONCLUSION

Molecular dynamics simulations on strained pillared-graphene nanostructures have shown some intriguing results. The lattice structure of the nanotube pillar responds differently to axial and torsional strains and subsequently causes a predominantly LO or iTO mode shift for axial and torsional strains, respectively. Simulations at various atomic positions in the bulk nanotube and PGN interface show that the LO mode shift is uniform spatially in the nanotube as axial strain is applied. In contrast, for torsional strain, iTO softening is comparatively stronger than LO stiffening. A contrast between the strain-TBR plots for both types of strain cogently suggests that iTO softening is more effective than LO softening in minimizing the thermal boundary resistance. In addition, interfacial modes respond differently to an axial strain when torsion is coupled with the axial strain. Through this novel study, we enhance the understanding of the correlation between the structure and the topology of strained PGN pillars, the shift of iTO and LO modes, and thermal boundary resistance at the interface.

ACKNOWLEDGMENTS

The codes used in this work were developed from a code provided by the Maruyama Group at the University of Tokyo. The main author was supported by the Nanyang Research Scholarship, and the work was funded by the MOE Tier 2 Fund.

¹See <http://www.itrs.net/Links/2010ITRS/Home2010.htm> for the International Technology Roadmap for Semiconductors (ITRS) 2010 update.

²D. Segal, A. Nitzan, and P. Hänggi, *J. Chem. Phys.* **119**, 6840 (2003).

³C. J. Glassbrenner and G. A. Slack, *Phys. Rev.* **134**, A1058 (1964).

⁴G. A. Slack, *J. Appl. Phys.* **35**, 3460 (1964).

⁵D. D. L. Chung, *Appl. Therm. Eng.* **21**, 1593 (2001).

⁶G. Chen and P. Hui, *Appl. Phys. Lett.* **74**, 2942 (1999).

⁷A. A. Balandin, S. Ghosh, W. Bao, I. Calizo, D. Teweldebrhan, F. Miao, and C. N. Lau, *Nano Lett.* **8**, 902 (2008).

⁸S. Berber, Y.-K. Kwon, and D. Tománek, *Phys. Rev. Lett.* **84**, 4613 (2000).

⁹P. Kim, L. Shi, A. Majumdar, and P. L. McEuen, *Phys. Rev. Lett.* **87**, 215502 (2001).

¹⁰J. Hone, M. Whitney, C. Piskoti, and A. Zettl, *Phys. Rev. B* **59**, R2514 (1999).

¹¹J. Che, T. Çağın, W. Deng, and W. A. Goddard III, *J. Chem. Phys.* **113**, 6888 (2000).

¹²J. Che, T. Çağın, and W. A. Goddard III, *Nanotechnology* **11**, 65 (2000).

¹³J. R. Olson, K. A. Topp, and R. O. Pohl, *Science* **259**, 1145 (1993).

¹⁴G. A. Slack, *J. Appl. Phys.* **35**, 3460 (1964).

¹⁵L. Wei, P. K. Kuo, R. L. Thomas, T. R. Anthony, and W. F. Banholzer, *Phys. Rev. Lett.* **70**, 3764 (1993).

¹⁶V. Varshney, S. S. Patnaik, A. K. Roy, G. E. Froudakis, and B. L. Farmer, *ACS Nano* **4**, 1153 (2010).

¹⁷F. D. Novaes, R. Rurali, and P. Ordejón, *ACS Nano* **4**, 7596 (2010).

¹⁸G. K. Dimitrakakis, E. Tylianakis, and G. E. Froudakis, *Nano Lett.* **8**, 3166 (2008).

¹⁹D. Kondo, S. Sato, and Y. Awano, *Appl. Phys. Express* **1**, 074003 (2008).

²⁰G. C. Loh, E. H. T. Teo, and B. K. Tay, *J. Appl. Phys.* **110**, 083502 (2011).

²¹X. Li, K. Maute, M. L. Dunn, and R. Yang, *Phys. Rev. B* **81**, 245318 (2010).

²²S. Bhowmick and V. B. Shenoy, *J. Chem. Phys.* **125**, 164513 (2006).

²³A. R. Abramson, C.-L. Tien, and A. Majumdar, *J. Heat Transfer* **124**, 963 (2002).

²⁴R. C. Picu, T. Borca-Tasciuc, and M. C. Pavel, *J. Appl. Phys.* **93**, 3535 (2003).

²⁵J. Geng and T. Chang, *Phys. Rev. B* **74**, 245428 (2006).

²⁶Y. N. Gartstein, A. A. Zakhidov, and R. H. Baughman, *Phys. Rev. B* **68**, 115415 (2003).

²⁷H. W. Zhang, L. Wang, J. B. Wang, Z. Q. Zhang, and Y. G. Zheng, *Phys. Lett. A* **372**, 3488 (2008).

²⁸H. Liang and M. Upmanyu, *Phys. Rev. Lett.* **96**, 165501 (2006).

²⁹D. W. Brenner, *Phys. Rev. B* **42**, 9458 (1990).

³⁰S. Nosé, *J. Chem. Phys.* **81**, 511 (1984).

³¹W. G. Hoover, *Phys. Rev. A* **31**, 1695 (1985).

³²M. S. Dresselhaus, G. Dresselhaus, R. Saito, and A. Jorio, *Phys. Rep.* **409**, 47 (2005).

³³C. Ren, W. Zhang, Z. Xu, Z. Zhu, and P. Huai, *J. Phys. Chem. C* **114**, 5786 (2010).

³⁴N. Wei, L. Xu, H.-Q. Wang, and J.-C. Zheng, *Nanotechnology* **22**, 105705 (2011).

³⁵G. P. Srivastava, *The Physics of Phonons* (Taylor & Francis, New York, 1990).

³⁶E. T. Swartz and R. O. Pohl, *Rev. Mod. Phys.* **61**, 605 (1989).

³⁷P. E. Hopkins, *J. Appl. Phys.* **106**, 013528 (2009).

³⁸T. E. Beechem, S. Graham, P. E. Hopkins, and P. M. Norris, *Appl. Phys. Lett.* **90**, 054104 (2007).

³⁹R. S. Prasher and P. E. Phelan, *ASME J. Heat Transfer* **123**, 105 (2001).

⁴⁰A. Majumdar and P. Reddy, *Appl. Phys. Lett.* **84**, 4768 (2004).

⁴¹P. E. Hopkins, P. M. Norris, R. J. Stevens, T. E. Beechem, and S. Graham, *J. Heat Transfer* **130**, 062402 (2008).

⁴²G. C. Loh, B. K. Tay, and E. H. T. Teo, *Appl. Phys. Lett.* **97**, 121917 (2010).