ESRF	**Experiment title:** Elastic constants from diffuse scattering at high pressure	**Experiment number**: HC 2492
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Report:

We have measured thermal diffuse scattering of single crystal MgO and Calcite at high pressures. Samples were of approximately 50x50x20 μm^3 size. We have used He loaded diamond anvil cells equipped with diamonds of 350 and 300 μm culets for MgO and Calcite, respectively, and Ruby as pressure standard. The beamline was operated at 20.0 keV x-ray energy, a focus of 5x15 μm^2 and a Pilatus W-300 detector system. Temperature of the sample was controlled by resistive heating of the pressure cells. The diffraction geometry was refined using reference measurements with CeO_2 powder and an Enstatite single crystal.

For MgO, we have measured at 0.67, 9.3, 28.4 and 43 GPa pressure at room temperature. Scattering intensities were collected in transmission geometry within an angular range of 70° with angular steps of 0.1° and at three different vertical detector positions.

For Calcite, we have measured at 0.25, 1.05 and 5.2 GPa pressure, at room temperature and 40°C. The angular range was 70° with angular steps of 0.1° and six different vertical detector positions.

Background measurements were performed for all angles and detector positions with measurements with the same cell and temperature, but beside the sample.

For data analysis, we have developed new software for patching and normalizing the diffraction pattern. 3D reconstruction of the reciprocal space and 3D intensity fitting were performed using the recently established method[1] as implemented in our open source software TDS2EL[2].

Preliminary data analysis was performed for MgO at 10 GPa. Scattering intensities around a Bragg reflection as obtained from the 3D reconstruction are illustrated in Figure 1 together with the best fit result.

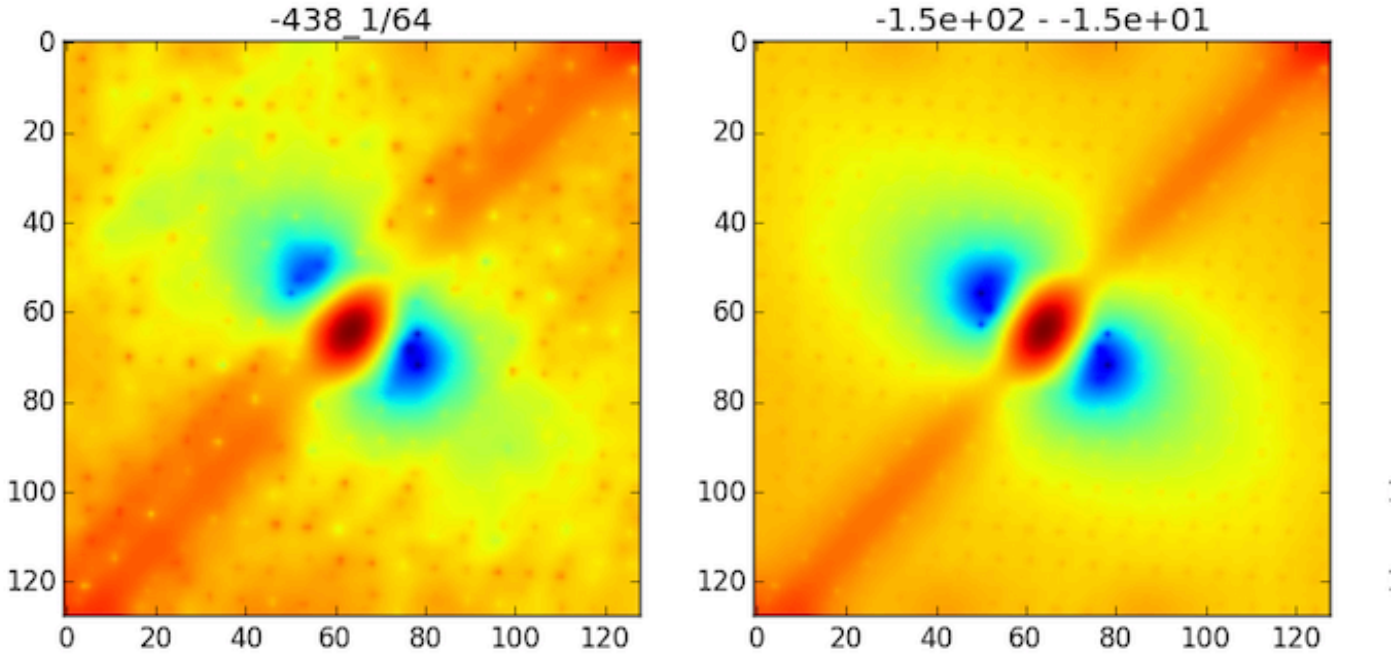

Figure 1. Graphical rendering of measured (left panel) and fitted (right panel) scattering intensities around a selected Bragg reflection of MgO at a pressure of 9.3 GPa. The red area in the centre represents the area in reciprocal space affected by elastic scattering due to the Bragg reflection which is excluded from the fit.

The obtained elastic constants from simultaneous fitting of the scattering intensity distribution around several Bragg reflections agree within 8% to literature values obtained by Brillouin light scattering[3].

In summary, this experiment proofs the feasibility of a quantitative analysis of x-ray diffuse scattering from high pressure measurements using diamond anvil cells. We have shown, that the full elasticity tensor can be obtained from such measurements. With further progress on the experimental setup it will be possible to determine the elasticity tensor to much higher precision. The required improvements are (i) a more precise measurement of incoming flux, (ii) quantitative absorption measurements of the direct beam and (iii) an optimized sample-detector distance. (i) and (ii) are required for a more precise normalisation of the scattering intensity, whereas (iii) will allow us to optimize the momentum resolution with respect to the probed volume in reciprocal space. Ideally, such experiment should be performed using a large CdTe single photon counting pixel detector without read-out noise. This would not only allow to decrease the collection time by one order of magnitude but at the same time enable measurements at an x-ray energy of 30 keV, where the spot size at ID27 is much smaller, thus allowing clean measurements also at more elevated pressure highly relevant for geophysical conditions. Suitable detector systems are commercially available for example from Dectris (Baden, Switzerland).

1. Wehinger, B., Mirone, A., Krisch, M. & Bosak, A. Full Elasticity Tensor from Thermal Diffuse Scattering. *Phys. Rev. Lett.* **118,** 035502 (2017).
2. Mirone, A. & Wehinger, B. TDS2EL documentation. (2017). Available at: http://ftp.esrf.fr/scisoft/TDS2EL/index.html. (Accessed: 7th September 2017)
3. Zha, C.-S., Mao, H. & Hemley, R. J. Elasticity of MgO and a primary pressure scale to 55 GPa. *Proc. Natl. Acad. Sci.* **97,** 13494–13499 (2000).