Xpress – Diffraction at Extreme Conditions

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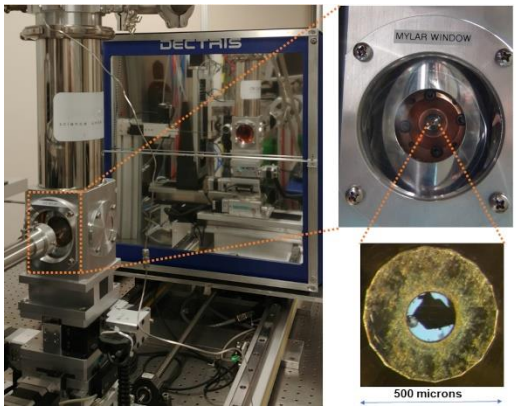
Material properties depends on their atomic-scale organization and a change in this organization can drastically affect the properties of the materials. One best example is the well-known forms of carbon: graphite, diamond, carbon-nanotubes *etc*. Pressure, an important thermodynamic variable, can very effectively modify the atomic-scale organization of materials. *In-situ* high-pressure (HP) diffraction studies permit to monitor the evolution of the atomic-scale structure to this finely controllable external tuning parameter. From 2018, with the availability of the Xpress beamline at Elettra, the HP diffraction community got yet another dedicated experimental set up at their disposal. The beamline utilizes the synchrotron radiation from a superconducting wiggler to produce a 25 keV monochromatic x-rays focused on a large area detector for the diffraction data acquisition in angle dispersive mode. This configuration allows powder and single crystal diffraction experiments [1] to be performed under HP conditions by using diamond anvil cells (DACs). The beamline station is equipped with state-of-the-art facilities for HP manipulation: online fluorescence spectrometer (ruby, Sm^{2+}:SrB_4O_7), automatic pneumatic membrane pressure controller, microscope (long working distance), microdriller etc. In addition to this, the beamline team, in collaboration with the Elettra's Research Engineers (RE) group, had developed a cryogenic loader [2] to permit the loading of a variety of gas media, such as Ar, N_2, O_2, CH_4, etc. We have also a commercial He gas loading system (Sanchez) dedicated to membrane-based DACs.



Cryostat facility permitting the high-pressure low-temperature diffraction investigations.

Xpress is part of a scientific partnership between India and Italy under a joint project between *Indian Institute of Science* Bengaluru and *Elettra-Sincrotrone* Trieste. We are slowly increasing our operational performances by adding new instrumentations to cover the "extreme" conditions, by allowing the simultaneous variation of pressure and temperature. Recently, we have added three new dedicated HP setups compatible to DAC: (i) a low-temperature closed cycle He-cryostat, reaching down to 10 K see Fig. 1; (ii) a high-temperature vacuum chamber, making use of internal and external heater, reaching up to 1000 K; and (iii) a micro Raman spectrometer with a DAC holder. Beamline data collection and control graphical user interface is being continuously improved by the Elettra's Information Technology group to handle well all these new developments, keeping the data collection user friendly.

Elettra is currently undertaking an upgrade program, Elettra 2.0, to reach an even brighter and coherent source. Under this project, Xpress beamline has received a new large area detector, PILATUS3 S 6M (DECTRIS). This development enabled reducing significantly the HP diffraction data collection time, as well as increasing the Q-range with significant improvement in the signal to noise ratio, compared to the previous detector (MAR345). As a consequence, the HP single crystal diffraction data collection, which is recently being highly sought after, become a routine possibility. We will discuss few recent scientific highlights from the beamline to demonstrate the current capabilities of the beamline.

[1] **Single-crystal diffraction at the high-pressure Indo-Italian beamline Xpress at Elettra, Trieste**, Lotti P., Milani S., Merlini M., Joseph B., Alabarse F., Lausi A., *Journal of Synchrotron Radiation*, Vol. 27, pp. 222-229 (2020), doi: 10.1107/S1600577519015170

[2] **Tuning Negative Thermal Expansion in AlPO4-17 by Insertion of Guest Molecules**, Gil Alabarse F., Baptiste B., Joseph B., Haines J., *Journal of Physical Chemistry Letters*, Vol. 13, pp. 9390-9395 (2022), doi: 10.1021/acs.jpclett.2c02718