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DEVELOPMENT OF A PHOTOELECTRON SPECTROMETER FOR HARD X-RAY PHOTON DIAGNOSTICS AT THE EUROPEAN XFEL

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Abstract

We developed an angle-resolved photoelectron spectrometer, based on the electron time-of-flight concept, for hard X-ray photon diagnostics at the European Free-Electron Laser. The instrument shall provide users and operators with pulse-resolved, non-invasive spectral distribution diagnostics, which in the hard X-ray regime is a challenge due to the poor cross-section and high kinetic energy of photoelectrons for the available target gases. We report on the performance of this instrument as obtained using hard X-rays at the PETRA III synchrotron at DESY. We demonstrate a resolving power of 10 eV at incident photon energies up to 20 keV.

INTRODUCTION

The unique properties of X-ray Free-Electron Laser (XFEL) radiation offering high-intensity and coherent X-ray pulses at Ångström wavelengths have found applications where the ability to take snapshots of samples at unprecedented molecular length and time scales provides new scientific insights. However, the stochastic nature of Self-Amplification of Spontaneous Emission (SASE) has the consequence that every photon pulse displays individual characteristics in terms of spectral distribution and intensity. At the European XFEL (EuXFEL) facility in Schenefeld, Germany, the X-ray photon diagnostics group (XPD) utilizes a variety of dedicated techniques for providing beam parameters [1]. For soft X-rays, the angle-resolved Photo-Electron Spectrometer (PES) with 16 electron Time-Of-Flight (eTOF) flight-tubes as dispersive elements provides pulse resolved photon energy and polarization diagnostics [2]. Electron spectrometers based on the eTOF principle have flight-tubes with applied voltages that decelerate the electrons. Fast electronics register the time difference from ionization to detection which is related to the kinetic energy of the photoelectrons. The PES, in Fig.1, which uses gas targets is non-invasive and has found applications for soft X-ray photon diagnostics and experiments [3, 4]. Adapting the PES concept to the hard X-ray range is not straightforward due to the poor ionization cross-section and very high kinetic energies of photoelectrons in that regime. This contribution describes the development of the new PES dedicated to photon diagnostics at hard X-rays and presents results from measurements at the beamline P09 at PETRA III [5].

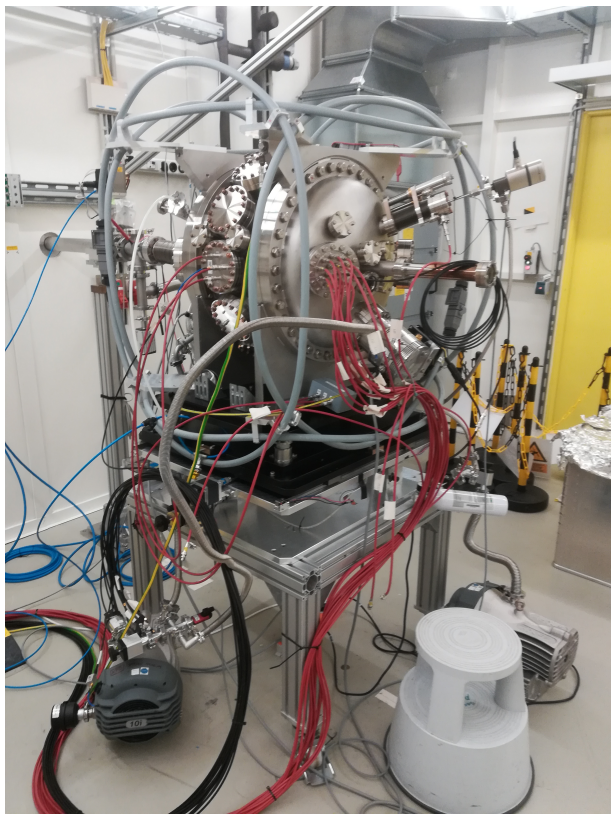

Figure 1: The hard X-ray PES installed at the P09 beamline at PETRA III. A target gas is injected into the center. Emitted photoelectrons are decelerated and focused through the electron optics of the flight-tubes before they reach the detector. Helmholtz coils encapsulate the device to cancel external magnetic fields, which otherwise influence the electron trajectories.

INSTRUMENT

A picture of the device installed at the P09 beamline is presented in Fig. 1. The spectrometer consists of 12 eTOF flight-tubes oriented perpendicular to the X-ray beam at angles of $0°, 30°, \ldots, 330°$. In order to maximize the flight-tubes performance as dispersive elements, while simultaneously focussing the photo-emitted electrons to the detector, we chose a design where the flight-tubes are divided in *retardation region* and *Einzel lens*, separated with a high transmission gold mesh to prevent field penetration between the two regions. An effusive gas jet is injected via a capillary in the interaction region where it interacts with the X-ray beam

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and photoelectrons are emitted. The interaction region has a ∅35 mm inner cylindrical diameter and encapsulates the source region to make it field-free. Following the IR are nine 2 mm thick electrodes where gradually higher potentials are applied. These 10 first electrodes are serially connected via 100 MΩ resistors to work as voltage dividers, thus within a short distance, a steep retardation is imposed capable of decelerating electrons from many keV to only a few 10 eV. Following the strong deceleration, electrons must be guided to the detector which is achieved by a three-element electrostatic Einzel lens. For a robust monolithic design, flight-tubes were machined out of aluminum so that each electrode segment is a round block with 12 conical holes that work as parts of the flight-tube. Electrodes are separated 1 mm from each other with PEEK spacers. To avoid oxidation, aluminum parts were chromatized with the surface treatment *SurTec 650* that ensures the preservation of the electrical conductivity. On both faces of the nested concentric flight-tube electrode cylinders, we have aluminum disks that work as shields. The vacuum vessel is made of non-magnetic stainless steel and care has been taken that all parts are non-magnetic. A 3D Helmholtz coil structure comprised of three mutually orthogonal pairs of coils surrounds the chamber and is used to compensate for the background magnetic field which otherwise would influence the electron trajectories. A fluxgate-type magnetometer (*Bartington Mag-03*) to monitor the magnetic field is mounted in a pocket flange to be as close as possible to the source region. The detectors are *Hamamatsu F9892-31* Micro Channel Plates (MCP) with 42 mm active area and 0.7 ns pulse width. For alignment of the instrument to the beam, the setup is supported by decoupled transverse and vertical translation motion stages controlled by stepper motors.

A target gas that is typically a noble gas is injected as an effusive jet in the interaction region via a ∅100 µm inner-diameter capillary. Target gas criteria are high cross section (σ) and low natural line-width (Γ) In the case of polarization studies also an anisotropy parameter (β) far from 0 becomes relevant. Furthermore the presence of Auger lines can be valuable for kinetic energy calibration of the spectrum.

Before installation in the EuXFEL SASE1 tunnel, the device was tested at the hard X-ray beamline P09 at PETRA III, DESY that offers high energy tuneability from 2.7 keV to 24 keV, full polarization control, high energy resolution and flux [5]. The Si(111) crystal monochromator with the energy bandwidth 1.3×10^{-4} was selected. The beam was uncollimated of size ~2.1 mm × 1.5 mm (V×H) FWHM and mirrors were used to suppress higher harmonics. Measurements were carried out when the machine was operating in timing mode at 5.2 MHz (192 ns pulse separation). For data acquisition a programmable four channel *Lecroy WavePro 725Zi* oscilloscope 2.5 GHz and 40 GS/s was used.

The CAD model was imported into the commercial software *SIMION 8.0* for electron trajectory simulations in order to quantify the performance and improve the design prior to manufacturing. The simulated spectra enables us to define a calibration function that transforms TOF to electron kinetic energy and further on to spectral distribution regardless of the target gas. The kinetic energy scale of the electron spectra were in addition calibrated by measuring the well-established Kr LMM Auger lines, thus confirming the simulations reliability for TOF to E_K calibration.

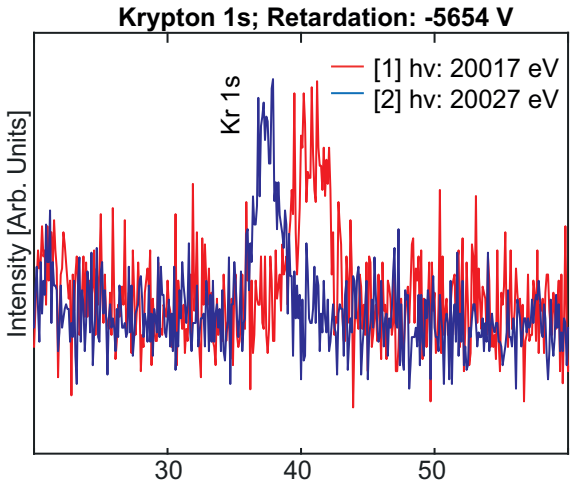

Figure 2: Kr 1s spectra collected at 20 017 eV (red) and 20 027 eV (blue) photon energy with fixed retardation voltage at −5654 V. Peaks are clearly shifted from which we estimate a resolving power of 10 eV.

Table 1: Photoelectron binding energy (E_B) and Lorentzian natural line broadening (Γ) in eV for the typical target gases: Xenon and Krypton.

Orbital	Xenon		Krypton	
	E_B [eV]	Γ [eV]	E_B [eV]	Γ [eV]
1s	34 565.13	9.6	14 327	2.65
2s	5452.57	2.76	1921.4	4.28
$2p_{1/2}$	5106.72	2.79	1730.90	1.31
$2p_{3/2}$	4786.47	2.60	1679.07	1.17

RESULTS AND ANALYSIS

For photon energies above 14 keV, Kr 1s is the most suitable choice. The binding energy is 14 327 eV and the natural line broadening is 2.65 eV (Table 1). Figure 2 presents Kr 1s TOF spectra for photon energies 20 017 eV (red) and 20 027 eV (blue). Here we have $\sigma = 0.008$ Mb. Retardation voltage is fixed at −5654 V. Peaks are clearly shifted from which we estimate a resolving power of 10 eV.

For the spectrometer to be valuable as a photon diagnostics device at EuXFEL it is important that it can perform single pulse diagnostics. In the 40 bunches mode, at 100 mA, P09 beamline at PETRA III provides $\sim 10^5$ photons per pulse. SASE1 beamline at EuXFEL provides $\sim 10^{12}$ photons per pulse. We estimate that at P09 we must collect data from $10^{12}/10^5 = 10^7$ pulses in order to reach comparable statistics as at the EuXFEL. Our spectrum corresponds to $\sim 10^7$ pulses. The integrated number of collected photoelectrons in the

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peak is ~200 which is sufficient to calculate the mean-value and standard deviation of the spectral distribution.

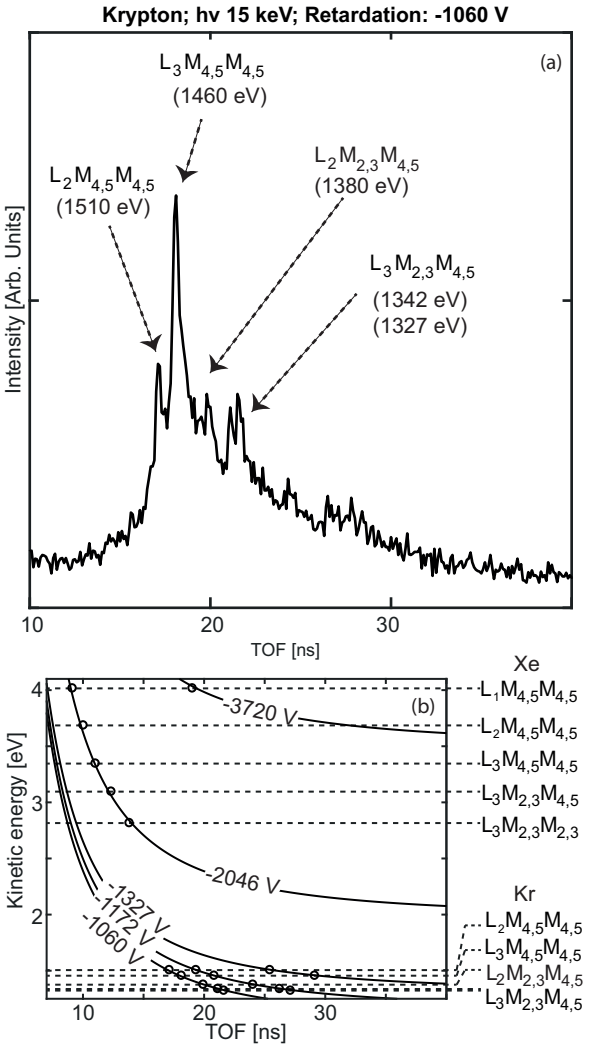

Figure 3: (a) Kr LMM Auger spectrum collected at 15 keV photon energy with target gas Krypton. (b) Comparison of simulated TOF to E_K calibration for different voltage settings and measured data from Kr LMM Auger lines and Xe LMM Auger lines.

Figure 3(a) presents an Auger spectrum at retardation voltage (−1060 V) where LMM line groups corresponding to transitions from vacancies in the L_2 and L_3 subshell can be resolved. The presence of Auger lines that are photon energy independent provides us with an intrinsic TOF to kinetic energy calibration. Furthermore, their polarization independence makes Auger lines suitable for the normalization of detector signals for polarimetry. Most dominating are $L_{2,3}M_{4,5}M_{4,5}$ but also $L_{2,3}M_{2,3}M_{4,5}$ have sufficient signal to noise ratio to be detected. Lower E_K leads to better resolution. Indeed, for the $L_3M_{2,3}M_{4,5}$ line group, two bands can be resolved, each corresponds to transitions to several different final states, dominated by $^1F_3$ and $^3D_3$. Figure 3(b) shows simulated TOF to E_K calibration curves for five different voltage settings compared with measured data from Kr LMM and Xe LMM auger lines. The agreement is excellent, thus we use Auger lines to confirm that our calibration procedure is correct.

CONCLUSION

We have created a novel design for an angular photoelectron spectrometer for the hard X-ray regime. We built and tested this device which is based on the well-known eTOF concept but allows for much higher photon energies thanks to a fundamentally new layout of the flight tubes. A resolving power of ~10 eV for up to 8.7 keV electron kinetic energy has been demonstrated and we have shown that the instrument is suitable for hard X-ray photon diagnostics for both spectral distribution and polarization. By comparing Auger lines with simulated spectra we have confirmed that simulations are reliable for kinetic energy calibration.

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