High Energy Laue X-ray Emission Spectrometer at the European XFEL

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X-ray emission spectroscopy (XES) is a powerful tool for electronic structure characterization, it has been widely used in the study of 3d transition elements, while the K-edge XES spectra of 4d elements were rarely reported [1], even though they are greatly important for phase transition, photocatalyst, biology, geochemistry and etc. One of the main reasons for this is that the K emission lines of 4d elements are usually larger than 16 keV [2] and the standard XES spectrometers (Johann and von Hamos) based on Bragg analyzers quickly loose efficiency when the photon energy is larger than 15 keV. Moreover, the fine structures of X-ray absorption spectroscopy for high-Z elements at high X-ray energies will be strongly submerged by the large core-hole lifetime broadening (Γ >10 eV when the absorption edge>30 keV), the high energy resolution fluorescence detected (HERFD) XAS [3] will be essential for the core-level spectroscopies for very hard X-ray, wherein the high efficiency emission analyzers become to be necessary.

The newly Laue analyzer was designed by FXE group of European XFEL and recently tested at SuperXAS of SLS(~10¹⁰ phs/sec). The analyzer has open window of 8×3 cm², radius of 1.5 m, thickness of 0.25 mm and an asymmetric angle of 2.5° for improving the efficiency, the static nor dynamic bender was chosen for more easy and productive commissioning. We have investigated the possibility of operating off of the Rowland circle to explore the dispersive capabilities, the analyzer can disperse fluorescence X-ray spatially according to its energy, and an algorithm to convert the emission image to spectrum was developed. In this arrangement, as shown in the Fig. 1, the valence to core (VtC) spectra for niobium (with K edge of 19 keV) samples can be visible ~10 mins at SuperXAS beamline. A resolution of 6.7 eV has been realized with the beam size of ~100 μ m, better resolution of ~2.5 eV is expected when reducing the beam size to ~20 μ m.



Figure 1. The VtC emission images and spectra of NbF₅ with 10 mins, 25 mins and 70 mins collection times. The spectra are converted from the image via a calibration method. [1] C. Doonan *et al.*, Inorg. Chem. 44, 2579 (2005).

[2] W. Elam et al., Radiat. Phys. Chem. 63, 121 (2002).

[3] M. Bauer, PCCP. 16, 13827 (2014); F. Lima, PCCP 15, 20911 (2013).