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Combined X-ray and neutron single-crystal diffraction in diamond anvil cells

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Owing to the tremendous development of radiation sources and area-sensitive detectors, single-crystal X-ray diffraction in diamond anvil cells (DAC) can now be performed on complex crystal structures to megabar pressures. However, there are hardly any single-crystal neutron diffraction studies in the DAC that would present complete structural refinements. The reason is that it is still difficult to study crystals with volumes below 1 mm3 due to the low flux of the neutron beams. The requirement for large samples hinders a combined use of X-ray and neutron single-crystals diffraction upon compression. The combination of both techniques is advantageous as neutron diffraction plays a crucial role in cases where X-ray diffraction fails to provide information on, for instance, magnetic (dis)order or hydrogen bonding.

We have developed *transmission* cells for both neutron and X-ray single-crystal diffraction. One of them is equipped with a membrane filled with the He gas that could be operated remotely. The same crystal in the same DAC can now be studied on laboratory X-ray diffractometers, synchrotron beamlines, and at neutron facilities. We have also worked out proper procedures to combine the neutron and X-ray data for joint refinements of the crystal structure.

We are now producing a new *transmission* DAC made of the Ni-Cr-Al alloy with very large opening angles that would allow a wider access to the reciprocal space, close to the one in our *panoramic* diamond anvil cell.

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