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Polycrystalline time-of-flight inelastic neutron scattering beyond the density of states

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Conventionally, experimental phonon dispersions are determined by inelastic neutron scattering on triple-axis spectrometers or by inelastic X-ray scattering, in both cases requiring single crystalline samples. When only polycrystals are available, the energy-dependent density of states (DOS) can be measured as an alternative.

Here I will make the point that the ($|\mathbf{Q}|$,E)-dependent spectral density, which is the primary quantity measured in coherent time-of-flight scattering on polycrystals, has a much greater information content than the DOS, to which it is customarily reduced, and that this information can be accessed by modelling the scattering signal. I will present applications of this technique to different systems and specifically show how the efficiency of the method makes it possible to perform temperature-dependent measurements with fine resolution, such as the behaviour of the phonon frequencies around the α-ɣ transition in elemental iron.

Fig. 1. Time-of-flight spectra of polycrystalline Nickel: measured (left) and simulated (right)

Summary

Topic

1. Theoretical and experimental methods

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