

A new high-pressure powder X-ray diffraction cell for soft materials

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High-pressure structural research on soft materials is a critical starting point for establishing structure–property relationships and for enabling targeted chemical improvements, with relevance to properties and applications including mechanical stability, energy storage, solid-state refrigeration, negative linear and area compressibility, and sensing. Diamond anvil cells (DACs) are traditionally the tool of choice for high-pressure diffraction experiments. While highly successful, DACs have been optimized primarily for reaching ever higher pressures. This presents challenges when studying soft materials, such as molecular crystals or soft coordination polymers, where even relatively low pressures can induce large structural responses.

In this presentation, I introduce a new high-pressure powder X-ray diffraction (HP-PXRD) cell designed for the characterization of soft crystalline materials under quasi-hydrostatic pressures up to 0.8 GPa. The cell enables HP-PXRD measurements with pressure increments as small as 50 bar and is compatible with automated cyclic measurement protocols. Its high resolution in the low-pressure regime makes the setup particularly suitable for soft, highly compressible materials. The performance of the cell is demonstrated using $\text{Ni}(\text{dmg})_2$ (dmg = dimethylglyoximate) and $\text{Fe}(\text{phen})_2(\text{NCS})_2$ as a benchmark. In going forward, we understand our cell as the starting point for a new direction in high-pressure research on soft materials, including molecular materials and soft coordination polymers.

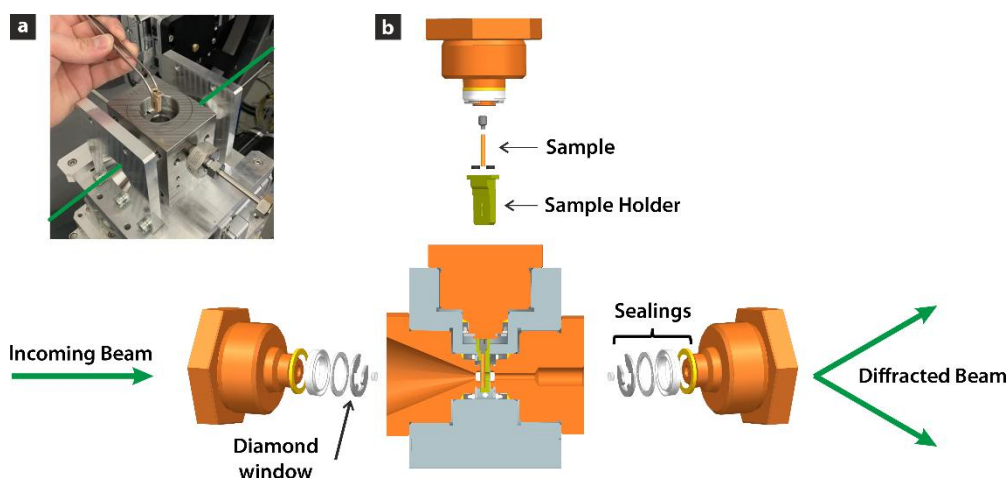


Figure 1. Photograph (a) and schematic (b) of our high-pressure powder X-ray diffraction cell as available at beamline P02.1 at DESY. Pressure is applied by increasing water pressure with an external pumping system. The sample, placed in a plastic capillary, is immersed in this water, and diffraction is measured through two diamond windows.