

High-pressure synthesis and diffraction studies on functional materials using *in situ* x-ray and neutron diffraction

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High-pressure diffraction studies of the crystal structures of functional materials can give important hints for the optimization of their properties and stability. Therefore, X-ray experiments on powders and single crystals are routinely performed using diamond anvil cells at laboratory X-ray and synchrotron sources. In neutron diffraction experiments, where mostly clamp cells and Paris Edinburg cells are used, the reachable pressure limit is much lower than in x-ray diffraction, due to the fact, that larger sample volumes are required because of low neutron fluxes. In addition, there are hardly any single-crystal neutron diffraction studies, which include a complete determination of the crystal structure.

On the other hand, high-pressure synthesis at variable temperatures in large volume devices not only offers the opportunity to characterize stability fields of different phases but also allows for the discovery of new (metastable) polymorphs with novel properties if the experiments are performed *in situ* at synchrotron or neutron sources.

We could recently show that a full structure determination in diamond anvil cells using the neutron single crystal diffractometer HeiDi at the Maier Leibniz Zentrum is feasible and can be performed in combination with temperatures down to 4 K [1,2]. In parallel, we also performed experiments in clamp cells at ILL at varying HP/LT conditions where larger sample volumes were used [3]. As the combination of X-ray and neutron single-crystal diffraction upon compression is highly advantageous, we also showed that it is feasible to study the same crystals using neutrons and x-rays in the same diamond anvil cell and could show that a joint refinement of the data is suitable [4].

We will illustrate the potential of high-pressure diffraction and synthesis with various examples. These include studies on the high-pressure low-temperature behavior of the crystal and magnetic structure of the unconventional superconductor CrAs [3,5], a comparison of the pressure- and temperature-induced transitions in spin crossover compounds [6], and the discovery of an unusual phase transition sequence in an incommensurately modulated binary vanadium oxide synthesized at high pressures and high temperatures [7].

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