	Experiment title: Inelastic X-ray scattering from polycrystalline samples as a mean of extraction of single crystal elastic moduli	**Experiment number**: HS 3051
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Shifts: 18	**Local contact(s)**: Bossak Alexei	*Received at ESRF:*

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Report:

The aim of the experiment was to establish an alternative method for the extraction of the phonon dispersion scheme and the single crystal elastic moduli, utilizing inelastic X-ray scattering (IXS) from polycrystalline samples. Polycrystalline hcp beryllium was chosen as test case because of its high inelastic scattering intensity.

The experiment was performed in transmission geometry, utilizing the Si(999) backscattering reflection of the monochromator and the analyzer (energy resolution of ~3 meV). Spectra for 18 angular settings of the spectrometer arm were recorded. The exact angular positions were chosen to uniformly cover the achievable momentum transfer range and to avoid Bragg peaks. A total of 90 IXS spectra were recorded, spanning a momentum transfer region from 19 nm^{-1} to 79.5 nm^{-1}. The IXS spectra were normalized to the incident photon flux and corrected for the different analyzer efficiencies, scattering volume, the scattering factor and the polarization of the incoming X-ray beam.

A map of the collected and normalized scattering intensities is shown in figure 1. The x-axis covers the momentum transfer range from the first Brillouin zone up to the density-of-state limit. The energy transfer from 0 meV to 92.5 meV is presented in the y direction. The right panel of figure 1 shows model calculations. A set of force constants [1] was used to calculate the phonon energy eigenvalues (E) and eigenvectors over the relevant momentum transfer range, Q, using the OpenPhonon programme [2]. IXS cross sections were determined for a set of crystallographic directions, corresponding to a uniform orientational sampling. The IXS intensity of the polycrystalline sample was then obtained by averaging these values. Finally, the resulting spectra (at fixed Q) were convoluted with the experimental resolution of 3 meV. The data is in good agreement with the model calculations. In the near future a least square fitting routine, refining the lattice dynamics model, will be available.

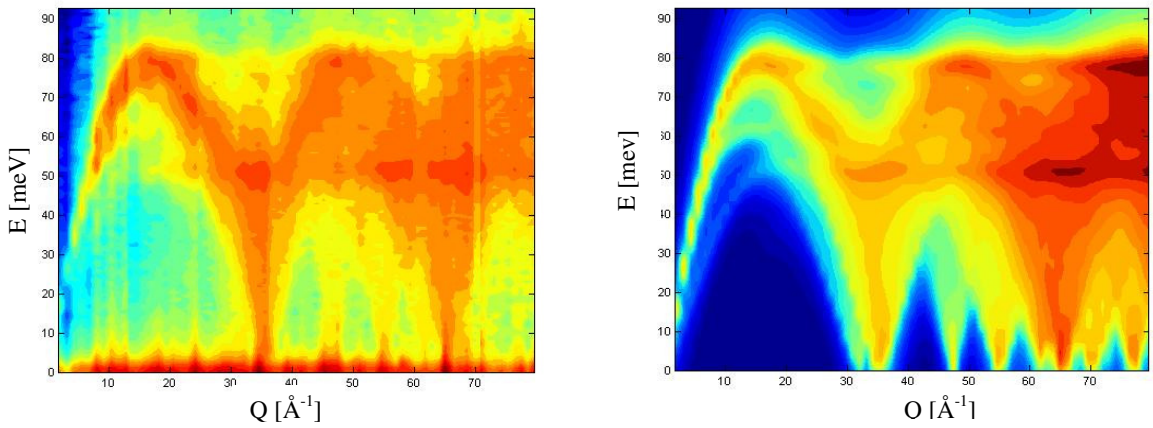

Figure 1: Inelastic X-ray scattering intensity for polycrystalline Beryllium. Left panel: experimental results; right panel: model

In order to have an appropriate sampling for the phonon density of state (VDOS) reconstruction, two angular settings were chosen. After appropriate summing of the spectra, the multiphonon term was eliminated simultaneously with the deconvolution of the data and the instrumental function, following the procedure described in [2]. The resulting VDOS of Beryllium is shown in figure 2. The determined experimental VDOS is in excellent agreement with calculations [3], thus allowing the precise determination of macroscopic parameters such as the Debye temperature and Debye velocity, the vibrational contribution to the specific heat and the internal energy (see Table 1).

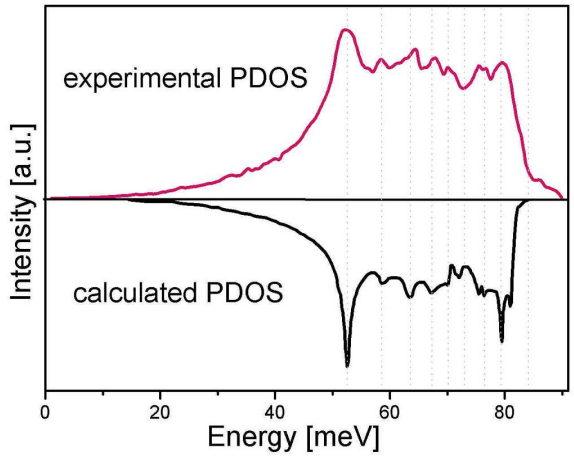

Figure 2. *Reconstructed and calculated VDOS of beryllium*

Experimental	*Literature*
Debye Temperature	
~ 1600 K	1462 K [5] 1160 K [6]
Debye velocity	
10.8 km/s	9.878 m/s [5] 7.840 m/s [6]

Table 1. *Selected macroscopic parameters for beryllium*

The derived Debye temperature is about 1600 K. Its value is about 10% higher than calculated from the elastic moduli [5] and much higher than that obtained from low temperature heat capacity measurements [6]. No adequate explanation for this discrepancy with heat capacity data is available at the present time.

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