Lattice Dynamics from X-Ray Thermal Diffuse Scattering under High Pressure

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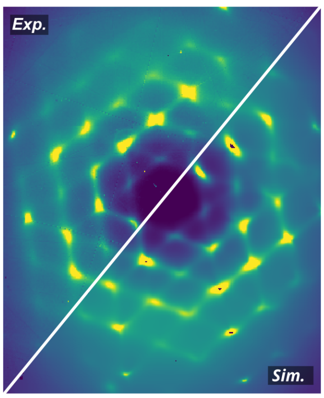
Abstract

Between the Bragg reflections in the X-ray diffraction pattern of any single crystal there exists a weak, continuous, diffuse pattern created by scattering of the X-rays by phonons (Fig. 1, left). This thermal diffuse scattering (TDS) pattern contains information about the lattice dynamics of the crystal. Technological advancements in the past 25 years have sparked renewed interest in TDS as an alternative to inelastic neutron and X-ray scattering techniques for studying the lattice dynamics of crystals [1, 2]. The principal advantage of using TDS is its far shorter data collection times when compared with inelastic scattering techniques. These short data collection times allow for more detailed studies of the lattice dynamics in crystalline systems as a function of pressure, temperature and/or other parameters. However, the data analysis involved with this technique is significantly more demanding.

We have been developing experimental and computational methods for the novel approach of collecting and analysing TDS data from single crystals inside diamond anvil cells (DACs) under compression. We have been taking advantage of the fast data collection associated with TDS techniques to determine full sets of phonon dispersion relations (Fig. 1, right) for a material at numerous different pressures with data collection times of the order of hours instead of days. Extensive model fitting is required to extract lattice dynamical information from the experimental data. In addition to the scattering from the sample, there are numerous sources of background signal, and particular attention must be paid to the Compton scattering and TDS signal from the diamond anvils in the DAC. We have found that modern, multi-panel phonon-counting detectors demand extra attention to the flat-field correction. Here we discuss experimental and data-analysis aspects of the TDS technique, and present first results on the lattice dynamics and pressure-induced anomalies in caesium metal and caesium iodide at pressures up to 10 GPa.



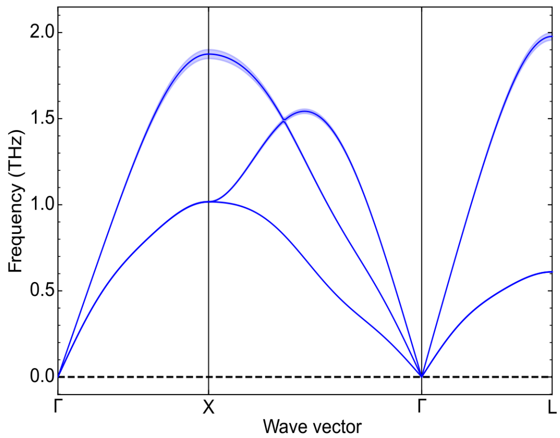


Fig. 1: (Left) Experimental and simulated TDS image of the high-pressure phase fcc caesium at 2.6 GPa and (right) the corresponding extracted phonon dispersion relations. The shaded bands indicate the numerical uncertainty of the phonon frequencies obtained.

References

[1] M. Holt *et al.*, Phys. Rev. Lett. **83**, 3317 (1999).

[2] R. Xu *et al.*, Z. Kristallogr. **220**, 1009 (2005).