Abstract Submitted
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Phonon Scattering Mechanisms in Thermoelectrics[1] OLIVIER DELAIRE, JIE MA, CHEN LI, ANDREW MAY, DAVID SINGH, GEORG EHLERS, DOUG ABERNATHY, BRIAN SALES, Oak Ridge National Lab — Improving our current microscopic understanding of thermal conductivity is needed to design more efficient thermoelectric materials. Thus, establishing a complete picture of phonon dispersions and mean-free-paths is crucial to provide a realistic microscopic characterization of phonon transport, against which theories can be tested. Thanks to recent advances in instrumentation, inelastic neutron scattering can map phonon dispersions and lifetimes across the entire Brillouin zone. As our studies illustrate, such measurements provide key insights about phonon scattering mechanisms, including phonon anharmonicity, electron-phonon coupling, and scattering by point defects or nanostructures. In addition, we perform first-principles simulations of atomic dynamics, including effects of anharmonicity and electron-phonon coupling, to quantitatively model the large experimental datasets. We present results from several studies of important thermoelectric materials [1,2], illustrating how this integrated approach can be used to reach a new level of microscopic understanding of thermal conductivity. [1] O. Delaire, J. Ma, K. Marty, et al. Nature Materials 10, 614 (2011). [2] J. Ma*, O. Delaire*, A. F. May et al. Nature Nanotechnology 8, 445 (2013).

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