1st Workshop for the Extreme Conditions Beamline (ECB) Discussion Summary

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The summary below describes the comments/questions that were raised during the discussion at the end of the 1st workshop for the ECB. The discussion was based on the following scientific and experimental focus proposed for P02.2 by the DESY staff. The list does not necessary present a priority list but could be used as a guideline for the development of the beamline, i.e. start with monochromatic and static high-pressure and -temperature experiments, followed in a second stage that provides pink beam Laue diffraction in conjunction with the dynamic sample environments (d-DAC and pulsed laser heating). The purpose of the discussion was to sharpen the scientific focus, and better define the experimental techniques / sample environments based on the needs of the community that will be using the new Extreme Conditions Beamline.

Experimental Techniques proposed for beamline P02.2

X-ray micro diffraction techniques for high-P & high/low-T experiments

⇒ **Monochromatic x-ray diffraction techniques (1st stage of development)**

- **A. Powder Diffraction (especially low Z materials)**
- **B. Single Crystal Diffraction (especially low Z materials)**
- **C. Amorphous Diffraction (Liquids, glasses and amorphous materials)**
- **D. Anomalous Diffraction (Single crystals at high-P in DAC)**
- **E. Diffuse Scattering (Single crystals at high-P in DAC)**

⇒ **Pink beam x-ray diffraction techniques (2nd stage of development)**

- **A. Single Crystal Diffraction (especially low Z materials)**

Sample Environments

⇒ **Sample Environments to conduct static pressure experiments (1st stage of development)**

- **A. High-pressure in the DAC**
- **B. High-pressure and -temperatures with the laser and resistive heated DAC**
- **C. Low temperature with the DAC in the He flow cryostat and the dilution refrigerator cryostat**
- **D. Paris Edinburgh Cell**

⇒ **Sample Environments for dynamic experiments (2nd stage of development)**

- **A. Time resolved pressure studies in the dynamic DAC (d-DAC)**
- **B. Higher P-, T-, t- studies with pulsed laser heated DAC**

Scientific and Experimental Focus of the ECB

There was consent that the 1st stage of development (monochromatic techniques) will provide standard techniques, while the 2nd stage of the development offers rather unique capabilities that would really set the ECB apart from other high-pressure beamlines. Thus, there was a call to accelerate the development of the pink beam options and make it available as soon as possible, even though this might delay the start of the standard monochromatic beamline operations, by at least 6 maybe 12 month.

Optics

Both experiments (Laser Heating, LH, and general purpose, GP) will use a shared KB mirror system with a variable focus as small as 2 μm. In addition both experiments will be equipped with a Compound Refractive Lenses (CRL) system optimized for the fixed energy conditions and with a set focus.

Sample environments

In general, standard sample environments and techniques should be copied from existing high-pressure facilities and focus the resources of the beamline on the development of new techniques such as single crystal laser heating, resistive heating and dynamic DAC. In the same context the beamline should publish which techniques will be available, standard and supported by the beamline stuff, for both experienced and inexperienced users.

LASER HEATING EXPERIMENTS

The position of the LH vs. the GP experiment was debated, i.e. weather it should be positioned upstream or downstream and if the two experiments could be located in two independently operating hutches within the currently available space in sector 2. In general it was suggested that the LH system should be untouched when switching between LH and GP experiment to avoid downtime during lengthy realignments. This is also true for the use of different type of DAC which could be easily accomplished when defining the type of DAC that can be used at the new ECB. There was a call to use the experience of the experts to build and optimize the LH system.

EXTERNAL RESISTIVE HEATING EXPERIMENTS

External heating in DAC is not available at any of the other 3rd generation facilities for general users. It was pointed out that providing the expertise and technical support for such experiments to the community would make the beamline very unique and attract many new users.

PARIS EDINBURGH CELL EXPERIMENTS

In the addendum to the Technical Design Report (TDR) for the ECB a setup for the use of the PE cell was requested, since a hard x-ray beamline is ideal for the study of liquids and one can use the PE to produced melts at high-pressure and simultaneous – temperature. PETRA III does own a V4 PE cell and the necessary soller slits to conducted melting experiment in e.g. on silicate melts. However, the community suggested that one should focus the capabilities for the general purpose experiment on high-pressure and low-temperature experiments and make the Paris-Edinburgh cell's (PE)

the lowest priority, especially since this technique is already established and available at ESRF and at Soleil. In addition the PE might exclude the operation of a potential four circle diffractometer that is optimized for DAC research on the beamline. A four circle diffractometer for high-pressure research is a capability that is currently not available at any of the European synchrotron facilities.

CRYOSTAT EXPERIMENTS

A cryostat setup for high-pressure experiments that can reach temperatures down to 1.9 K is seen as very desirable experimental capability for the general purpose experiment. However, there will be more beamlines at PETRA III that can accommodate DAC in the cryostats and thus it was suggested that cryostats for DAC research should be able to fit on different beamlines.

FOUR CIRCLE DIFFRACTOMETER

The high-pressure single crystal community in Europe is in need of a beamline that offers a four circle diffractometer optimized for high-pressure and preferentially equipped with a small cryostat. Such a setup would make the general purpose experiment of the ECB very unique. The setup should be build on the general purpose experiment despite the availability of four circle diffractometers on other beamlines, because the sphere of confusion of less then 1 micron for all three circles, phi, chi, and omega is needed to conducted very high-pressure experiments.

Infrastructure

The community attested that the infrastructure is crucial for a successful operation of an ECB. In particular the availability of online and offline laser systems such as a Ruby pressure measuring system with high spatial resolution or a portable laser heating system that could be used offline or be installed on other beamlines should be a high priority. In addition it was seen as absolutely crucial to have a gas loading facility on site.

Software

The availability of software for motor control, scanning and data analysis right from the start of the commissioning is very crucial for the successful start of the beamline. In order to minimize the commissioning phase, the beamline should copy as much software as possible from other successful operating high-pressure beamlines.

Miscellaneous

Webpage of the beamline should have information for users such as timeline, protocols, DAC types compatible, etc.. Furthermore, there should be additional but smaller workshops on the various subjects such as low-temperature and high-pressure as well as for the users of the Paris Edinburgh Cell. Obvious opportunities are satellite meetings to the Annual HASYLAB User’s Meeting. Finally, it was suggested to form design teams for the different experimental setups that will actively be involved in the design and guidance for the different techniques. Members of these groups should be very experienced users and that will use the system on a regular basis.