"My little synchrotron-at-home" - Bruker D8 Venture/X-ray Atlas - the ultimate home-lab high-pressure crystallography solution

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Over the last two decades the great majority of high-profile crystallographic studies in mineral physics have been performed at synchrotron facilities. Besides the obvious advantages of much higher incident beam intensity, small focal spot size, and adjustable energy, synchrotron instruments were the only ones to provide the accuracy of motorized sample positioning, ability to monitor intensity of the X-ray beam passing through diamond anvil cell (used both for DAC alignment, as well as for correcting measured intensity data) and availability of online pressure measurements based on ruby fluorescence. All of these components make the experiments with miniscule mineral crystals enclosed in diamond anvil cells more reliable and dramatically increase the data quality. While the synchrotron beam flux and focal size cannot be matched on home-lab-based instruments, significant improvements in microfocus X-ray sources and 2-dimensional detector technology for X-ray diffraction make experiments in the 0-50 GPa range feasible on home lab instruments.

X-ray Atlas is an NSF-funded, instrument development project aimed at creating a "little synchrotron at home" solution for single crystal diamond anvil cell experiments. Within this project, we are customizing a commercial instrument, Bruker D8 Venture single-crystal diffractometer with a fixed-chi 3-circle goniometer, innovative PHOTON-II CPAD detector, and IμS 3.0 AgKα Incoatec microfocus source with Helios focusing optics. The instrument has been outfitted with all the typical synchrotron high-pressure apparatus, while preserving all of the original standard crystallographic functionality. The X-ray Atlas instrument is controlled via the robust, EPICS protocol used on many synchrotron beamlines, and allows scripting from Python, IDL, or most other languages. It features an alternative heavy duty long translation-range motorized sample platform that can easily accommodate heavy megabar-type DACs, and allows automated, motorized X-ray beam intensity scanning. X-ray Atlas is also equipped with high resolution online optical observation and spectroscopy system enabling accurate measurement of ruby fluorescence signals. With these custom solutions, sub-100um focused beam size, 22.144 keV incident energy and 1.2 x 10^9 photons/s mm^2 intensity, the X-ray Atlas system is still fully compatible with Bruker APEX 3 data analysis software, and allows taking advantage of all the advanced structure determination features, including innovative structure solution algorithms, processing of twinned, multi-crystal and modulated structure data, etc. Lab-based experiments up to 50 GPa with synchrotron-sized high-pressure single-crystal samples of even triclinic symmetry have been successfully performed. The poster will present benchmark results demonstrating accurate sample alignment with X-ray beam intensity scanning, accurate ruby fluorescence measurements, and structure solution from in situ high-pressure data collected at high pressure on crystals of complex mantle silicate minerals.