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Cem Sevik, Alper Kinaci, Justin B. Haskins, and Tahir Çağın

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Influence of disorder on thermal transport properties of Boron Nitride nanostructures

Cem Sevik

*Artie McFerrin Department of Chemical Engineering,
Texas A&M University, College Station, TX 77845-3122,
USA & Advanced Technologies Research Center, Anadolu University, Eskisehir, 26470, Turkey*

Alper Kinaci

Material Science and Engineering, Texas A&M University, College Station, TX 77845-3122, USA

Justin B. Haskins

*Artie McFerrin Department of Chemical Engineering,
Texas A&M University, College Station, TX 77845-3122, USA*

Tahir Çağın*

*Artie McFerrin Department of Chemical Engineering & Material Science and Engineering,
Texas A&M University, College Station, TX 77845-3122, USA
(Dated: May 23, 2012)*

The impact of isotopes on thermal transport in boron nitride nanotubes (BNNTs) and boron nitride white graphene (BNWG) is systematically studied *via* molecular dynamic (MD) simulations. By varying the concentration of the ^{10}B isotope in these materials, we find that thermal conductivity ranges from 340 to 500 $\text{Wm}^{-1}\text{K}^{-1}$, closely agreeing with experimental observations for isotopically pure and natural (19.9% ^{10}B) BNNTs. Further, we investigate the interplay between dimension and isotope disorder in several C based materials. Our results show a general trend of decreasing influence of isotope disorder with dimension of these materials.

I. INTRODUCTION

Recent technological advances in the synthesis of boron nitride isomorphs of carbon nanostructures^{1,2} have led to special interest in these materials for applications such as high temperature catalysts and photovoltaic devices.³ Several experiments have been carried out concerning mechanical, structural, and thermal properties of these nanomaterials,^{4–17} the results of which parallel to that of their carbon counterparts.^{18–26} Isotopic disorder, however, has been reported to significantly deteriorate the thermal transport properties in BN based nanomaterials.²⁷ Several authors^{28,29} have speculated that this effect is the main mechanism responsible for the degradation of lattice thermal conductivity (κ) in boron nitride nanotubes (BNNTs) especially considering the much higher natural abundance of isotopes in boron compared to carbon. Recent studies performed using an atomistic Green's function transport formalism (AGTF) coupled with first principles phonon data have predicted that the isotopic purification enhances $[(\kappa^{\text{pure}}/\kappa^{\text{natural}} - 1) \times 100]$ the room temperature ballistic thermal conductivity more than $\sim 400\%$ and $\sim 150\%$ in C (with 10.7% of ^{14}C isotope) and BN (with 18.8% of ^{10}B isotope) based nanotubes respectively.³⁰ It is claimed that the ratio $(\kappa^{\text{pure}}/\kappa^{\text{natural}})$ is not a strong function of contact resistance because of the small diameter of single wall nanotubes. The source of such a significant decrease in thermal conductivity with isotope disorder has been correlated to diffusive scattering rather than an increase in disorder-induced localization effects as reported elsewhere.²⁹ In a subsequent work, using a similar method, Savić *et al.* discussed isotope, anharmonic and intershell scattering in isotopically disordered BNNTs. Although the simulations were done for single wall nanotubes, intershell effects are considered with a scaling factor emanating from the ratio of multiwall and single wall nanotube diameters. The introduction of this scaling factor produced good agreement with the previous thermal conductivity measurements in multiwall BNNTs.²⁷ The authors concluded that anharmonic and intershell scattering could not be determinant factors in reduction of κ without shadowing isotopic effects. In another study, utilizing the exact numerical solution of phonon Boltzmann Transport Equation (PBTE), Lindsay and Broido³¹ reported an enhancement in room temperature thermal conductivity ranging from 26% for a system size of 1 μm to 37% for a system size of 10 μm when natural (19.9% ^{10}B , 80.1% ^{11}B) and pure (100% ^{11}B) forms of single layer hexagonal BN (white graphene) are considered. These results are also close to the magnitude of reduction predicted in experiments carried out with BNNTs.²⁷ Compared to C based materials, one can speculate the difference in mass of boron and nitrogen will cause a major reduction in κ ; however, it is not clear that further mass differences due to isotopes of boron should lead to drastic reductions in room temperature lattice thermal conductivity of these materials.

In order to investigate the effect of boron isotopes on room temperature lattice thermal conductivity of BN nanostructures, we have performed equilibrium molecular dynamics simulations utilizing the Einstein relation. We have considered different concentrations and masses for boron isotopes. In addition to BN based systems we have also studied their C isomorphs, and have predicted a significant difference between the responses of different dimensional systems, namely nanotube, graphene, and diamond, to isotopic disorder. The rest of the paper is organized as follows. After describing the models and methods used in this study, we demonstrate the suitability of our optimized potential parameter set (OPS)³² for studying thermal transport properties of BN nanostructures. This is followed by a detailed description of how the isotopic disorder affects the thermal transport on BN nano structures and a comparison to their C isomorphs.

II. METHOD

Lattice thermal conductivity, κ , of a system can be calculated by using Green-Kubo theorem^{33–35} or Einstein relation³⁶ in equilibrium MD. In this study, Einstein relation, see Eq. 1, has been employed with a modified energy moment, \mathbf{R} , that is applicable to periodic boundary conditions. The details for the calculation of \mathbf{R} was given in elsewhere.^{37,38} Volume and average temperature of the system and Boltzmann constant are represented by V , T and k_B respectively in Eq. 1. The volumes of the nanotubes and graphene are defined as $2\pi r l \Delta$, and $(lw \times \Delta)$, where r is the nanotube radius, w is the graphene width, l is the structure length, and Δ , 0.335 nm, is the mean Van der Waals diameter for B, N and C atoms of BNWG and graphene.

$$\kappa = \frac{1}{Vk_B T^2} \lim_{t \rightarrow \infty} \frac{1}{2t} \left\langle [\mathbf{R}(t) - \mathbf{R}(0)] \otimes [\mathbf{R}(t) - \mathbf{R}(0)] \right\rangle \quad (1)$$

Molecular dynamics simulations are performed in the microcanonical (NVE) ensemble for 5 ns with a time step of 0.5 fs. Each data point for κ is obtained by averaging the results of six distinct simulations which have different initial particle velocities. In isotopically disordered systems, the isotope distribution considered is random. The standard deviation of these six calculations is shown as the error on data points.

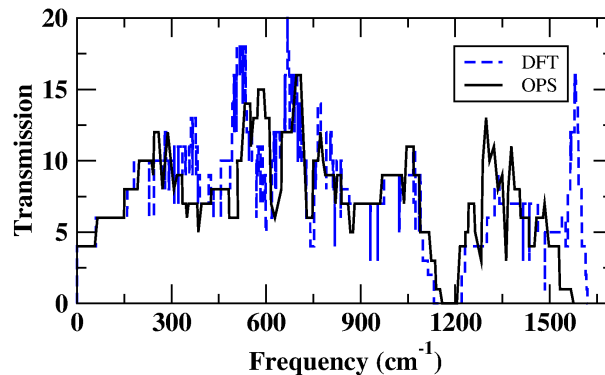


FIG. 1. (Color online) A comparison of the phonon transmission function of BNNT(8,0) calculated from DFT²⁸ and the optimized Tersoff potential used in this work.

Empirical potentials are generated to mimic particle interactions. These potentials have been shown to produce very accurate ground state forces and equation of states. This in turn gives reliable phonon dispersion and anharmonic behavior. Thus, empirical potentials can be used in several methods such as molecular dynamics for correct definition of particle motion and Boltzmann transport³¹ and Green's function³⁹ for dependable phonon band structure. These potentials inherently contain anharmonicity which can be extracted via higher order (third, fourth, fifth etc.) derivatives of potential energy.⁴⁰ The derivatives can also be related to phonon-phonon interactions^{31,41} and be used in BTE. As the order of energy derivatives considered in BTE calculation increases, more phonon-phonon processes (three-, four-, ..., n-phonon) can be included and thus a better accuracy is obtained in calculations.

In molecular dynamics, all phonon-phonon processes, defect scattering, boundary scattering etc. are innate to the calculation. It can be assumed that the natural evolution of the dynamics through thermal excitations possesses the anharmonic behavior of the potential. So, molecular dynamics is very flexible in simulation of complex systems and calculation of total lattice thermal conductivity. But it is inflexible in modularity in examining the effect of structural features from a single simulation. As a result, complexities should be investigated separately if one needs individual contributions. The classical nature of MD inhibits the phonon population from strictly obeying Bose-Einstein statistics. Classical distribution lets all phonons to be excited equally. This generally results in reduction of group velocities below Debye temperature (T_D) because relatively flat optical modes are equally emphasized as relatively steep acoustic modes in phonon dispersion. However, this reduction is balanced by an increase in heat capacity such that the results are comparable to experiments as shown by many previous studies.^{38,42,43} Briefly, it has been claimed that the MD predictions for lattice conductivity can be credible above $T_D/10$.^{41,44} This conclusion is parallel with a previous discussion of the relationship between the quantum canonical correlation function and the classical heat current autocorrelation function.^{18,45}

As described above, accurate description of phonon dispersion, corresponding group velocities and equation of states are critically important in thermal transport calculations.^{46,47} In this study, a recently optimized Tersoff type potential (OPS) which yields very accurate results for both dynamical, mechanical and thermal transport properties of BN nanostructures, is used.³² For instance, the calculated phonon transmission data for BNNT(8,0), shown in Fig. 1, is in good agreement with first principles results reported by Savić *et al.*²⁸

III. RESULTS AND DISCUSSIONS

A. BN nanostructures

In studying isotope effect, we have built BNNT and BNWG structures with varying concentrations of randomly distributed ¹¹B or ¹⁰B isotopes, as see in Fig. 2 (a). First, it is important to note that pure BNNTs and BNWG (formed with 100% ¹¹B or ¹⁰B) have the largest values of κ , while the maximum reduction from isotope scattering is found in the materials with an equal ratio of ¹¹B and ¹⁰B. The enhancement of κ for a pure sample (100% ¹¹B) over isotopically disordered system as a function of isotope concentration, n_i , can be given as $[(\kappa^{pure}/\kappa^{natural}(n_i) - 1) \times 100]$. Based on this formula, our calculations show 27% and 33% enhancement in BNNTs and BNWG respectively noting that the results for nanotubes are given as an average of (10,0) and (10,10) types. These results are fairly close to recently reported PBTE calculations³¹ on a single layer hexagonal BN structure (~ 26 -37% increase).

As a test case, we calculated the effect of isotope disorder considering the unstable isotopes, ⁸B and ⁹B, as well. Our

results show that when the mass of the scarce isotope decreases further in the natural composition, linear decreases are observed in thermal conductivities of both BNNT and BNWG, as seen in Fig. 2 (b). The slopes of these lines are only 9% different from each other but still for almost isotopes BNWG has smaller thermal conductivity. Even when ^8B is used, the reduction in room temperature lattice thermal conductivity of isotopically disordered BNNTs and BNWG is still smaller than the amount of reduction predicted in ballistic thermal conductivity of BNNTs (AGTF based calculations).³⁰

The equal mass case (i.e. atomic weight of B = atomic weight of N) is another interesting point in understanding the effect of mass difference on the lattice thermal conductivity of BN structures. In a previous study, a hypothetical case was investigated where a single mass ($x = 12\text{u}$) is used for all B and N atoms.³² Such an equality increased the thermal conductivity more than 20% compared to hetero-mass system composed of ^{11}B and ^{14}N only. Here, two additional systems are considered. First, all atom masses are equated to 14u . The resulting thermal conductivity of this system is $549 \pm 61 \text{ W/m}^{-1}\text{K}^{-1}$ which represents a similar increase when all masses are 12u . Second, only 19.9% of the ^{11}B is replaced with ^{14}B . In this case, the calculated thermal conductivity is $264 \pm 36 \text{ W/m}^{-1}\text{K}^{-1}$. At first, it may be expected that this value should be larger than the κ for the system without isotopic disorder since it is also a two-mass system and there is less mass difference between B and N atoms in total. However, the broken order due to randomly distributed ^{14}B at boron site results in stronger phonon scattering. Still, B(19.9% ^{14}B +80.1% ^{11}B)N has larger thermal conductivity than the system containing ^8B with the same concentration although both structures have $|3\text{u}|$ difference from ^{11}B . It could be concluded that lowering mass difference system wide may improve the thermal conduction as predicted by Rayleigh model, but the random distribution of isotopes limits the improvement over the isotopically pure structures.

The reported experimental values for isotopically pure and natural BNNTs at 300 K are ~ 300 and $\sim 200 \text{ Wm}^{-1}\text{K}^{-1}$, respectively.²⁷ This range has been supported by AGTF results;²⁸ however, these computations have considered a scaling factor in order to represent the multiwall nanotubes that are used in the experiment. Our simulations predict the κ of BNNTs between $350\text{-}400 \text{ Wm}^{-1}\text{K}^{-1}$, which is directly comparable with both the experimentally reported value (i.e. if only outer shell in multiwall nanotube is active in heat conduction) and those calculated by an exact numerical solution of the PBTE.³¹ The similarity in percent changes in thermal conductivity due to isotope disorder with the PBTE is not surprising because, in principle, both method obtain anharmonic behavior from the same source, namely interatomic potential. Moreover, it should be noted that both our and Lindsay-Borido's potentials have similar forms. The differences in absolute values of thermal conductivity in these two studies should be caused by the difference in phonon populations and the order of included phonon-phonon interactions. As mentioned before, the classical approach used here equipartitions energy into the phonon modes, whereas in PBTE, Bose-Einstein statistics was used. Also, only three-phonon processes are considered in Ref. 31. On the other hand, the effect of anharmonic scattering seems to be the main cause of the lower impact of isotopic scattering in our calculations, 33% enhancement, in comparison to 50% in AGTF calculations.²⁸ In Ref. 28 anharmonic relaxation is considered through an empirical relation⁴⁸ and it is claimed to be less pronounced compared to isotope disorder.

The effect of isotopic disorder for different temperatures is also investigated as depicted in Fig. 3. Here, the convergence of the lattice thermal conductivity of pure and natural BNNTs with temperature reveals the dominant effect of scattering due to anharmonic interactions over isotopic scattering at temperatures above 350 K. Inversely, the larger difference in thermal conductivities of pure and natural systems at lower temperatures suggests that isotopic disorder has more influence in ballistic thermal transport.

B. C nanostructures

It has been shown that the natural abundance of ^{13}C isotopes ($\sim 1.1\%$) in diamond results in $\kappa^{\text{pure}}/\kappa^{\text{isotopic}}$ ratio of 1.3-1.4.^{45,49} This prepotent change compared to 27-33% enhancement in κ of isotope enriched BN nanostructures have encouraged us to further investigate the phenomenon in carbon nanotubes (10,0), graphene and diamond. Different concentrations from 1 to 20% ^{13}C isotope is randomly distributed in C based structures, and the corresponding lattice thermal conductivities are evaluated. Both Tersoff's original potential⁵⁰ and Lindsay-Broido's optimized Tersoff potential⁴⁰ for planar systems are considered in these calculations. In Fig. 4 we present the percent increase in lattice thermal conductivity of the given structures. Just like the BN case, the reduction in the κ due to the presence of isotopes is not as strong as suggested in previous literature for 1D and 2D nanomaterials. On the other hand, the thermal conductivity of diamond is severely reduced even at 1% ^{13}C isotope in accordance with the computational findings of Che *et al.*⁴⁵ and experimental results of Morelli *et al.*⁴⁹ Moreover there seems to be an order in the way isotopic disorder decreases κ in different dimensional structures *i.e.* the diamond (3D) is affected the most and nanotube (1D) is affected the least from the presence of isotopes. Classical simulations represent a relationship between average isotope-isotope distance and thermal conductivity. As the average separation between isotopes is shortened, the mean relaxation time for isotope scattering will be lowered. This will give a lower thermal conductivity according

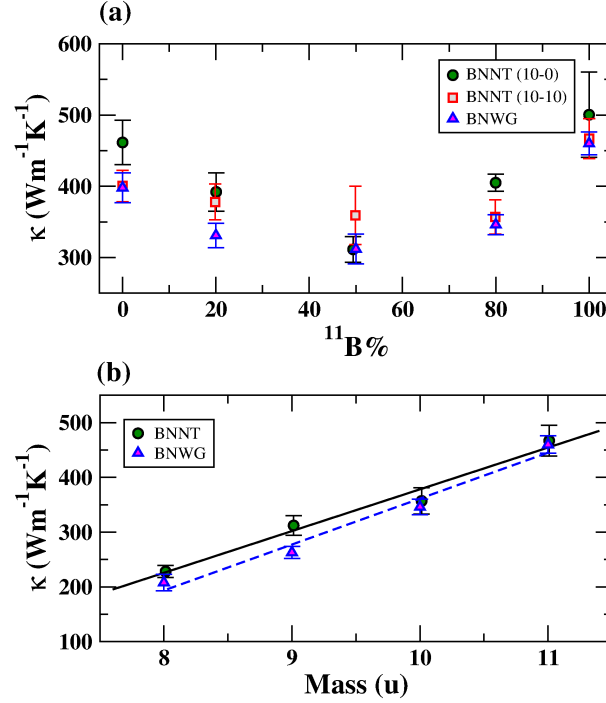


FIG. 2. (Color online) (a) Room temperature lattice thermal conductivity of isotopically disordered zig-zag and armchair BNNTs and BNWG for various ¹⁰B and ¹¹B ratios. (b) Evaluation of lattice thermal conductivity of natural (formed with 19.9% ¹⁰B and 80.1% ¹¹B) BNNT and BNWG with different isotope masses, x .

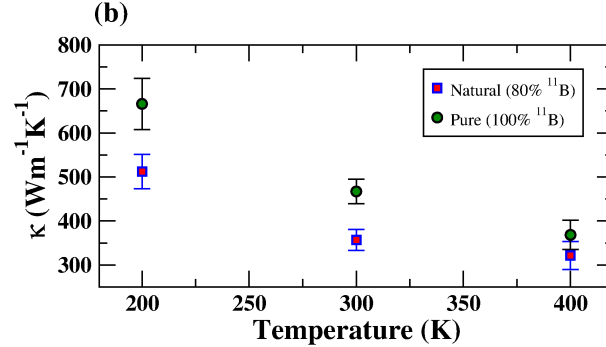


FIG. 3. (Color online) Evaluation of lattice thermal conductivity of natural (formed with 19.9% ¹⁰B and 80.1% ¹¹B) and pure (formed with 100% ¹¹B) BNNTs with temperature.

to fundamental kinetic theory. For instance, if one assumes an isotope concentration of 0.001, the average linear spacing (l) between the isotopes in nanotube, graphene and diamond becomes ~ 108 , 54 and 17.8 Å. The variation of l among systems can be given as $l_{\text{tube}} > l_{\text{graphene}} > l_{\text{diamond}}$. Thus, current results about the dimensionality influence on the κ of isotopically disordered systems can be explained by the difference in mean isotope-isotope separation. If Fig. 2 (a) is reexamined on the basis of this information, one can see a similar case where BNNT(10,0) has almost always higher thermal conductivity than BNNT(10,10) and BNWG. Only at 50% ¹¹B BNNT(10,10) which may be due to an averaging problem and more simulation may be needed at this point. Furthermore the κ s obtained for BNNT(10,10) and BNWG are close to each other which is again expected since the l_{tube} is ~ 62.3 Å for BNNT(10,10).

IV. SUMMARY AND CONCLUDING REMARKS

In this work we present molecular dynamics thermal conductivity calculations on BN and C based materials with disorder arising from isotopes. We predict a room temperature κ on the order of 450 - 500 Wm⁻¹K⁻¹ and

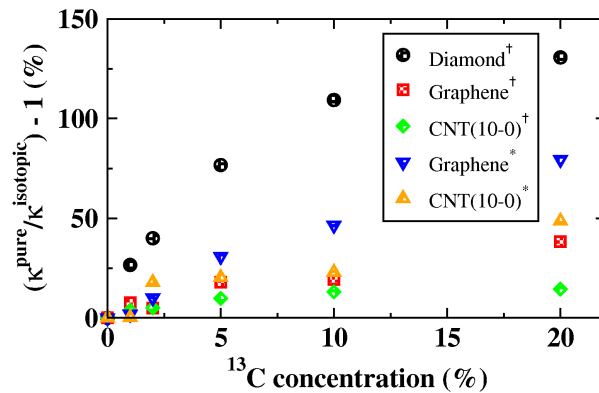


FIG. 4. (Color online) Percent enhancement in the lattice thermal conductivities of isotopically enriched carbon based materials (diamond, graphene and 10-0 CNT) with respect to isotopically disordered systems at various isotope concentrations. Here, (†) and (*) denote that the particle interactions are defined via original and optimized Tersoff potentials respectively.

340-400 $\text{Wm}^{-1}\text{K}^{-1}$ for isotopically pure (100% ^{11}B) and natural (80% ^{11}B) BNNTs and BNWG. This agrees well with the experiments on BNNT that yield values²⁷ on the order of 200-300 $\text{Wm}^{-1}\text{K}^{-1}$. By observing the temperature dependence of BNNTs, we have shown that the influence of isotopes on κ increases at lower temperatures, suggesting the ballistic regime is more susceptible to isotopic scattering. The isotope effect clearly contributes to the reduction of κ , and may have a larger effect on transport in the low-temperature regime. As a result of computations on various dimensional boron nitride and carbon based materials we predict an ascending trend in the effect of isotopic disorder from 1- to 3-dimensional structures in classical regime. This tendency can be explained on the account of average isotope-isotope separation where smaller distances reduces relaxation length ultimately decreasing lattice thermal conductivity.

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* tcagin@tamu.edu

- ¹ S. Iijima, *Nature* **354**, 56 (1991).
- ² R. Saito, G. Dresselhaus, and M. S. Dresselhaus, *Carbon Nanotubes: Synthesis, structure, properties, and applications* (Springer-Verlag, Berlin, 2001).
- ³ M. L. Cohen and A. Zettl, *Phys. Today* **63**, 34 (2010).
- ⁴ C. Y. Zhi, Y. Bando, C. C. Tang, Q. Huang, and D. Golberg, *J. Mater. Chem.* **18**, 3900 (2008).
- ⁵ W.-Q. Han, L. Wu, Y. Zhu, K. Watanabe, and T. Taniguchi, *Appl. Phys. Lett.* **93**, 223103 (2008).
- ⁶ C. Zhi, Y. Bando, C. Tang, H. Kuwahara, and D. Golberg, *Adv. Mater.* **21**, 2889 (2009).
- ⁷ Y. Lin, T. V. Williams, and J. W. Connell, *J. Phys. Chem. Lett.* **1**, 277 (2010).
- ⁸ H. Zeng, C. Zhi, Z. Zhang, X. Wei, X. Wang, W. Guo, Y. Bando, and D. Golberg, *Nano Lett.* **10**, 5049 (2010).
- ⁹ A. Nag, K. Raidongia, K. P. S. S. Hembram, R. Datta, U. V. Waghmare, and C. N. R. Rao, *ACS Nano* **4**, 1539 (2010).
- ¹⁰ N. G. NG Chopra, R. J. Luyken, K. Cherrey, V. H. Crespi, M. L. Cohen, S. G. Louie, and A. Zettl, *Science* **269**, 966 (1995).
- ¹¹ D. Pacile, J. C. Meyer, C. O. Girit, and A. Zettl, *Appl. Phys. Lett.* **92**, 133107 (2008).
- ¹² D. Golberg, Y. Bando, Y. Huang, T. Terao, M. Mitome, C. Tang, and C. Zhi, *ACS Nano* **4**, 2979 (2010).
- ¹³ R. S. Lee, J. Gavillet, M. L. d. l. Chapelle, A. Loiseau, J.-L. Cochon, D. Pigache, J. Thibault, and F. Willaime, *Phys. Rev. B* **64**, 121405 (2001).
- ¹⁴ L. Song, L. Ci, H. Lu, P. B. Sorokin, C. Jin, J. Ni, A. G. Kvashnin, D. G. Kvashnin, J. Lou, B. I. Yakobson, and P. M. Ajayan, *Nano Lett.* **10**, 3209 (2010).
- ¹⁵ Y. Shi, C. Hamsen, X. Jia, K. K. Kim, A. Reina, M. Hofmann, A. L. Hsu, K. Zhang, H. Li, Z.-Y. Juang, M. S. Dresselhaus, L.-J. Li, and J. Kong, *Nano Lett.* **10**, 4134 (2010).
- ¹⁶ Z.-G. Chen, J. Zou, G. Liu, F. Li, Y. Wang, L. Wang, X.-L. Yuan, T. Sekiguchi, H.-M. Cheng, and G. Q. Lu, *ACS Nano* **2**, 2183 (2008).
- ¹⁷ D. Golberg, Y. Bando, C. Tang, and C. Zhi, *Adv. Mater.* **19**, 2413 (2007).
- ¹⁸ J. Che, T. Çağın, and W. A. Goddard III, *Nanotechnology* **11**, 65 (2000).
- ¹⁹ P. Kim, L. Shi, A. Majumdar, and P. L. McEuen, *Phys. Rev. Lett.* **87**, 215502 (2001).
- ²⁰ S. Berber, Y. Kwon, and D. Tomaneck, *Phys. Rev. Lett.* **84**, 4613 (2000).
- ²¹ N. Mingo and D. Broido, *Nano Lett.* **5**, 1221 (2005).
- ²² R. S. Prasher, X. J. Hu, Y. Chalopin, N. Mingo, K. Lofgreen, S. Volz, F. Cleri, and P. Keblinski, *Phys. Rev. Lett.* **102**, 105901 (2009).
- ²³ T.-Y. Choi, D. Poulikakos, J. Tharian, and U. Sennhauser, *Nano Lett.* **6**, 1589 (2006).
- ²⁴ A. A. Balandin, *Nat. Mater.* **10**, 569 (2011).
- ²⁵ W. Li, H. Sevinçli, G. Cuniberti, and S. Roche, *Phys. Rev. B* **82**, 041410 (2010).
- ²⁶ C. Sevik, H. Sevinçli, G. Cuniberti, and T. Çağın, *Nano Letters* **11**, 4971 (2011).
- ²⁷ C. W. Chang, A. M. Fennimore, A. Afanasiev, D. Okawa, T. Ikuno, H. Garcia, D. Li, A. Majumdar, and A. Zettl, *Phys. Rev. Lett.* **97**, 085901 (2006).
- ²⁸ I. Savić, D. A. Stewart, and N. Mingo, *Phys. Rev. B* **78**, 235434 (2008).
- ²⁹ C. W. Chang, W. Q. Han, and A. Zettl, *J. Vac Sci & Tech B* **27**, 199 (2009).
- ³⁰ I. Savić, N. Mingo, and D. A. Stewart, *Phys. Rev. Lett.* **101**, 165502 (2008).
- ³¹ L. Lindsay and D. A. Broido, *Phys. Rev. B* **84**, 155421 (2011).
- ³² C. Sevik, J. B. Haskins, A. Kinaci, and T. Çağın, *Phys. Rev. B* **84**, 085409 (2011).
- ³³ M. S. Green, *J. Chem. Phys.* **22**, 398 (1954).
- ³⁴ R. Kubo, *J. Phys. Soc. Japan* **12**, 570 (1957).
- ³⁵ R. Zwanzig, *Annu. Rev. Phys. Chem.* **16**, 67 (1965).
- ³⁶ E. Helfand, *Phys. Rev.* **119**, 1 (1960).
- ³⁷ A. Kinaci, J. B. Haskins, and T. Çağın, arXiv:1201.6684v3 [physics.chem-ph] (2012).
- ³⁸ J. Haskins, A. Kinaci, and T. Cagin, *Nanotechnology* **22**, 155701 (2011).
- ³⁹ H. Sevinçli, W. Li, N. Mingo, G. Cuniberti, and S. Roche, *Phys. Rev. B* **84**, 205444 (2011).
- ⁴⁰ L. Lindsay and D. A. Broido, *Phys. Rev. B* **81**, 205441 (2010).
- ⁴¹ J. E. Turney, E. S. Landry, A. J. H. McGaughey, and C. H. Amon, *Phys. Rev. B* **79**, 064301 (2009).
- ⁴² P. K. Schelling, S. R. Phillpot, and P. Keblinski, *Phys. Rev. B* **65**, 144306 (2002).
- ⁴³ A. J. H. McGaughey and M. Kaviani, *Int. J. Heat Mass Tran.* **47**, 1783 (2004).
- ⁴⁴ C.-L. Tien, A. Majumdar, and F. M. Gerner, eds., *Microscale Energy Transport* (Taylor and Francis, Washington, 1998).
- ⁴⁵ J. Che, T. Çağın, W. Deng, and W. G. III, *J. Chem. Phys.* **113**, 6888 (2000).
- ⁴⁶ P. Carruthers, *Rev. Mod. Phys.* **33**, 92 (1961).
- ⁴⁷ J. B. Haskins, A. Kinaci, C. Sevik, H. Sevinçli, G. Cuniberti, and T. Çağın, *ACS Nano* , 3779 (2011).
- ⁴⁸ P. G. Klemens and D. F. Pedraza, *Carbon* **32**, 735 (1994).
- ⁴⁹ D. T. Morelli, J. P. Heremans, and G. A. Slack, *Phys. Rev. B* **66**, 195304 (2002).
- ⁵⁰ J. Tersoff, *Phys. Rev. B* **39**, 5566 (1989).