A case study of novel X-ray Optics for FEL sources

2013 J. Phys.: Conf. Ser. 425 052013

(http://iopscience.iop.org/1742-6596/425/5/052013)

A case study of novel X-ray Optics for FEL sources

J Rehanek[a], F Schäfers[a], H Löchel[a], A Firsov[a], J Grünert[b], W Freund[b], C Ozkan[b], S Molodtsov[b], A Erko[a]

[a]Institute for Nanometre Optics and Technology, HZB – BESSY II, Albert-Einstein-Strasse 15, 12489 Berlin, Germany
[b]European XFEL GmbH, Albert-Einstein-Ring 19, 22761 Hamburg, Germany

Email: Jens.Rehanek@helmholtz-berlin.de

Abstract. We suggest optical schemes for the European X-ray Free Electron Laser facility (XFEL.EU) in Hamburg: a single element X-ray spectrometer on the basis of a reflection zone plate (RZP) for single-shot diagnostics; and a two-element soft X-ray spectrometer on the basis of two RZPs to carry out Resonant Inelastic X-ray Scattering (RIXS) experiments. With this setup, a full map of the sample spectrum is obtainable in a single measurement. The main advantage of using zone plates is the possibility to enable dispersion and focusing in one step. Moreover, highest possible X-ray transmission is achieved by using the minimum number of optical elements. Taking into account the European XFEL beam parameters, our simulations, concerning the RIXS experiment, produced very promising results, reaching an energy resolution (E/ΔE) of up to 30,000 at photon energy of 1 keV. When applied as a single shot spectrometer the energy resolution for RZP is of the same order of magnitude.

1. Reflection zone plates (RZP)

We present ray trace calculations [1] for optical schemes that could be applicable at the European X-ray Free Electron Laser facility (XFEL.EU) in Germany: a single-element X-ray spectrometer on the basis of a reflection zone plate; and a two-element soft X-ray spectrometer to carry out Resonant Inelastic X-ray Scattering (RIXS) experiments, based on the use of two RZPs. For the latter, RZPs are used as both a monochromator and an analyzer of the scattered light, instead of a combination of mirrors, monochromator and a diffraction grating, as proposed in an original optical layout by Strocov [2]. In this way, we receive a full 2-D map of the sample spectrum in a single shot exploring the unique property of zone plates: their ability to disperse and focus a photon beam in one step. In addition, RZPs provide reasonable energy dispersion and attain the highest possible X-ray transmission [3]. Their use may reveal many ways of application in this field – e.g. as a spectrometer on a pulse-to-pulse basis for the European XFEL [4]. They are already implemented as focusing elements in the femtosecond-slicing beamline at BESSY-II [3]. The spectrometer would enable us to perform highly-efficient time-resolved fluorescence experiments. Furthermore, the highest possible X-ray transmission can be attained due to the use of fewer elements. The principle of reflection zone plates is extensively described in [5]. Fig. 1 shows the optical principle. An RZP is a cross-section or cut through the 3-dimensional ellipsoid, formed around the two foci of a transmission zone plate (TZP). The Reflection Zone Plate is a projection of the TZP onto a reflecting surface. The reflection is based upon diffraction and interference. It consists of alternating reflective and non-reflective zones (shown as grey or white areas). In this way, it is comparable to a 2-dimensional variable line spacing (VLS)-grating focusing in 2-D.

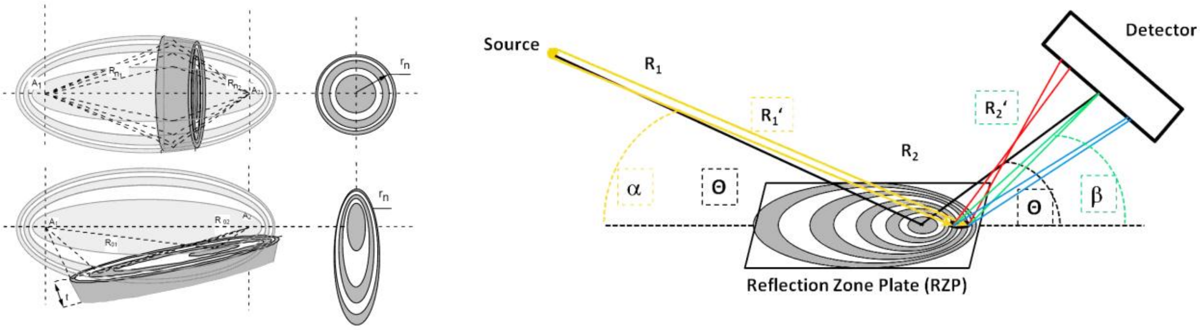

Figure 1: (top-Left): 3D sketch of the zone structure of a transmission zone plate and its circular cross-section; (bottom-Left): 3D structure of an RZP and its elliptical cross-section; (Right): by illumination of an off-center part of the RZP the zero order can be suppressed (by deflection into another direction than higher orders). Three energies spatially separated at the detector are shown in color. (R_1/R_2 – entrance-/exit-arm to the center of the RZP; R_1'/R_2' – entrance-/exit-arm to center of illuminated part; Θ – incidence angle of central ray to the RZP-center; α/β – entrance-/exit-angle at center of illuminated part).

2. Applications of RZP at XFEL

In this section, two different applications of RZPs as x-ray optical elements at synchrotrons and XFELs will be discussed. In both cases, the ability of RZPs to combine focusing and dispersion in one step is exploited.

2.1. An "online" single shot spectrometer

We propose the use of a Reflection Zone Plate for online diagnostics of the FEL pulses at the European XFEL in Hamburg. The SASE 3 undulator delivers soft x-ray radiation in the energy range between 0.26 keV and 3 keV. The proposed optical setup is sketched schematically in Figure 2. A double (plane) mirror arrangement at a variable grazing incidence angle creates a vertical offset from the direct FEL-pulse. It leads the beam to the monochromator as well as the user experiment.

When the second mirror is structured with a zone plate, the zero-order beam path to the experiment is not affected. The 1^{st} order diffracted beam will be spatially separated from the zero-order beam and the dispersed radiation hits a detector array. To prevent a damage of the detector a diagnostic spectrometer should have low diffraction efficiency. Therefore, the modulation profile of the mirror surface should only be on the order of 1-2 nm. Low efficiency of the RZP will not affect the primary beam, but is sufficient for the monitoring purpose. In this way we could obtain a very useful device for getting the entire spectral information from shot-to-shot of the XFEL, without damaging the detector. The use of an RZP-structure with higher efficiency would be conceivable in combination with a slit. This slit would be positioned in the focal plane of the RZP, acting as an exit slit of a monochromator to select a certain wavelength out of the dispersion plane.

In Fig. 2, right side, the calculated energy resolution of such a device is plotted. This result was obtained by raytracing [1] the proposed optical setup. Three closely spaced energies of 1000 eV ± 25 meV are spatially separated at the detector by 20 µm. Hence, a moderate detector pixel size of 20 µm in dispersion direction is sufficient to obtain an energy resolution of E/ΔE = 40,000. Nevertheless, to provide necessary time resolution, the energy resolution of the spectrometer must be optimized to the FEL pulse duration.

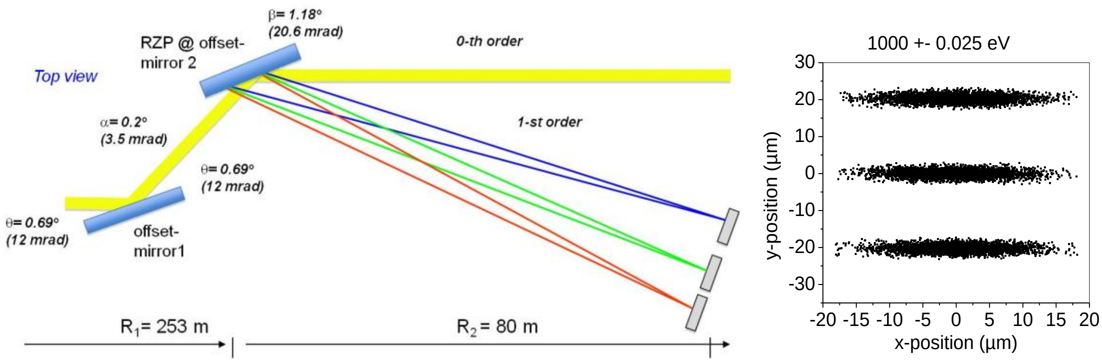

Figure 2: (Left): schematic setup of the RZP spectrometer for single shot diagnostic of XFEL pulses; (Right): result of ray tracing simulation. (Raytrace-parameters: point source of 34 µm x 34 µm (FWHM) cross section and with divergence of 1 µrad x 1 µrad (FWHM), RZP: R_1 = 253 m, R_2 = 80 m, "d_{av}" = 160 lines/mm, length = 155mm). Spot pattern at the detector for three energies of 1 keV ± 25 meV). A detector with a pixel size of 20 µm is sufficient to obtain an energy resolution E/ΔE = 40 000.

2.2. *RIXS at XFEL*

The second proposed application of RZPs concerns RIXS experiments as currently performed at synchrotron radiation sources as well as similar experiments planned for FEL radiation. The principle of RIXS is described in [6].

In the RIXS setup, described by Strocov [2], "a monochromator produces in its (stigmatic) focal plane a line image of light with vertical dispersion in energy $h\nu_{in}$. A refocusing KB optics…brings this image into a line focus on the sample." To collect the scattered fluorescence light from the sample, a vertically focussing mirror and a VLS grating focus and disperse horizontally onto a 2D position sensitive detector.

We propose to replace these five elements by only two Reflection Zone Plates, one before and one after the sample, to combine all dispersing, reflecting and focussing features into just two optical elements. Fig. 3 shows the schematic setup. The first RZP creates a dispersion plane and has its focus on the sample vertically. The second RZP is oriented perpendicular to the first one, in order to bring the scattered light from the sample and focus it on to a position sensitive detector; thus, giving a well-resolved RIXS intensity distribution in 2D. It is generally true that the transmission of a two-element system is much higher than that of a five-element one.

In this way, we obtain information of both incoming and outgoing energy distribution of the sample. With this simple setup, only a 2D-detector is necessary to obtain information about the entire spectrum in a single measurement/FEL shot.

Fig. 4 shows the ray tracing results of such a setup. Three closely spaced energies of 1000 eV ± 20 meV are well separated on a 2D-detector. Raytracing a 'white' energy band of 1000 eV ± 0.1 eV through this setup yields an energy resolution of E/ΔE ≈ 33,000 at the design energy assuming (realistic) slope errors of 0.1 arcsec on both RZPs. Thus, a 2D-detector with moderate pixel size of 10 µm x 10 µm is sufficient to resolve the incoming image.

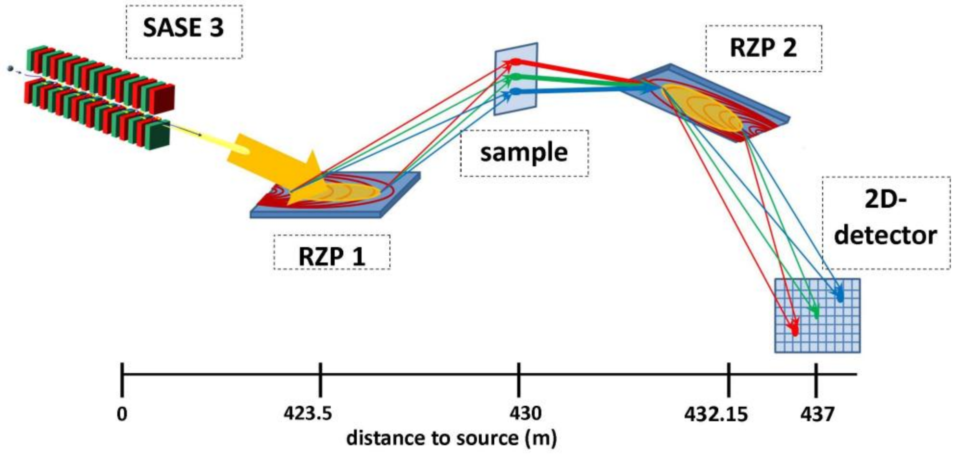

Figure 3: Proposed setup for energy resolved RIXS experiments at the XFEL SASE3 undulator beamline, using two RZPs only.

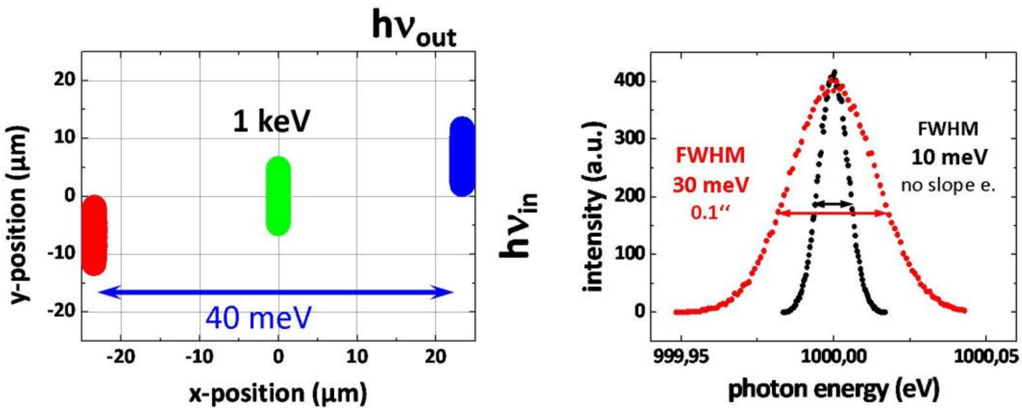

Figure 4: Left: 2D-Energy dispersion on a 2D-detector for the setup of Fig. 3. The centre energy of 1 keV (green) and the neighbouring energies ±20 meV away (red, blue) are dispersed in two dimensions by the two perpendicularly orientated RZPs. Right: Energy distribution of an intrinsically 'white' energy band of 1000 eV ± 0.1 eV behind a pinhole of 10 x 10 µm². Black curve: calculation of the RZP optics without slope errors. Red curve: includes a slope error of 0.1 arcsec.
(Raytrace parameters: point source with the size of 34x34µm² (FWHM) and with divergence of 1µrad² (FWHM), RZP1: α=0.2°, β=2.9°, d_{av}=0.1µm, size=400x3mm² (LxW), R_1=423m, R_2=7m, RZP2: α=4.5°, β=2°, d_{av}=0.5µm, size=10x3mm², R_1=2m, R_2=5m).

3. Summary

In conclusion, we have presented applications of RZPs as spectrometers for FEL-radiation on a shot-to-shot basis. RZPs combine focusing and dispersion in one step, as a result reducing the number of optical elements. They allow strong demagnification, consequently small focal size and a high resolution.

The first application is an online spectrometer that will enable non-destructive shot-to-shot diagnostic of FEL pulses.

The second application allows obtaining a full 2D-map of the entire RIXS-spectrum in a single FEL-shot, by using only two RZPs as optical elements. The reduction of the number of optical elements in a beamline would satisfy the purpose of conserving the unique properties of FELs such as their high coherence.

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