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Multiphonon: Phonon Density of States tools for Inelastic Neutron Scattering Powder Data

Jiao Y. Y. Lin[1], **Fahima Islam**[1], **and Max Kresh**[1]

1 Oak Ridge National Laboratory

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Software

- Review
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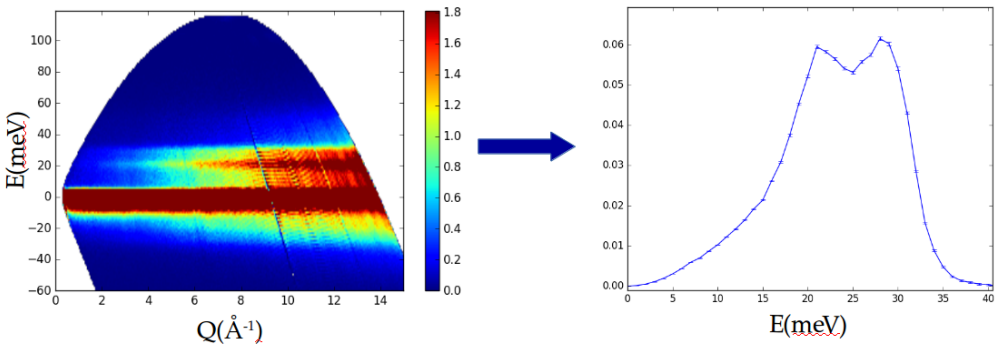
Summary

The multiphonon python package calculates phonon density of states, a reduced representation of vibrational property of condensed matter (see, for example, Section "Density of Normal Modes" in Chapter 23 "Quantum Theory of the Harmonic Crystal" of (Ashcroft and Mermin 2011)), from inelastic neutron scattering (see, for example (B. Fultz et al. 2006–2016)) spectrum from a powder sample. Inelastic neutron spectroscopy (INS) is a probe of excitations in solids of vibrational or magnetic origins. In INS, neutrons can lose(gain) energy to(from) the solid in the form of quantized lattice vibrations – phonons. Measuring phonon density of states is usually the first step in determining the phonon properties of a material experimentally. Phonons play a very important role in understanding the physical properties of a solid, including thermal conductivity and electrical conductivity. Hence, INS is an important tool for studying thermoelectric materials (Budai et al. 2014, Li et al. (2015)), where low thermal conductivity and high electirical conductivity are desired. Study of phonon entropy also made important contributions to the research of thermal dynamics and phase stability of materials (B. Fultz 2010, bogdanoff2002phonon, swan2006vibrational).

The algorithm implemented in this package is a self-consistent, iterative procedure that finishes when the measured INS spectrum can be accounted for by the one-phonon scattering, multi-phonon scattering, and multiple scattering from the deduced phonon density of states, under the incoherent approximation (Appendix of (M. Kresch et al. 2007) and Section 6.5 "Calculation of Multiphonon Scattering" of (B. Fultz et al. 2006–2016)).



The multiphonon package takes the inelastic neutron scattering spectrum, shown on the left, and produces the phonon density of states shown on the right.

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