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High-pressure crystallographic studies in diamond anvil cells using neutrons at HEIDI

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High-pressure single-crystal X-ray diffraction in diamond anvil cells (DAC) using laboratory and synchrotron facilities can now be performed on complex crystal structures that are twinned or modulated. However, there are hardly any single-crystal neutron diffraction studies in the DAC with complete structural refinements. Even at the most advanced neutron facilities, it is difficult to investigate crystals with volumes below 1 mm3 due to low neutron fluxes. The requirement for large samples also hinders a joint use of X-ray and neutron single-crystals diffraction upon compression. The combination of both techniques is highly advantageous for detailed studies on crystalline compounds with magnetic (dis)order and/or on compounds containing light elements. Recently, we have started to explore the feasibility of neutron measurements in the DAC on the single-crystal diffractometer HEIDI at the Heinz Maier-Leibnitz Zentrum in Garching that offers the benefit of short wavelengths with high fluxes. Currently, the minimum crystal size that could be studied there in a DAC is about 0.1 mm3. We have developed optimized DACs for measurements at room and low temperatures in the transmission and radial (panoramic) neutron scattering geometries. Some of these DACs could well be used for combined X-ray and neutron investigations. The diffraction data collected at HEIDI can be used for full and reliable structure refinements.

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