Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Scattering phase space and Brillouin zone integrations toward understanding phonon thermal transport properties[1] LUCAS LINDSAY, Oak Ridge National Laboratory — Phonon-phonon interactions arising from lattice anharmonicity most often provide the dominant resistance for thermal energy transfer in semiconductors and insulators. These interactions are governed by fundamental energy and crystal momentum conservation conditions, which define the amount of scattering available to phonons, and thus dictate mode lifetimes and thermal conductivity (k). This work will discuss how various aspects of phonon dispersions determine phase space and k, specifically applied to light atom materials: LiH and LiF. Also, various Brillouin zone integration schemes used to define this phase space and other phonon properties will be discussed, for example, as they are applied to calculate k accumulation with mean free path for Si and MgO.

[1]L. L. acknowledges support from the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division for work done at ORNL.

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Date submitted: 04 Nov 2016 Electronic form version 1.4