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Direct Calculation of Modal Contributions to Thermal Conductivity via Green-Kubo Modal Analysis WEI LV, ASEGUN HENRY, Georgia Inst of Tech — In studying the physics of thermal conductivity, tremendous progress has been made over the last 20 years toward understanding lattice thermal conductivity in crystalline solids. However, most of the existing methods are based on "phonon gas model", which is the dominant paradigm. It essentially treats vibrations as gas particles, which scatter with each other. This analogy works well for crystals, but it hinges on the assumption that particle velocity being well defined. Because amorphous materials and molecules lack periodicity, it is difficult to define the phonon velocity. We used molecular dynamics simulations and a new formalism for calculating the modal contributions to thermal conductivity to study the amorphous materials, a-Si and a-SiO2. It is the first method that is able to obtain the modal details of phonon transport in amorphous materials including full anharmonicity. This method offers a different perspective on phonon-phonon interactions and allows for direct calculation of phonon contributions to thermal conductivity, which will advance our understanding of the phonon transport mechanism and facilitate heat transfer applications in disordered solids and polymers.

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