

Abstract Submitted
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Green-Kubo Modal Analysis ASEGUN HENRY, Georgia Institute of Technology — A new method for direct calculation of the modal contributions to thermal conductivity, which is termed Green-Kubo modal analysis (GKMA) will be presented. The GKMA method combines the lattice dynamics formalism with the Green-Kubo formula for thermal conductivity, such that the thermal conductivity becomes a direct summation of modal contributions, where one need not define the phonon velocity. As a result, the GKMA method can be applied to any material/group of atoms, where the atoms vibrate around stable equilibrium positions, which includes crystalline line compounds, non-stoichiometric compounds, random alloys, amorphous materials and even rigid molecules. By using molecular dynamics simulations to obtain the time history of each mode's contribution to the heat current, one naturally includes anharmonicity to full order and can obtain insight into the interactions between different modes through the cross-correlations. Several example materials will be discussed and the specific attention will be devoted to new fundamental questions that arise from the changes in mode character that occur in disordered systems. The GKMA method provides new insight into the nature of phonon transport, as it casts the problem in terms of mode-mode correlation instead of scattering, and provides a general unified formalism that can be used to understand phonon-phonon interactions in essentially any class of materials or structures where the atoms vibrate around stable equilibrium sites.

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