### BL08W High Energy Inelastic Scattering

#### 1. Introduction

High-energy X-ray diffraction (HEXRD) and the total scattering method are techniques that require a stable, high-energy X-ray beam. BL08W is particularly well-suited for this purpose, as it employs a wiggler source combined with a Si (400) monochromator, delivering a high-flux X-ray beam with an energy of 115 keV.

# 2. Rearrangement of HEXRD experiment Setup at BL08W

Until 2023, the HEXRD method was integrated with the sample stage of the magnetic Compton scattering (MCP) setup. However, switching between methods required significant time, with each change taking at least a full day to complete, including the necessary beam calibration. As the number of HEXRD users increased, efforts were made to separate the HEXRD setup from the MCP setup, allowing each system to operate independently.

Recently, the experimental setups at EH1 and EH2 have been restructured. As of 2023, EH1 now hosts HCP, CSI, and XRF measurements, whereas EH2 is dedicated to MCP and HEXRD experiments. Figure 1(a) illustrates the current layout of EH2, where the space is divided into two sections: the front side is allocated for the MCP setup, whereas the back is designated for the HEXRD setup. To optimize the use of space, the HEXRD setup now includes three additional stages, an optic stage, a sample stage, and a detector stage, along with an Xray slit system [Fig. 1(b)]. The slits and these stages enable the beam calibration and experiments of the HEXRD system to be performed independently of the Compton scattering methods and remain permanently in their designated positions. This advancement has significantly reduced the beam calibration time, streamlining the overall process.

In more detail, a laser aligned with the X-ray beam, an ionization chamber, and a two-slit system are incorporated into the optical stage for the HEXRD setup. The front 4-jaw slits shape the beam, whereas the second slit acts as a pinhole to block any unwanted scattering. The sample stage has an area of 500 mm  $\times$  600 mm with a large Z direction translation range of up to 250 mm, enabling it to accommodate various operando reactors for experiments. The long Y direction translation detector stage permits the detector to be moved along the beam direction, which supports data collection from different q-ranges. In addition to the arrangement of the experimental hutch, the motor setup and experimental control area are now completely separated from the Compton scattering setup, establishing а fully independent configuration for the long-term development [Fig. 1(c)].



#### (a) EH2 at BL08W

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X-ray diffraction setup

for Diffraction / Total scattering methods

#### (b) HEXRD at EH2, BL08W



(c) Experimental control area for HEXRD



Fig. 1 (a) Current configuration of EH2 for both MCP and HEXRD methods. (b) Three stages are incorporated for the HEXRD setup at EH2, BL08W. (c) Experimental control area is restructured for HEXRD users at BL08W.

## 3. New long translation detector stage for HEXRD

The new detector stage, with its 1200 mm translation range along the X-ray beam direction, provides the flexibility to tune the q-range and angular resolution of diffraction patterns [Fig. 2(a)]. This capability is well-suited for studies using both HEXRD and total scattering (TS) methods. A larger sample-to-detector distance (SDD) enhances the angular resolution of the scattering pattern, which is essential for detailed analysis in the low q-range to reveal fine structural details. Conversely, a closer SDD facilitates the collection of a wider q-range, which is crucial for pair distribution function (PDF) analysis via TS patterns. Meanwhile, enhanced angular resolution at a large SDD further enriches HEXRD studies, providing valuable insights into the average structure of materials [Fig. 2(b)]. This flexibility enables users to conduct both XRD and TS experiments at the beamline during a single beamtime session.

(a) Long translation of detector stage



(b) Different angular resolution



Fig. 2. (a) The long translation of the detector stage allows both XRD and TS methods at the same beamline. (b) Two XRD patterns collected at min. and max. SDD with the new detector stage show different angular resolutions on patterns.

Currently, the maximum SDD (1360 mm) allows a q-min of 0.15 Å<sup>-1</sup>, whereas the minimum SDD (630 mm) enables effective signal detection up to a q-max of 32 Å<sup>-1</sup> (Table 1). Different q-range scattering patterns are applicable to various disciplines. For example, analyzing amorphous samples requires a specific minimum q-range to perform accurate PDF analysis. In contrast, measurements involving nanosized crystalline

samples benefit from a higher maximum q-range to obtain detailed information on shorter bond lengths and conduct a comprehensive Fourier transform on the TS patterns. The newly configured detector stage is expected to benefit a broader user base.

Table 1. X-ray diffraction patterns collected at different sample-to-detector distances and the q-ranges covered.

SDD	q-range	Method	Material system
1360 mm	0.15 – 15 Å <sup>-1</sup>	XRD	All kinds
830 mm	0.25 – 24 Å <sup>-1</sup>	TS	All kinds
630 mm	0.3 – 32 Å <sup>-1</sup>	TS	Nano materials

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