Proceedings of the 12th International Conference on Fluid Flow, Heat and Mass Transfer (FFHMT 2025)
July 15, 2025 - July 17, 2025 | Imperial College London Conference, London, United Kingdom
Paper No. 156
DOI: 10.11159/ffhmt25.156

Thermal Conductivity of Disordered Media from Quasi-Phonon Modes

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Extended Abstract

Introduction: The theory of phonons is successful in predicting the thermal conductivity of non-metallic crystalline materials. Making an analogy to the kinetic theory of dilute gases, the isotropic thermal conductivity of a crystal can be expressed as $\kappa = \frac{1}{3}\sum_{n=1}^{3}\int_0^{\infty} c\,(\omega)v(\omega)l(\omega)d\omega$, where c is molar specific heat, v is the phonon group velocity and l is the phonon mean free path, each evaluated for distinct phonon modes with frequency ω. In most cases, the dominant contribution arises from the acoustic modes that have non-trivial group velocities. Extending the theory to disordered media such as liquids or glasses is challenging. First, the phonon dispersion curves are not satisfactorily resolved using the traditional approach which rests on translational symmetry arising from the periodicity of a repeating unit cell. Second, some of the phonon group velocities are deemed to be too high for amorphous solids such as silica [1]. Interestingly, a recent analysis shows that thermal conductivity of a large number of liquids can be predicted using the phonon gas model [2].

Method: In this work we extend our recent effort on using current correlations [3] to extract quasi-phonon modes of two disordered systems – ***i***) a model glass former and ***ii***) a graphite system that is structurally disordered from radiation damage. First, we show that the Fourier modes of the atomic species current, without using a repeating unit cell, are shown to be theoretically and numerically equivalent to phonon modes that are derived through the dynamical matrix approach for crystalline materials. We also show that the eigen decomposition can be advantageously used to identify the phonon modes from different atomic species in a multicomponent system. Next, we compute the isotropic quasi-phononic thermal conductivity using the integral form and compare it with a direct evaluation using the Green-Kubo formalism.

The model glass former is a binary system with parameters provided by Kob and Andersen [4]. The radiation-damaged graphitic system is prepared through large scale non-equilibrium cascade simulation. After equilibration, a primary knock-on atom that is placed at the center of the simulation box receives excess momentum along a certain specified direction. This initially creates a transient liquid-like state, which condenses to a solid state with a number of quasi-stable atomic scale defects following an ultra-fast cooldown phase.

Results: Using the Fourier modes, we extract the quasi-phonon modes for the model glass former and the disordered graphitic system. In both systems, the phonon dispersion curves are non-repeating; for amorphous systems there can be gaps for certain optic branches that do not contribute significantly to thermal transport. Our analysis shows that the thermal conductivities computed from the quasi-phonon modes are numerically close to those obtained from the direct GK method. Of particular interest are the modal frequencies and wavevectors, which contribute most to the thermal conductivity. We will also highlight the origin of phonon bands and the spread in frequencies that are conspicuous for disordered systems. In conclusion, we show that the kinetic theory of phonons can be used to compute the thermal conductivity of disordered media.

References

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