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

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1 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 [1]), from inelastic neutron scattering (see, for example [2]) 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 [3, 4], 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 [5, 6, 7].

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 [8] and Section 6.5 "Calculation of Multiphonon Scattering" of [2]).

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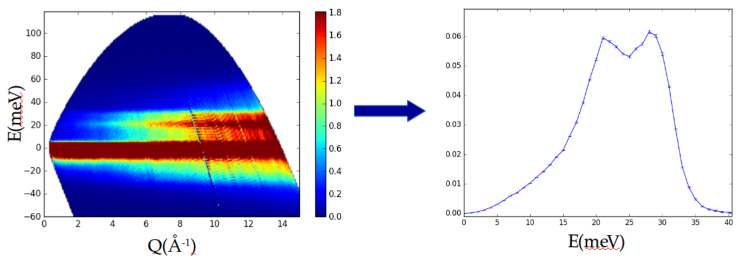

Figure 1: The multiphonon package takes the inelastic neutron scattering spectrum, shown on the left, and produces the phonon density of states shown on the right.

2 Notice of Copyright

3 Acknowledgements

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