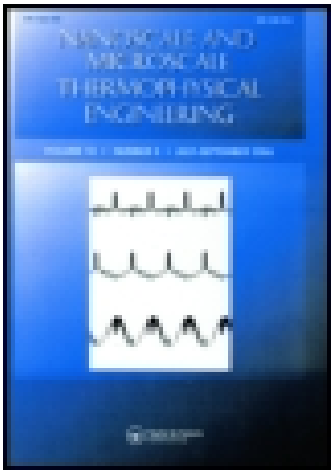

Nanoscale and Microscale Thermophysical Engineering

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/umte20

Explicit Treatment of Hydrogen Atoms in Thermal Simulations of Polyethylene

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Published online: 13 May 2009.

To cite this article: Asegun Henry & Gang Chen (2009) Explicit Treatment of Hydrogen Atoms in Thermal Simulations of Polyethylene, Nanoscale and Microscale Thermophysical Engineering, 13:2, 99-108, DOI: 10.1080/15567260902834707

To link to this article: http://dx.doi.org/10.1080/15567260902834707

Nanoscale and Microscale Thermophysical Engineering, 13: 99–108, 2009

ISSN: 1556-7265 print / 1556-7273 online
DOI: 10.1080/15567260902834707

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EXPLICIT TREATMENT OF HYDROGEN ATOMS IN THERMAL SIMULATIONS OF POLYETHYLENE

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Most atomistic simulation studies of polyethylene employ a united-atom representation to reduce complexity and computational costs. The ramifications of such an approximation have been discussed with respect to structural properties but have not been examined with respect to thermal properties. Here we investigate the consequences of simplified united-atom representations by comparing results from the Kirkwood model to molecular dynamics simulations and lattice dynamics calculations based on a more recent potential, which treats all atoms explicitly. Our results indicate that an explicit treatment of all degrees of freedom is necessary and that significant errors can arise if united-atom approaches are used.

KEY WORDS: molecular dynamics, thermal conductivity, polymer, phonon transport

INTRODUCTION

Polyethylene (PE) is one of the most widely used and simplest polymers. Due to its wide range of applications in many industries, there has been significant effort devoted to modeling and understanding its structural and mechanical properties [1–10]. More recently, the idea of increasing the thermal conductivity of PE through increased alignment of the constituent PE molecules has been suggested from experiments [2, 7]. One experiment demonstrated that the thermal conductivity of bulk PE can be increased by more than two orders of magnitude by mechanically stretching the samples [2].

From a modeling perspective, atomistic simulations can provide useful insight into the associated heat conduction phenomena that give rise to this strong effect. We are aware, however, of only one investigation involving thermal simulations of PE, by Freeman et al. [3]. This study employed the Kirkwood model [4], which uses a united-atom (UA) representation to describe the vibrational modes of the PE chain molecule in two dimensions. UA models reduce the total number of degrees of freedom in a molecular dynamics simulation by lumping atoms together to form a single pseudo-atom rigid body. In the case of the Kirkwood model for PE [4], each hydrogen atom is

Received 24 September 2008; accepted 19 February 2009.
This article was presented at the 6th U.S.–Japan Joint Seminar on Nanoscale Transport Phenomena, July 13–16, 2008, in Boston, MA, USA.
We acknowledge financial support from NSF (CBET0829932) and a DOE computational science graduate fellowship to A.H. We also acknowledge computational resources provided by Intel Corporation and Sandia National Laboratories.
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lumped together with a carbon atom to form CH_2 pseudo-atom units, such that the total number of degrees of freedom is reduced by a factor of three. The UA representation also allows for a time step that is approximately four times larger, because the high-velocity hydrogen motions no longer need explicit treatment. These two benefits together allow for at least an order of magnitude reduction in computational cost compared to a fully explicit treatment of each atomic species. The cost in accuracy for UA representations of PE, however, may outweigh the computational benefits. Sumpter et al. [8] have discussed the ramifications of this simplification on the structural properties of PE. In this article we consider how the UA simplification affects the accuracy and realism of thermal simulations of PE.

The phonon thermal conductivity of crystalline materials is proportional to the phonon specific heat C, group velocities v, and relaxation times τ—($\kappa \propto C \cdot \mathrm{v}2 \cdot \tau$). In modeling thermal conductivity, it is important to model these key properties accurately [11]. The first two properties are largely determined by the accuracy of the phonon dispersion. If the frequency spectrum of the vibrational states is not represented accurately by the associated phonon dispersion of the model, significant errors can arise in the temperature dependence of the specific heat. Additionally, if the slopes of phonon branches ($\mathrm{v} = {}^{\partial\omega}/_{\partial\mathbf{k}}$) are not accurately described by the model, large errors can accumulate in the thermal conductivity. Of particular concern are the acoustic phonons, which are expected to have the largest impact on the thermal conductivity, because of their high velocities and longer relaxation times. Here it is important to note that a factor of three error in a particular mode's group velocity can lead to almost an order of magnitude error in its contribution to thermal conductivity. This is because thermal conductivity is nominally proportional to the square of the group velocity, which consequently has the largest impact on the results. We therefore emphasize that accurate description of acoustic phonon group velocities is of crucial importance. The other property of central importance is that of the phonon relaxation time, which is inherently related to how accurately the material's anharmonicity is described by the atomistic potential energy model.

In a PE crystal we would expect a wide range of vibrational frequencies, due to the high-frequency vibrations of the lightweight hydrogen atoms. One might also expect, by inspection of Fermi's golden rule [12], that the strongest phonon scattering interactions (transition rates) occur between phonons of similar frequency. One can therefore argue that higher frequency optical modes in PE may have a little interaction with acoustic phonons, which are the primary heat carriers. This idea can also be reasoned classically by internal resonances in nonlinear oscillator [13] chains and mode coupling analysis of heat conduction in 1D lattices [14–22]. In the particular case of simulating the thermal conductivity of a single PE chain molecule, one might also expect that higher frequency optical modes will not scatter the low-frequency non-attenuating modes observed in previous studies of anomalous heat conduction in 1D lattices [14–22]. From this line of reasoning, it could be argued that an explicit treatment of hydrogen atoms is not necessary for accurate modeling of thermal transport in PE and thus a UA representation is satisfactory.

On the other hand, there are several reasons why this type of approximate representation may not be satisfactory. For one, reports on classical nonlinear systems have shown that nonlinearity (anharmonicity) in the forces can also allow for significant interactions between high- and low-frequency modes [23]. A second reason is that explicit treatment of all vibrational degrees of freedom is essential for realistic and

accurate description of the normal mode eigenvectors, which generally involve the motion of every degree of freedom [24]. Another reason why explicit treatment of hydrogen atoms in PE might be particularly necessary is because the relative displacement of hydrogen atoms can alter the carbon-carbon interaction between adjacent CH_2 monomers. Lastly, the explicit treatment of hydrogen is necessary for an accurate representation of the specific heat, because the highest frequency vibrations are only expected to become active at high temperatures, above 1000 K. In this article we compare several features of the Kirkwood model for PE [4], which employs the UA approximation, to that of the adaptive intermolecular empirical bond order (AIREBO) potential [25], through molecular dynamics simulations and lattice dynamics calculations. Our simulation results indicate that although explicit treatment of hydrogen may not be necessary for accurate description of some structural and mechanical properties of PE, it is essential for simulations of thermal transport.

MODEL AND SIMULATION PARAMETERS AND ANALYSIS

To describe the interatomic forces, we used the adaptive intermolecular empirical bond order (AIREBO) potential [25], which is based on the highly successful second-generation reactive empirical bond order (REBO) potential developed by Brenner [26]. The REBO term [26] employs a short-ranged cutoff of $\sim$2 Å and is primarily designed to reproduce an accurate energetic description of various covalently bonded hydrocarbon configurations. The REBO term in this regard was fit to various quantum mechanical and experimental results [26]. The major advancement of the AIREBO potential is that it adds a long-range Lennard-Jones term for intermolecular van der Waals interactions and an explicit four-body dihedral term for preferred bonding angles in polymer systems [25]. The Kirkwood model [4], on the other hand, consists of simple harmonic bond stretching and harmonic bond bending interactions in two dimensions. In this sense, the Kirkwood model was not built from quantum mechanical chemical bonding considerations. Nonetheless, Freeman et al.'s [3] use of the Kirkwood model is the most realistic thermal simulation of PE to date [22, 27].

In this article we first used lattice dynamics calculations to determine the phonon dispersion relations and mode eigenvectors [24]. From these results we then ran molecular dynamics simulations of single PE chains in the LAMMPS software package, developed at Sandia [28]. All simulations were run at constant energy, volume, and number of particles (microcanonical) and used a time step of 0.25 fs. Periodic boundary conditions were employed along the length of the chain and all simulations were started with the equilibrium (minimum energy) zigzag lattice positions and random velocities corresponding to a quantum corrected [29] room temperature.

Upon calculation of the atomic trajectory a modal analysis technique was employed to study the energy fluctuations of each normal mode. We first compute the mode amplitudes,

$$X_{\mathbf{k},p}(t) = \sum_{j}^{N} \sqrt{\frac{m_j}{N}} \cdot \left(\mathbf{r}_j(t) - \mathbf{r}_{j0}\right) \cdot \mathbf{p}^*_{\mathbf{k},p} e^{\left(i \cdot \mathbf{k} \cdot \mathbf{r}_{j0}\right)} \tag{1}$$

where m_j is the mass of atom j, $\mathbf{r}_j(t)$ is its time-dependent location, $\mathbf{r}_{j0}$ is its equilibrium position, and $\mathbf{p}^*_{\mathbf{k},p}$ is the mode eigenvector for a mode with wave vector $\mathbf{k}$

and polarization p. We then calculate each normal mode's total energy at every time step,

$$E_{\mathbf{k},p}(t) = \frac{1}{2}\omega^2_{\mathbf{k},p} X_{\mathbf{k},p}(t) \cdot X^*_{\mathbf{k},p}(t) + \frac{1}{2}\dot{X}_{\mathbf{k},p}(t) \cdot \dot{X}^*_{\mathbf{k},p}(t) \tag{2}$$

where ω is the mode's angular frequency. These results can then be used to calculate mode autocorrelation functions. The integration of these autocorrelations leads to phonon relaxation times for each mode, as proposed by Ladd and Moran [30], furthered by McGaughey and Kaviany [31], and then used in silicon by Henry and Chen [32]. Direct evaluation of the relaxation times and thermal conductivity, however, was not specifically of interest in the present work. What was of primary interest was whether or not the interactions between low-frequency acoustic modes and higher frequency optical modes were significant. We evaluated the strength of these interactions quantitatively by computing the Fourier transform of the temporal mode energy fluctuations $\delta E_{\mathbf{k},p}(t) = E_{\mathbf{k},p}(t) - \langle E_{\mathbf{k},p} \rangle$,

$$F_{\mathbf{k},p}(\nu) = \int_{-\infty}^{\infty} \delta E_{\mathbf{k},p}(t) \cdot \exp(-i \cdot 2\pi\nu \cdot t) \cdot dt \tag{3}$$

where ν is the mode frequency. As other phonons scatter temporally with a particular mode they impart fluctuations at their own oscillation frequencies onto the modal amplitudes of the mode under consideration. The fluctuations in $\delta E_{\mathbf{k},p}(t)$ come from various scattering interactions with other modes in the system. These fluctuations ultimately cause the mode autocorrelation to decay, resulting in a finite relaxation time. If there are significant interactions between low-frequency acoustic modes and higher frequency optical modes, we would expect non-zero frequency components in the corresponding optical frequency range when evaluating Eq. (3) for acoustic modes. If, however, the nonlinearity of the AIREBO potential is not sufficient to cause significant interactions between these two groups of phonons, we would expect a single peak in $F_{\mathbf{k},p}(\nu)$ at the corresponding frequency for the mode being studied.

RESULTS

The phonon dispersion for a single polyethylene chain is shown in Figure 1. This figure shows curves calculated from the AIREBO potential [25], the Kirkwood model [4], and experimental data for phonon frequencies in bulk PE [33]. The AIREBO potential, which uses an explicit treatment of hydrogen atoms, shows significant improvement in the description of phonon frequencies, as compared to Kirkwood's UA model. Most notable is the agreement between the experimental data [33] from bulk PE and the AIREBO potential. Although there is deviation at higher wave vectors, the AIREBO potential predicts the correct shape and magnitude of the acoustic phonon branches, whereas the Kirkwood model is less accurate.

The normalized specific heat per mode for both models is shown in Figure 2, along with the bulk specific heat predicted by the AIREBO model and inferred from ab initio data [1] on the bulk PE dispersion. This figure shows that by employing a UA representation, the Kirkwood model overpredicts the specific heat per mode by more

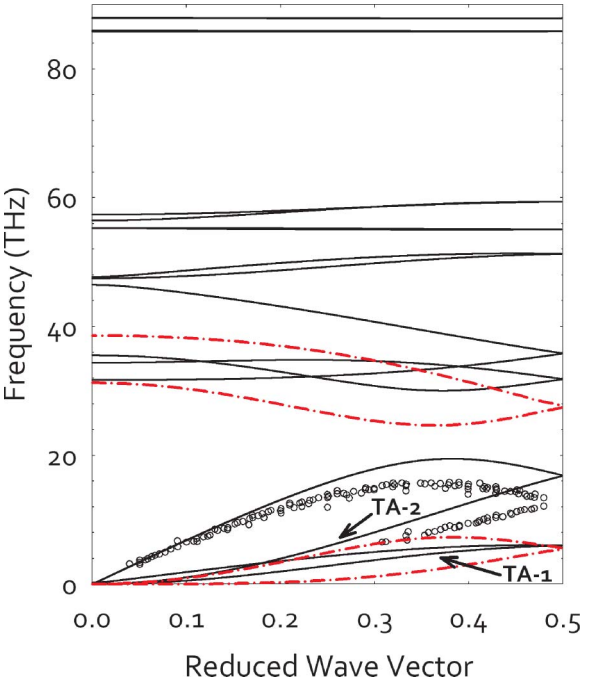

Figure 1 Phonon dispersion of a single polyethylene chain calculated with the AIREBO potential (solid lines) and the Kirkwood model (dashed lines). Arrows indicate the two nondegenerate transverse acoustic polarizations. Experimental data [33] for phonon frequencies in bulk polyethylene are also shown (open circles).

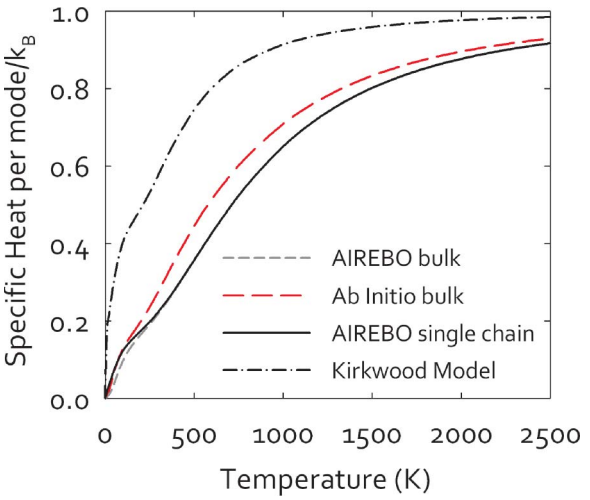

Figure 2 Normalized specific heat per mode. The specific heat of a single polyethylene chain calculated from the AIREBO potential (solid line) and the Kirkwood model (dash-dot line) is shown in comparison with the bulk phonon dispersion calculated from the AIREBO potential (short dashed line) as well as result inferred from the bulk phonon dispersion predicted by ab initio calculations (long dashed line).

than a factor of two at room temperature. This is due to the fact that the highest frequency vibrations associated with the hydrogen vibrations are not described in the UA representation. As a result, several high-frequency phonon branches are left out and the specific heat approaches its maximum at a much lower temperature. The AIREBO model, however, is much more accurate, but differs from the ab initio [1] calculations by ~20–30% in certain regimes. Nonetheless, Figure 2 shows that without explicit inclusion of hydrogen atoms, the specific heat per mode is overpredicted at lower temperatures. It is also important to note that the results in Figure 2 are based on the specific heat per mode and not the total specific heat. This normalization was used to show the ramifications of the discrepancy in frequency spectra for the two models.

The panels of Figure 3 show the Fourier transform of the mode energy fluctuations for several low-frequency transverse acoustic modes, which are indicated in Figure 1. These plots of $F_{\mathbf{k},p}(\nu)$ show that there is significant interaction between the low-frequency acoustic modes and higher frequency optical phonons. It is also evident from Figure 3 that the degree of scattering interaction decreases with acoustic mode frequency. Although this effect may not arise in simpler models [4, 14–18, 20, 22, 27, 34–42], the chemical bonding description of the AIREBO potential [25] shows that scattering from optical phonons between 30 and 60 THz is nonnegligible.

To further illustrate where this nonlinear interaction comes from, Figure 4 shows how the potential well between neighboring carbon atoms is altered when the z-component of a bonded hydrogen atom is displaced by 0.1 Å. This plot shows that

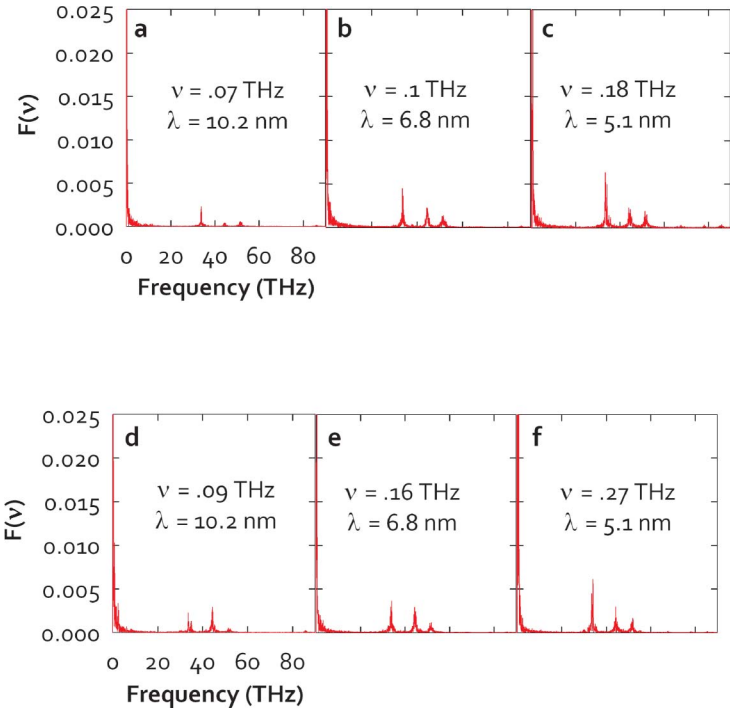

Figure 3 Fourier transform of the temporal mode energy fluctuations of transverse acoustic modes. Panels a, b, and c show data for modes in the TA-1 polarization, and panels d, e, and f show data from the TA-2 polarization. The corresponding mode frequencies and wavelengths are indicated in each panel.

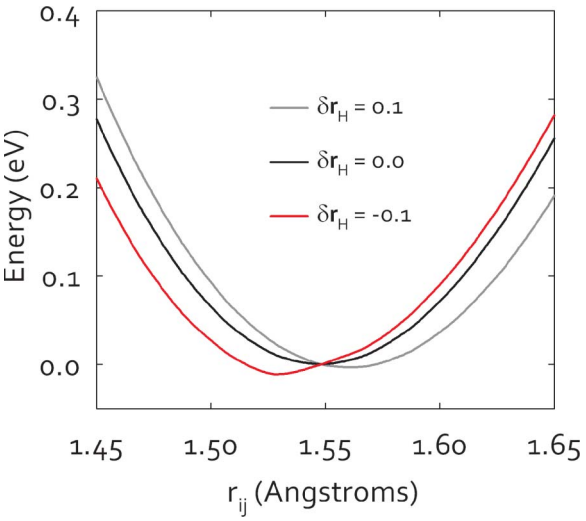

Figure 4 Potential energy well between two bonded carbon atoms in polyethylene as predicted by the AIREBO potential. Each curve indicates how the potential well is affected by a 0.1 Å displacement of a bonded hydrogen atom in the z-direction (along the chain axis). The hydrogen atom displacements are indicated in the legend.

the minimum position of the C-C bond changes with the respective position of the hydrogen atoms. Figure 4 also shows that the asymmetric shape (anharmonicity) of the well is also affected by the hydrogen atom displacement. It is this type of coupling between hydrogen and carbon atoms in the potential that allows interactions between higher frequency optical phonons and low-frequency acoustic modes to occur

To further illustrate the impact that optical phonons have on lower frequency acoustic modes, we show two example normal mode autocorrelations for transverse acoustic modes at short times in Figure 5. This figure shows that there are two

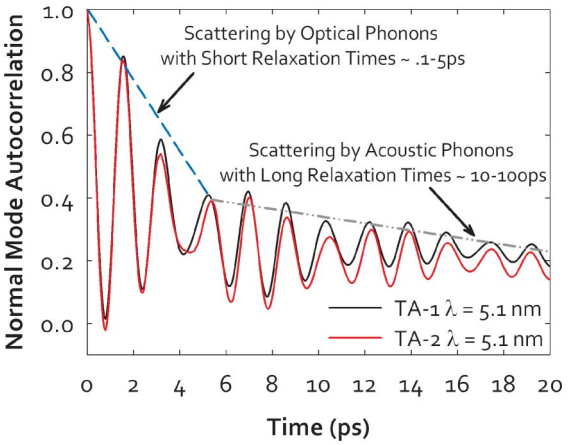

Figure 5 Normal mode autocorrelation for two transverse acoustic modes, based on molecular dynamics simulations with the AIREBO potential. The two distinct timescales for the autocorrelation decay are indicated.

timescales associated with the decay of acoustic phonons. The first short time decay is due to optical phonons, which have short relaxation times on the order of .1–5 ps. The second timescale for the mode decay is due to interactions with other much lower frequency acoustic modes, which have relaxation times on the order of 10–100 ps. This sharp initial decay indicates that optical phonons cause significant energy dissipation in the low-frequency modes at room temperature.

CONCLUSION

The evidence from our molecular dynamics simulations and lattice dynamics calculations suggest that explicit inclusion of hydrogen atoms is necessary for thermal simulations of PE. Our phonon dispersion results indicate that every degree of freedom is necessary to accurately predict the phonon dispersion. The specific heat calculations suggest that UA approaches can also incorrectly allocate the specific heat and may lead to overprediction at lower temperatures. The normal mode analysis indicated that realistic anharmonicity can allow for significant interactions between phonons with more than two orders of magnitude difference in frequency. These results all suggest that an explicit treatment of hydrogen atoms is necessary for accurate modeling of PE's thermal properties. Some of these observations may also be relevant for other polymer systems where the vibrational frequencies span multiple orders of magnitude. Thus, the validity of UA representations in thermal simulations is highly questionable, because our results indicate that all degrees of freedom are necessary for realistic depiction of phonon transport in PE.

REFERENCES

1. G.D. Barrera, S.F. Parker, A.J. Ramirez-Cuesta, and P.C.H. Mitchell, The Vibrational Spectrum and Ultimate Modulus of Polyethylene, *Macromolecules*, vol. 39, pp. 2683–2690, 2006.
2. C.L. Choy, Y.W. Wong, G.W. Yang, and T. Kanamoto, Elastic Modulus and Thermal Conductivity of Ultradrawn Polyethylene, *Journal of Polymer Science: Part B: Polymer Physics*, vol. 37, pp. 3359–3367, 1999.
3. J.J. Freeman, G.J. Morgan, and C.A. Cullen, Thermal Conductivity of a Single Polymer Chain, *Physical Review B*, vol. 35(14), pp. 7627–7635, 1986.
4. J. Kirkwood, The Skeletal Modes of Vibration of Long Chain Molecules, *Journal of Chemical Physics*, vol. 7, pp. 506–509, 1939.
5. J. Ramos, J.F. Vega, D.N. Theodoru, and J. Martinez-Salazar, Entanglement Relaxation Time in Polyethylene: Simulation versus Experimental Data, *Macromolecules*, vol. 41, p. 2959, 2008.
6. C. Schneider, M. Schwetz, H. Munstedt, and J. Kaschta, The Axial Velocity Distribution of a Polyethylene Strand during Extrusion: Simulation and Comparison with Measurements, *Mechanics of Time-Dependent Materials*, vol. 8, pp. 215–224, 2004.
7. E. Skow, Processing and Thermal Properties of Molecularly Oriented Polymers, Master's thesis, Massachusetts Institute of Technology, Cambridge, MA, 2007.
8. B.G. Sumpter, D.W. Noid, G.L. Liang, and B. Wunderlich, Atomistic Dynamics of Macromolecular Crystals, *Advances in Polymer Science*, vol. 116, pp. 27–58, 1994.
9. V. Vao-soongnern, P. Doruker, and W.L. Mattice, Simulation of an Amorphous Polyethylene Nanofiber on a High Coordination Lattice, *Macromolecular Theory and Simulations*, vol. 9(1), pp. 1–13, 1999.

10. X.-B. Zhang, Z.-S. Li, Z.-Y. Lu, and C.-C. Sun, The Crystallization of Low-Density Polyethylene: A Molecular Dynamics Simulation, *Polymer*, vol. 43, pp. 3223–3227, 2002.
11. G.P. Srivastava, *Physics of Phonons*, Adam Hilger, New York, 1990.
12. P.L. Hagelstein, S.D. Senturia, and T.P. Orlando, *Introductory Applied Quantum and Statistical Mechanics*, John Wiley & Sons, Hoboken, NJ, 2004.
13. A.H. Nayfeh and D.T. Mook, *Nonlinear Oscillations*, Wiley-IEEE, Hoboken, NJ, 1995.
14. G. Casati, J. Ford, F. Vivaldi, and W.M. Visscher, One-Dimensional Classical Many-Body System Having a Normal Thermal Conductivity, *Physical Review Letters*, vol. 52(21), pp. 1861–1864, 1984.
15. E. Fermi, J. Pasta, and S. Ulam, Studies of Nonlinear Problems. I, Los Alamos Report No. LA1940, 1955.
16. B. Li and J. Wang, Anomalous Heat Conduction and Anomalous Diffusion in One-Dimensional Systems, *Physical Review Letters*, vol. 91(4), p. 044301, 2003.
17. B. Li, H. Zhao, and B. Hu, Can Disorder Induce a Finite Thermal Conductivity in 1D Lattices?, *Physical Review Letters*, vol. 81(1), pp. 63–66, 2001.
18. N. Li, P. Tong, and B. Li, Effective Phonons in Anharmonic Lattices: Anomalous vs. Normal Heat Conduction, *Europhysics Letters*, vol. 75(1), pp. 49–55, 2006.
19. O. Narayan and S. Ramaswamy, Anomalous Heat Conduction in One-Dimensional Momentum-Conserving Systems, *Physical Review Letters*, vol. 89(20), p. 200601, 2002.
20. T. Prosen and D. K. Campbell, Normal and Anomalous Heat Transport in One-Dimensional Classical Lattices, *Chaos*, vol. 15, p. 015117, 2005.
21. H. Shiba and N. Ito, Anomalous Heat Conduction in Three-Dimensional Nonlinear Lattices, *Journal of the Physical Society of Japan*, vol. 77(5), p. 054006, 2008.
22. J.-S. Wang and B. Li, Intriguing Heat Conduction of a Chain with Transverse Motions, *Physical Review Letters*, vol. 92(7), p. 074302, 2004.
23. T.J. Anderson, A.H. Nayfeh, and B. Balachandran, Coupling between High-Frequency Modes and a Low-Frequency Mode: Theory and Experiment, *Nonlinear Dynamics*, vol. 11, pp. 17–36, 1996.
24. M.T. Dove, *Introduction to Lattice Dynamics*, Cambridge University Press, New York, 1993.
25. S. Stuart, A.B. Tutein, and J.A. Harrison, A Reactive Potential for Hydrocarbons with Intermolecular Interactions, *Journal of Chemical Physics*, vol. 112(14), pp. 6472–6486, 2000.
26. D.W. Brenner, O.A. Shenderova, J.A. Harrison, S.J. Stuart, B. Ni, and S.B. Sinnott, A Second-Generation Reactive Empirical Bond Order (REBO) Potential Energy Expression for Hydrocarbons, *Journal of Physics: Condensed Matter*, vol. 14, pp. 783–802, 2002.
27. J.-S. Wang and B. Li, Mode-Coupling Theory and Molecular Dynamics Simulation for Heat Conduction in a Chain with Transverse Motions, *Physical Review E*, vol. 70, p. 021204, 2004.
28. S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, *Journal of Computational Physics*, vol. 117, pp. 1–19, 1995.
29. S. Volz and G. Chen, Molecular-Dynamics Simulation of Thermal Conductivity of Silicon Crystals, *Physical Review B*, vol. 61, pp. 2651–2656, 2000.
30. A.J.C. Ladd, B. Moran, and W.G. Hoover, Lattice Thermal Conductivity: A Comparison of Molecular Dynamics and Anharmonic Lattice Dynamics, *Physical Review B*, vol. 34(8), pp. 5058–5064, 1986.
31. A.J.H. McGaughey and M. Kaviany, Thermal Conductivity Decomposition and Analysis Using Molecular Dynamics Simulations Part I. Lennard-Jones Argon, *International Journal of Heat and Mass Transfer*, vol. 47, pp. 1783–1798, 2004.
32. A.S. Henry and G. Chen, Spectral Phonon Transport Properties of Silicon Based on Molecular Dynamics Simulations and Lattice Dynamics, *Journal of Computational and Theoretical Nanoscience*, vol. 5, pp. 141–152, 2008.

33. D.A. Braden, S.F. Parker, J. Tomkinson, and B.S. Hudson, Inelastic Neutron Scattering Spectra of the Longitudinal Acoustic Modes of the Normal Alkanes from Pentane to Pentacosane, *J. Chem. Phys*., vol. 111, p. 429, 1999.
34. C. Giardina, R. Livi, A. Politi, and M. Vassalli, Finite Thermal Conductivity in 1D Lattices, *Physical Review Letters*, vol. 84, pp. 2144–2147, 1999.
35. S. Lepri, R. Livi, and A. Politi, Heat Conduction in Chains of Nonlinear Oscillators, *Physical Review Letters*, vol. 78(10), pp. 1896–1899, 1997.
36. S. Lepri, R. Livi, and A. Politi, On the Anomalous Thermal Conductivity of One-Dimensional Lattices, *Europhysics Letters*, vol. 43(3), pp. 271–276, 1998.
37. S. Lepri, R. Livi, and A. Politi, Thermal Conduction in Classical Low-Dimensional Lattices, *Physics Reports*, vol. 377, pp. 1–80, 2003.
38. B. Li, L. Wang, and B. Hu, Finite Thermal Conductivity in 1D Models Having Zero Lyapunov Exponents, *Physical Review Letters*, vol. 88(22), p. 223901, 2002.
39. T. Prosen and D. K. Campbell, Momentum Conservation Implies Anomalous Energy Transport in 1D Classical Lattices, *Physical Review Letters*, vol. 84(13), pp. 2857–2860, 2000.
40. A.V. Savin and O.V. Gendelman, Heat Conduction in One-Dimensional Lattices with On-Site Potential, *Physical Review E*, vol. 67, p. 041205, 2003.
41. A.V. Savin, L.I. Manevich, P.L. Christiansen, and A.V. Zolotaryuk, Nonlinear Dynamics of Zigzag Molecular Chains, *Physics - Uspekhi*, vol. 42(3), pp. 245–260, 1999.
42. A.V. Savin, G.P. Tsironis, and A.V. Zolotaryuk, Heat Conduction in One-Dimensional Systems with Hard-Point Interparticle Interactions, *Physical Review Letters*, vol. 88(15), p. 154301, 2002.