

Predicting Vibrational Mean Free Paths in Disordered Systems

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Abstract

Understanding thermal transport in crystalline systems requires detailed knowledge of phonons, which are the quanta of energy associated with atomic vibrations. By definition, phonons are non-localized vibrations that transport energy over distances much larger than the atomic spacing. For disordered materials (e.g., alloys, amorphous phases), with the exception of very long wavelength modes, the vibrational modes are localized and do not propagate like phonons. The Einstein model assumes that the mean free path of these localized vibrations is the average interatomic distance and that their group velocity is equal to the speed of sound. The Cahill-Pohl model assumes that the mean free path of the localized modes is equal to half of their wavelength. While these approach can be used to estimate the thermal conductivity of disordered systems, they only provide a qualitative description of the vibrations that contribute to the lattice thermal conductivity. Using lattice dynamics calculations and molecular dynamics simulations on Lennard-Jones crystalline, alloy, and amorphous systems, we predict and characterize the contributions from phonons and localized vibrations to lattice thermal conductivity.

I. INTRODUCTION

The thermal conductivity of amorphous solids display unique temperature dependance compared to ordered solids.¹ Cahill argued that the lattice vibrations in a disordered crystal are essentially the same as those of an amorphous solid.²

Measurements by all the refs from Galli paper, including Moon.³⁻⁹ The key to understanding such measurement is to estimate a MFP for the vibrational modes in disordered systems.

The goal of this work is to predict the MFP of vibrational modes in disordered systems. Simple Lennard-Jones systems will be studied. A perfect LJ crystal are alloyed with a species of differing mass and amorphous samples are prepared. Thermal transport will be studied to quantify and characterize the ordered and disordered contributions to lattice thermal conductivity. In particular, a more rigorous way to classify vibrational modes in disordered alloys and amorphous samples as phonon-like or diffuson will be investigated. These results will be compared to the phenomenological Einstein and Cahill-Pohl models,^{???}.

The vibrational modes in these systems are characterized in the limit of propagating (phonon) and non-propagating (diffuson) modes by predicting the mode lifetimes and estimating their mean free paths. Estimating an effective dispersion relation is necessary for calculating an effective group velocity for disordered, which is crucial for transforming lifetimes to MFPs. The spectrum of phonon MFPs and the accumulated thermal conductivity are predicted for a model of amorphous silicon. Predictions of thermal conductivity using a boundary scattering model demonstrates

II. THERMAL CONDUCTIVITY PREDICTIONS FROM MOLECULAR DYNAMICS

The thermal conductivity of amorphous solids at low temperatures contain quantum statistical effects.¹ Molecular dynamics simulations are not able to capture quantum statistical effects.

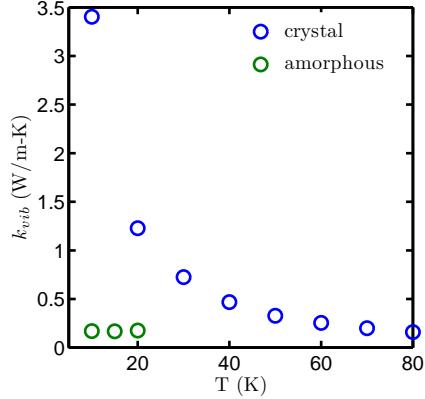


FIG. 1: The temperature dependence of crystalline and amorphous Lennard-Jones samples predicted using MD simulations and the Green-Kubo method.[?] For the crystal the vibrational conductivity follows a $1/T$ scaling (consistent with the phonon-phonon lifetime scaling in Eq. (??)) , while the amorphous vibrational conductivity is temperature independent. Both of these trends are due to the lack quantum mechanical effects in the classical MD simulations.

III. KINETIC THEORY

k = sum over modes

For a perfect system, all vibrational modes are phonons.

$$k_{vib,\mathbf{n}} = \sum_{\boldsymbol{\kappa}} \sum_{\nu} c_{ph}(\boldsymbol{\kappa}_{\nu}) \mathbf{v}_{g,\mathbf{n}}^2(\boldsymbol{\kappa}_{\nu}) \tau(\boldsymbol{\kappa}_{\nu}) . \quad (1)$$

Of particular interest if the phonon mean free path (MFP),

$$\Lambda(\boldsymbol{\kappa}_{\nu}) = |\mathbf{v}_g| \tau(\boldsymbol{\kappa}_{\nu}) , \quad (2)$$

which requires a group velocity.

A. Cahill-Pohl Model

Einstein model:

The group velocity for all the modes is equal to the speed of sound and the mean free path is given by the average interatomic spacing.^{2,11}

Cahill-Pohl (CP) model:

The group velocity for all the modes is equal to the speed of sound and the lifetime is given by the inverse of the mode frequency.²

(half the mode wave-length)

In the Cahill-Pohl model,⁷ the group velocity of all the vibrational modes is assumed to be the sound speed,

$$v_g = v_s \propto \sqrt{B_{glass}/\rho}, \quad (3)$$

and the phonon mean free paths scale with the wavelength of the mode,

$$\Lambda_{glass} = \lambda/2. \quad (4)$$

This approach can be used to estimate a lower limit to the vibrational conductivity in amorphous and disordered systems.^{2,12} However, theory,¹³ experimental measurements,¹⁴ and simulation results¹⁵ show that this approach can give only a qualitative description of the vibrations which contribute to the thermal conductivity in disordered systems.

IV. ALLEN-FELDMAN THEORY

The models for phonon scattering mechanisms described in Section ?? are successful for dilute alloys ($c < 0.1$).^{7,8} However, as the alloy concentration is increased, the vibrational modes become localized and non-propagating and a new description of the vibrational modes which carry the heat is required. For even more disordered systems, such as amorphous materials, the thermal transport is modeled using completely localized vibrations (called *diffusons*) which propagate diffusively, as phonons do.⁷ However, the propagation of these diffusons is (typically) much slower than the propagation of phonons which are able to carry heat over long distances before scattering. Thus, the vibrational conductivity

of amorphous phase is typically several orders of magnitude less than crystalline phase.⁷ The diffuson theory of Allen and Feldman is different than the phenomenological models discussed in Section VIII in that the only allowed wavevector is strictly $\kappa = 0$ since the system is disordered. In reality, the vibrational conductivity has contributions from very-long wavelength phonon-like modes (see Section ??). The disordered contribution to vibrational conductivity, k_{AF} , is given by

$$k_{AF} = \sum_i C(\omega_i) D_{AF}(\omega_i) \quad (5)$$

where $C(\omega_i)$ and $D_{AF}(\omega_i)$ are the diffuson mode specific heat and diffusivity. The vibrational conductivity at low temperatures in disordered and amorphous materials is due to the low temperature behavior of the specific heat $C(\omega_i)$, which is dictated by Bose-Einstein statistics.⁷ The theory of Allen and Feldman is purely harmonic. In the classical harmonic limit, $C(\omega_i) = k_B$ and k_{AF} is temperature independent, which can be used to understand the amorphous LJ temperature independence of vibrational conductivity in Section ??.

Diffusons, locons and propagons¹⁰.

A. AF Diffusivity

Allen Feldman theory¹³.

Feldman measure the DOS using the average level spacing.¹⁶

Predictions for a-Si, also effects of mass disorder.¹⁷: is Di pinned near a value of Di (1/3)va?

$$D = 1/3v_s a$$

It was noticed by Birch and Clark (1940), and by Kit- tel (1948) that in glasses (T) at T \gtrsim 20K could be interpreted as the specific heat C(T)/V multiplied by a temperature-independent diffusivity D of order $a^2 D / 3$ where a is an interatomic distance. In the phonon-gas model, this would correspond to $1/a$, too small to justify use of the model. The success of this observation implies that the dominant normal modes in a glass are of the D variety, not P because P implies $1/a$, and not L because L implies $D = 0$ until anharmonic corrections are added which make D depend on T . This successful (and we believe, essentially correct) interpretation lost favor after Anderson localization was understood, because a misconception arose that the P/D boundary (which certainly lies low in the spectrum of a

glass) should lie close to the E/L boundary.

B. Phonon Diffusivity

Taking the phonon mode specific heat to be $c_{ph}(\kappa_\nu) = k_B$, the phonon mode specific vibrational conductivity (Eq. (??)) can be written as

$$k_{vib,n} = \sum_{\kappa} \sum_{\nu} k_B D_{ph}(\kappa_\nu), \quad (6)$$

and the vibrational conductivity is determined by the phonon mode diffusivities, defined as

$$D_{ph}(\kappa_\nu) = v(\kappa_\nu)^2 \tau(\kappa_\nu). \quad (7)$$

This concept is useful for understanding how the relevant phonon properties (lifetime and group velocity) affect the thermal transport. It is also useful for comparing the relative transport strength of diffusons and phonons. Fig. 10 plots the phonon and diffuson mode diffusivities of a 256 atom LJ crystal and amorphous system at T = 20 K. The number of vibrational modes is the same for these two systems, but the relative magnitudes of the diffusivities vary greatly. The phonons diffusivities are generally greater than the diffuson diffusivities. However, Brioullin zone boundary (see Section A 3) phonon modes have a finite lifetime but vanishing group velocities, giving $D_{ph}(\kappa_\nu) = 0$.? For crystalline systems with many atoms in the unit cell, the presence of optical phonon modes begins to trap heat in low-group velocity branches ($D_{ph}(\kappa_\nu) \approx 0$, see Section ??), making the distinction between phonons and diffusons difficult. Based on their contribution to vibrational conductivity, these low diffusivity optical phonons are thermally indistinguishable from diffusons. The parameters defining the phonon diffusivity (phonon lifetime and group velocity) are generally well-understood. In particular, design strategies to minimize both of these parameters exist (see Sections ?? and ??). However, the design strategies to control the diffusons diffusivities (D_{AF}) are not well understood.? ? The diffuson theory does not consider the effects of anharmonicity, which can be investigated using a combination of MD simulations and LD calculations.?

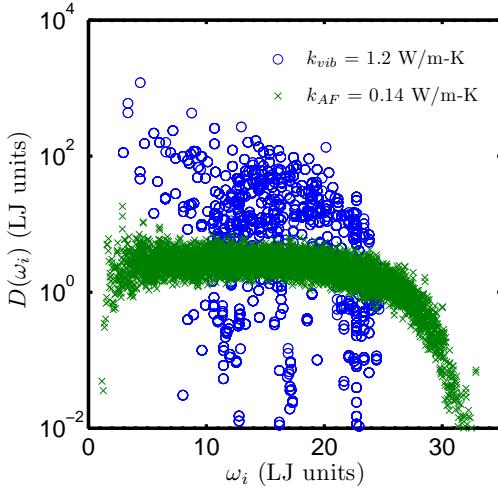


FIG. 2: plot comparison of phonon diffusivity versus AF mode diffusivity for a 256 atom LJ crystal and amorphous system. For both systems, the total number of vibrational modes is the same.

V. PHONONS IN AMORPHOUS MATERIALS

The diffuson theory is different than the phenomenological models discussed in Section VIII in that the only allowed wavevector is strictly $\kappa = 0$ since the system is disordered. In reality, the vibrational conductivity has contributions from very-long wavelength phonon-like modes. Accordingly, the total vibrational conductivity in a disordered or amorphous system is the sum of contributions from diffusons and phonons,

$$k_{vib} = k_{AF} + k_{ph}. \quad (8)$$

Using the Green-Kubo method (see Section ??), the total vibrational conductivity of amorphous Lennard-Jones argon has been predicted to be $k_l = 0.17$ W/m-K. The diffuson contribution is predicted to be $k_{AF} = 0.14$ W/m-K, which suggests $k_{ph} = 0.03$ W/m-K. Similar atomistic predictions have been made for amorphous silicon, where the phonon contribution was shown to be $k_{ph} = 0.5k_{vib}$.? However, the definition of the allowed wavevectors, and hence the phonon properties of the amorphous system, is not well understood.?

VI. LIFETIMES OF DISORDERED MODES

Lifetimes in amorphous silicon predicted before using a normal mode approach, but mode-by-mode properties were not presented.¹⁸

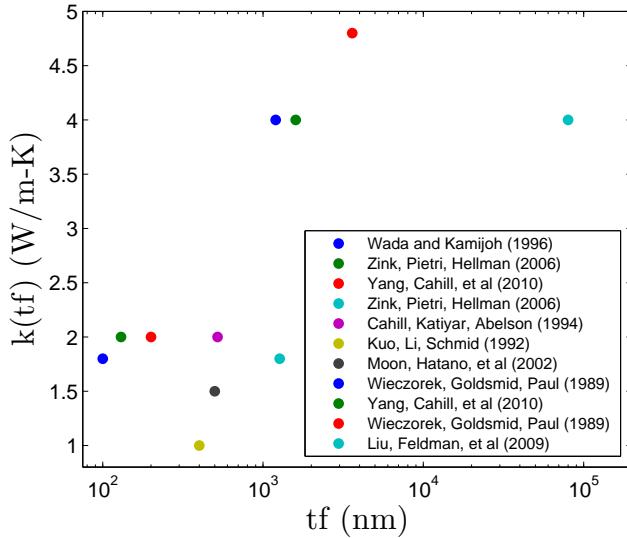


FIG. 3: film thickness dependant thermal conductivity of a-Si from experiment.

Lifetimes were predicted using anharmonic lattice dynamics, but no thermal transport properties were predicted.¹⁹

Thermal diffusivity was predicted for a percolation network which showed Rayleigh type scattering dependance in the low-frequency limit.²⁰

Thermal diffusivity has been predicted using a wave-packet method

The lifetimes of vibrational modes in a-Si were predicted using normal mode decomposition.²¹

A. MFPs in Disordered Systems

B. Ioffe-Regel Limit

C. Characterization of Vibrational Modes

If determined by the Ioffe-Regel limit, $\tau(\kappa) < 1/\omega(\kappa)$.²³ However, for thermal transport analysis this definition is not useful on its own. Show that Anderson localization is exponential dependence of mode excitation on distance from some local center¹⁶. If Ioffe-Regel limit is

According to Cahill, the lifetimes of vibrations in amorphous materials is taken to be one half the period, $\tau = \pi/\omega$.²⁴

Determine by mean free path condition:

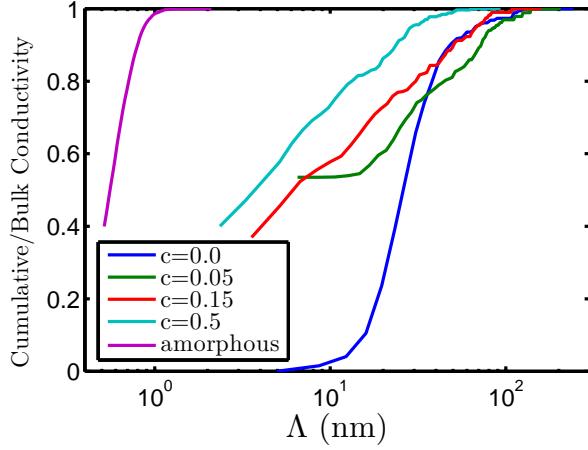


FIG. 4: plot comparison of phonon diffusivity versus AF mode diffusivity for a 256 atom LJ crystal and amorphous system. For both systems, the total number of vibrational modes is the same.

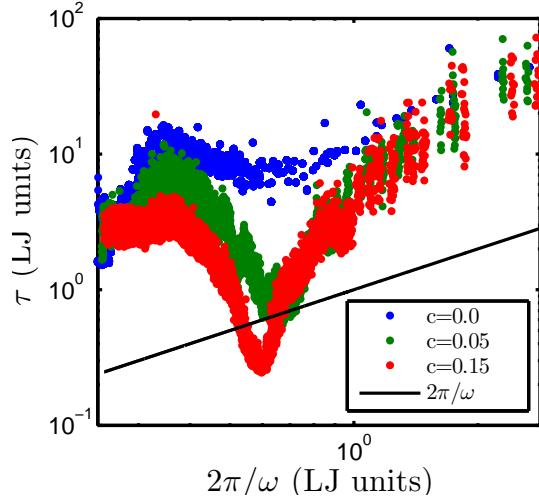


FIG. 5: film thickness dependant thermal conductivity of a-Si from experiment.

$$\Lambda > \lambda$$

Requires a

Participation ratio: For a finite system, the participation is limited by system size. evolution of a vibrational wave packet on a disordered chain.²⁵, shows participation ratio limitation. Also²⁶.

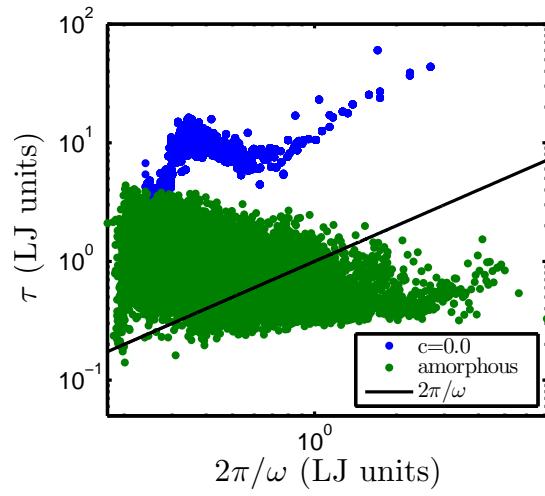


FIG. 6: film thickness dependant thermal conductivity of a-Si from experiment.

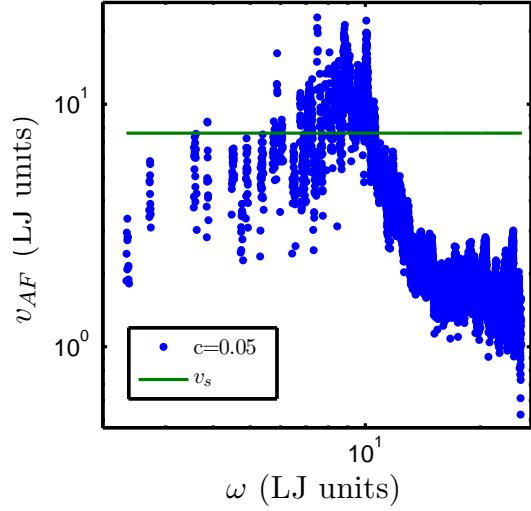


FIG. 7: AF effective velocity

VII. EFFECTIVE MODE VELOCITY

A. AF Velocity

- measured using NMD and anharmonic MD. - extract effective Diffuson velocity, compare to sound speed

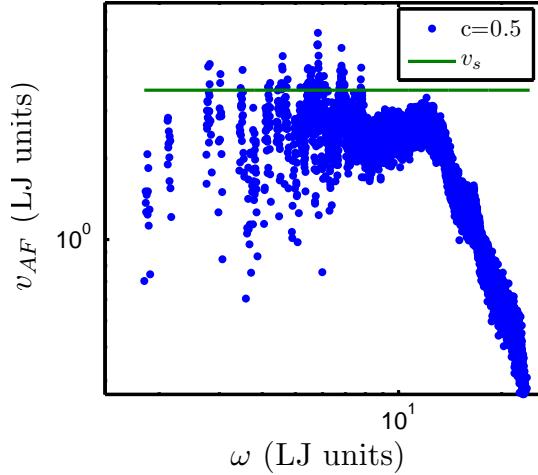


FIG. 8: AF effective velocity

B. Dynamic Structure Factor

If all modes are summed over, this gives the frequency spectrum needed to construct a (nonstationary) propagating state with a pure wave vector \mathbf{Q} and pure longitudinal or transverse polarization¹⁷. Locations of spectral peaks are peaked like acoustic dispersion branches. Only low-frequency vibrations have an (approximate) wavevector in disordered systems, and there is no theorem guaranteeing this.¹⁶

However, it is very difficult to distinguish between localized and extended modes at high frequencies on the basis of their $S(k, \nu)$ functions, as illustrated by the very similar scattering functions for a 67-meV localized and a 63-meV extended mode in Fig. 3(b).²⁷

The dynamic structure factor can be useful for demonstrating the plane-wave character of low-frequency vibrations. However, on a mode-by-mode basis, it is unable in general to characterize a given mode as either localized or delocalized. In fact, results for frequency modes in a disordered system

VIII. ROLE OF ANHARMONICITY IN DISORDERED THERMAL TRANS- PORT

- run harmonic FC MD, predict thermal conductivity using GK
- compare anharmonic GK, harmonic GK, and AF predictions. May possibly need to run "stiffer" system to compare with $k_{si} = k_{ph} + k_{AF} = 0.5 + 0.5$.

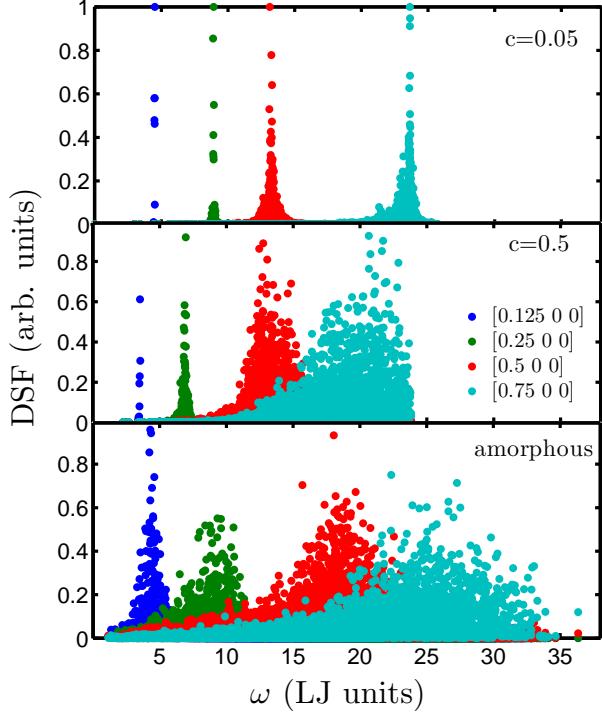


FIG. 9: dynamic structure factor for LJ alloys and amorphous solids.

Appendix A: Predicting Vibrational Lifetimes

1. Normal Mode Decomposition

Normal mode decomposition and its limitations.²²

If $\gamma(\kappa_\nu) > \omega(\kappa_\nu)$, then the vibrational mode is overdamped. Discuss why real-space method is necessary in this case.

2. Vibrations in Ordered and Disordered Solids

In a crystal (periodic) system, the vibrations of atoms are described by a basis of eigenfunctions called phonon normal modes, which are determined by the properties of the crystal (see Appendix A3). The eigenvalues of this basis are the phonon mode frequencies (energies).^{??} The atomic velocities can be represented by the velocity normal mode coordinate, defined as[?]

$$u_\alpha(l; t) = \sum_{\kappa', \nu}^{N, 3n} \frac{1}{\sqrt{m_b N}} \exp[i\kappa' \cdot \mathbf{r}_0(l)] e^*(\kappa'_\nu) \dot{q}(\kappa_\nu; t). \quad (\text{A1})$$

Here, $\dot{q}(\kappa_\nu; t)$ represents the kinetic energy $T(\kappa_\nu; t)$ of the mode with phonon frequency $\omega_0(\kappa_\nu)$ by?

$$T(\kappa_\nu; t) = \frac{\dot{q}^*(\kappa_\nu; t) \dot{q}(\kappa_\nu; t)}{2}. \quad (\text{A2})$$

The phonon mode kinetic energies $T(\kappa_\nu; t)$ are used to calculate the phonon spectral energy density in Appendix A 2.

3. Predicting Phonon Lifetimes using Spectral Energy Denisty

The phonon normal mode coordinate is,

$$\dot{q}(\kappa_\nu; t) = \sum_{\alpha, b, l}^{3, n, N} \sqrt{\frac{m_b}{N}} \dot{u}_\alpha(l_b; t) e^*(\kappa_\nu \cdot \mathbf{r}_\alpha(l)) \exp[i\kappa \cdot \mathbf{r}_0(l)], \quad (\text{A3})$$

which form the basis for vibrations in ordered materials and represents the phonon mode kinetic energy. The normal mode kinetic energy can be transformed from the time domain t to the frequency domain ω by Parseval's theorem,[?]

$$T(\kappa_\nu; \omega) = \lim_{\tau_0 \rightarrow \infty} \frac{1}{2\tau_0} \left| \frac{1}{\sqrt{2\pi}} \int_0^{\tau_0} \dot{q}(\kappa_\nu; t) \exp(-i\omega t) dt \right|^2. \quad (\text{A4})$$

Here, $T(\kappa_\nu; \omega)$ represents the spectral energy of the phonon normal mode with frequency $\omega(\kappa_\nu; \omega)$. Following the derivation in Appendix ??, one arrives at the expression for the SED of a single phonon mode,

$$T(\kappa_\nu; \omega) = \frac{C_0(\kappa_\nu)}{2} \frac{\Gamma(\kappa_\nu) / \pi}{[\omega_0(\kappa_\nu) - \omega]^2 + \Gamma^2(\kappa_\nu)}, \quad (\text{A5})$$

which is a Lorentzian function with center at $\omega_0(\kappa_\nu)$ and a half-width at half-maximum (linewidth) of $\Gamma(\kappa_\nu)$ and $C_0(\kappa_\nu)$ is a constant. We know from anharmonic lattice dynamics theory that the phonon linewidth is related to the phonon lifetime, $\tau(\kappa_\nu)$, by?[?]

$$\tau(\kappa_\nu) = \frac{1}{2\Gamma(\kappa_\nu)}. \quad (\text{A6})$$

The MD simulations we perform here are classical. For a classical system in the harmonic limit (i.e., temperature approaching zero) there is an equipartition of energy and $\sum_\nu^{3n} T(\kappa_\nu; \omega) = \sum_\nu^{3n} V(\kappa_\nu; \omega)$.[?] In an anharmonic system (i.e., a MD simulation), the assumption of equipartition of energy can be tested by predicting the system-level specific

FIG. 10: The SED (Φ) for the first three polarizations at the wavevector $[\pi/4a, \pi/4a, \pi/4a]$ for LJ argon at a temperature of 20 K. There are two degenerate transverse acoustic polarizations and one longitudinal acoustic polarization (of higher frequency).⁷ When fitting the SED, the different polarizations can be fit individually using single Lorentzian peaks or as a superposition of peaks. Here the two peaks are fit individually with Φ plotted as a superposition. The predicted lifetimes of these polarizations, which are inversely proportional to the peak widths Γ , are provided in the legend.

heat. By assuming equipartition of energy, the phonon SED at a particular wavevector is

$$\Phi(\kappa, \omega) = 2 \sum_{\nu}^{3n} T(\kappa; \omega) = \sum_{\nu}^{3n} C_0(\nu) \frac{\Gamma(\nu) / \pi}{[\omega_0(\nu) - \omega]^2 + \Gamma^2(\nu)}, \quad (\text{A7})$$

which is a superposition of $3n$ Lorentzian functions with centers at $\omega_0(\nu)$ (one for each polarization). For simplicity, we refer to $\Phi(\kappa, \omega)$ as Φ . Given a set of atomic velocities, Φ can be calculated using Eq. (??) and (??), and then fit using Eq. (??) to extract the phonon properties $\omega_0(\nu)$ and $\tau(\nu)$.

4. Allowed Wavevectors in Ordered Systems

The phonon spectral energy is defined for the allowed wavevectors of a crystal, which can be specified from the crystal structure's Bravais lattice and its basis, i.e. unit cell. A D -dimensional Bravais lattice is a collection of points with positions

$$\mathbf{u}_0(l) = \sum_{\alpha}^D N_{\alpha} \mathbf{a}_{\alpha} \quad (\text{A8})$$

where N_{α} and the summations if over the lattice vectors, \mathbf{a}_{α} .⁷ The basis (or unit cell) is the building block of the crystal and they are arranged on the points defined by the Bravais lattice. The equilibrium position of any atom in the crystal can be described by

$$\mathbf{u}_0(b) = \mathbf{u}_0(l) + \mathbf{u}_0(b) \quad (\text{A9})$$

where $\mathbf{u}_0(l)$ is the equilibrium position of the l^{th} unit cell and $\mathbf{u}_0(b)$ is the equilibrium position of the b^{th} atom in the unit cell relative to $\mathbf{u}_0(l)$. For the LJ systems studied

here, the cubic conventional cells are used with four atoms per unit cell.⁷ For our MD simulations, cubic simulation domains with periodic boundary conditions are used with $N_1 = N_2 = N_3 = N_0$.^{7, 8} The allowed wavevectors for such crystal structures are

$$\boldsymbol{\kappa} = \sum_{\alpha} \mathbf{b}_{\alpha} \frac{n_{\alpha}}{N_{\alpha}}, \quad (\text{A10})$$

where \mathbf{b}_{α} are the reciprocal lattice vectors⁷ and $-N_{\alpha}/2 < n_{\alpha} \leq N_{\alpha}/2$, where n_{α} are integers and N_{α} are even integers.⁷ The wavevectors are taken to be in the first Brioullin zone.⁷

Allowed Wavevectors in Disordered Materials

Strictly speaking, the only allowed wavevector in a disordered system is the gamma point ($\boldsymbol{\kappa} = [000]$). As such, the lattice dynamics calculations are performed at the gamma point:

5. Thermal Conductivity

Once the lifetimes (MFPs) and group velocities of all vibrational modes in the Brillouin zone are obtained, the bulk thermal conductivity in direction \mathbf{n} , $k_{\mathbf{n}}$, can be calculated from⁷

$$k_{\mathbf{n}} = \sum_{\boldsymbol{\kappa}} \sum_{\nu} c_{ph}(\boldsymbol{\kappa}) v_{g,\mathbf{n}}^2(\boldsymbol{\kappa}) \tau(\boldsymbol{\kappa}). \quad (\text{A11})$$

Here, c_{ph} is the phonon volumetric specific heat and $v_{g,\mathbf{n}}$ is the component of the group velocity vector in direction \mathbf{n} . Since the systems we consider are classical and obey Maxwell-Boltzmann statistics,⁷ the specific heat is k_B/V per mode in the harmonic limit where V is the system volume. This approximation is used here and has been shown to be suitable for LJ argon⁷ and SW silicon.⁷ The group velocity vector is the gradient of the dispersion curves (i.e., $\partial\omega/\partial\boldsymbol{\kappa}$), which can be calculated from the frequencies and wavevectors using finite differences. In this work, the group velocities are calculated using finite difference and quasi-harmonic lattice dynamics because a very small finite difference can be used which reduces the error.⁷ To predict a bulk thermal conductivity, it is necessary to perform a finite simulation size scaling procedure as discussed in Appendix B.

FIG. 11: Thermal conductivity predictions for LJ argon calculated using phonon lifetimes predicted by Φ and Φ' .? (a) The finite simulation-size scaling extrapolation?⁷ is used to compare the results to bulk predictions made using the Green-Kubo method. (b) The bulk results for Φ and Green-Kubo are in good agreement temperatures of 20 and 40 K with those of other atomistic simulation methods.[?]

Appendix B: Finite Simulation-Size Scaling for Thermal Conductivity

For the LJ argon system studied in Section ??, a finite simulation-size scaling procedure?^{??} is used to compare the thermal conductivity predictions from Φ and Φ' to those from the Green-Kubo method. The scaling procedure is demonstrated in Fig. 12. The thermal conductivity is predicted from Φ or Φ' and MD simulations with $N_0 = 4, 6, 8$, and 10. The bulk conductivity, k_∞ , is then estimated by fitting the data to

$$1/k = 1/k_\infty + A/N_0, \quad (\text{B1})$$

where A is a constant. This procedure is necessary because the first Brillouin zone is only sampled at a finite number of points for a finite simulation size, with no contribution from the volume at its center. To predict a bulk thermal conductivity, it is important to sample points near the Brillouin zone center, where the modes can have large lifetimes and group velocities.^{??}

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