

References:

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Keywords: high-pressure structural analysis; phase transitions; coordination number

MS18-O5

Thermal diffuse scattering. A novel approach for probing elasticity at extreme conditions

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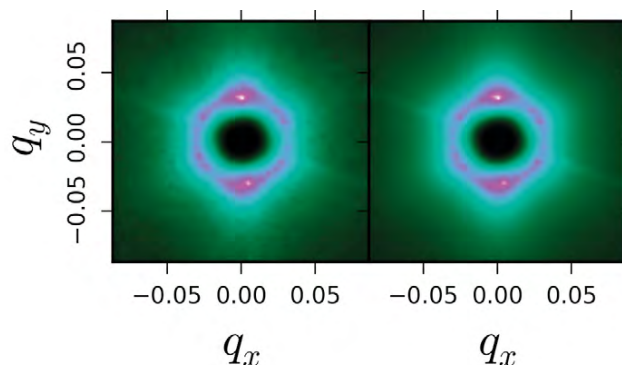
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I will present a novel and fully quantitative analysis of thermal diffuse x-ray scattering. High-precision measurements of diffuse scattering intensities together with a rigorous data analysis now allow for the determination of the full elasticity tensor in a single crystal diffraction experiment [1], see Figure 1.

Our approach enables a reliable and model-free determination of the elastic properties and can be performed together with crystal structure investigation in the same experiment. Elastic moduli can be extracted from small single crystals of arbitrary symmetry, shape and optical properties and will allow for significant progress in the study of the elastic behaviour of minerals at geophysical relevant conditions, structural phase transitions and fundamental interactions of phonons with other quasi-particles. I will furthermore show that this approach can be applied to high pressure, where the simultaneous measurement of structure and elasticity provides the possibility to establish a primary pressure scale from a single measurement.

Figure 1. Measured (left panel) and calculated (right panel) thermal diffuse scattering from calcite at $T = 170$ K. The images show a cross-section of the reciprocal space in Cartesian coordinates, in the vicinity of the $[1, 0, 16]$ reflection. Scattering intensities are shown on a linear color scale from black (zero) to white (maximum intensity).



References:

- [1] Björn Wehinger, Alessandro Mirone, Michael Krisch and Alexei Bosak, Full Elasticity Tensor from Thermal Diffuse Scattering, *Phys. Rev. Lett.* 118, 035502 (2017). Keywords: diffuse scattering, elasticity

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