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HIGH-PRESSURE CRYSTALLOGRAPHIC STUDIES IN DIAMOND ANVIL CELLS USING X-RAYS AND NEUTRONS

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A diamond anvil cell (DAC) is the most versatile tool to study structures and physical properties of (non-)crystalline materials at high pressures. The range of experimental techniques in a DAC is very broad: synchrotron and X-ray diffraction, inelastic X-ray scattering, optical and vibrational spectroscopies, etc. However, the main disadvantage of the DAC is a limited sample volume that is available in the sample chamber. Owing to the development of modern two-dimensional detectors and radiation sources, high-pressure single-crystal X-ray diffraction in the DAC using laboratory and synchrotron facilities can now be performed on complex crystal structures that are twinned or modulated. On the other hand, there are hardly any single-crystal neutron diffraction studies in the DAC that would present complete structural refinements. Up to now, even at the most advanced neutron facilities it is difficult to routinely study crystals with volumes below 1 mm3 due to the low flux of the neutron beams. The requirement for large samples 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, as neutron diffraction plays a crucial role in those cases where X-ray diffraction fails to provide information on, for instance, magnetic order or 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 (MLZ) in Garching (Germany) that offers the benefit of various short wavelengths with high fluxes. We have now developed optimized DACs for measurements on crystals smaller than 0.1 mm3 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.

Recent Publications

1. Friese, K., Grzechnik, A., Posse, J.M., Petricek, V. (2013) - Refinement of high-pressure single-crystal diffraction data using Jana2006 – High Pressure Research, 33, 196.
2. Friese, K., Grzechnik, A. (2014) – Twinning and pseudosymmetry under high pressure – Z. Kristallogr.229, 158.
3. Grzechnik, A., Ueda, Y., Yamauchi, T., Hanfland, M., Hering, P., Potapkin, V., Friese, K. (2015) - Structural stability of the Wadsley-type bronzes -Ag0.33V2O5 and -Li0.33V2O5 on compression: a break-down of the two-leg ladder system in the non-superconducting high-pressure phase of -Li0.33V2O5 – Phys. Rev. B 91, 174113.
4. Grzechnik, A., Yeon, J., zur Loye, H.-C., Friese, K. (2016) - High-pressure behaviour of Cs2V3O8 – J. Solid State Chem. 238, 252-258.
5. Friese, K., Khaidukov, N., Grzechnik, A. (2016) - Twinned CsLn2F7 compounds (Ln = Nd, Gd, Tb, Er, Yb): the role of a highly symmetrical cation lattice with an arrangement analogous to the Laves phase MgZn2 – Z. Kristallogr., 231, 631-639.

Biography

Andrzej Grzechnik is a staff scientist at the Institute of Crystallography, RWTH Aachen University (Germany). He has completed his PhD in chemistry from the Arizona State University in 1996. Since then, he has been working on various topics in the fields of crystallography, materials science, solid state chemistry, condensed matter physics, and applied mineralogy. He has served as a board member of various scientific meetings and review panels. Currently, he is a Chair of the Special Interest Group on Crystallography of Functional Materials (SIG#12) of the European Crystallographic Association.

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