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An inverse problem framework for extracting phonon properties from thermal spectroscopy measurements

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Proper characterization of phonons, which are quantum mechanical quasi-particles responsible for transfer of heat in solids, is crucial in design of nano-electronic devices, thermoelectric devices, and biological/chemical sensors. Thermal spectroscopy has been established as a promising experimental method to study phonon properties by measuring thermal responses of materials at sub-millimeter scales. While there have been significant advances enhancing the reliability and accuracy of this experimental technique, the inverse problem of extracting phonon properties from the experimental observations remains an open problem.

We show that by formulating the inverse problem as a non-convex optimization and combining Nelder-Mead algorithm with a graduated optimization framework, phonon properties can be extracted from transient thermal spectroscopy measurements. The proposed technique solves the inverse problem by iterating between solutions of the forward (relaxation) problem and thus requires solutions that capture the mode-dependent physics; these solutions can be either analytical or numerical, including stochastic.

In this presentation we focus on applications of this technique to the extraction of phonon properties using deviational Monte Carlo simulations of the Boltzmann Transport Equation (BTE) and inverse Fourier transform to solve the forward problem. We show that the proposed method can be used to extract phonon relaxation times, free path distribution, and solid-solid interface transmissivities.