Dedicated software for diffractive optics design and simulation

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Abstract. An efficient software package for the structure design and simulation of imaging properties of diffraction optical elements has been developed. It operates with point source and consists of: the ZON software, to calculate the structure of an optical element in transmission and reflection; the KRGF software, to simulate the diffraction properties of an ideal optical element with point source; the DS software, to calculate the diffraction properties by taking into consideration material and shadowing effects. Optional software allows simulation with a real non-point source. Zone plate thickness profile, source shape as well as substrate curvature are considered in this calculation. This is especially important for the diffractive focusing elements and gratings at a total external reflection, given that the lateral size of the structure can be up to 1 m. The program package can be used in combination with the Nanomaker software to prepare data for ion and e-beam surface modifications and corrections.

1. Introduction
Availability of suitable diffractive VUV and X-ray optics is the basis for further breakthroughs in measurement techniques, especially for time-resolved spectroscopy. The quality of achievable results depends first and foremost on the availability of high-quality optical components like gratings or diffractive focusing elements. Focused on these topics interdisciplinary research efforts are established at radiation sources, including the Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB, the former BESSY II, Germany), XFEL (Germany), Soleil (France), MAX-4 (Sweden), and facilities with – high harmonic generators (HHG) in Germany, France, Sweden, and Switzerland.

The necessary radiation for experiments is delivered by either synchrotron beamlines or laboratory sources – HHG. In order to focus light, optimum advantage must be taken of its interactions with matter, such as diffraction, reflection and refraction. There is a variety of X-ray focusing optical systems, such as mirrors [1], zone plates [2], refractive lenses [3] and multilayer Laue lenses [4].

Development and fabrication of focusing elements for “soft” and “hard” X-ray radiation focuses on achieving a spatial resolution in the nanometer range. This spatial resolution could be achieved by using planar zone plates [5], the Kirkpatrick-Baez scheme [6]. Good results were obtained using capillaries [7], refractive focusing optical elements [8] and total reflection zone plate (TRZP) [9].

These optical elements are presently the best high-resolution optical elements used in x-ray microscopy and micro-probing. However, the creation of innovative radiation sources with high power
density (FELs) that enable us to conduct experiments with time-resolutions of $10^{-15}$ and even $10^{-18}$ s, imposes new requirements for diffraction focusing optics: firstly, radiation stability; secondly, high efficiency; thirdly, high energy resolution; and fourthly, time resolution.

Very promising devices, which simultaneously meet all the above-listed requirements, are reflection focusing elements [9, 10]. Elliptical zone plates fabricated on a total external reflection mirror surface, referred to as “reflection zone plates” (RZP), can be effectively used for x-ray monochromatization and beam focusing at photon energies below 20 keV. It is important to use off-axis RZPs in order to achieve optimum energy and spatial resolution.

2. Software package

An efficient software package was developed for the structure design and simulation of the imaging properties of diffraction optical elements. It operates with a point source and consists of several parts:

- the ZON software, to calculate the structure of an optical element in transmission and reflection;
- the KRGF software, to simulate the diffraction properties of an ideal optical element with point source;
- the DS software, to calculate the diffraction properties by taking into consideration material and shadowing effects.

Optional software enables simulations with a real non-point source. ZP thickness profile, source shape as well as substrate curvature are considered in this calculations. This is especially important for the diffractive focusing elements (DOE) and gratings at a total external reflection, given that the lateral size of the structure can be up to one meter.

The main advantage of the KRGF software is a new method for fast calculation of the Kirchhoff integral [11]. The program allows us to obtain individual diffraction patterns from real lenses and analyze their changes at different lens positions starting from the ideal position with respect to an incident X-ray beam. A standard method of calculation is to add up the secondary point sources in the ZP plane. A disadvantage of this method is that it is time-consuming. A real ZP has about thousand zones and the amount of data required to describe its topology comprises up to 500 MB. The main idea for fast calculation of the Fresnel-Kirchhoff integral (FKI) is to reduce a 2D FKI to a 1D integral along the zone boundaries thus decreasing the number of calculations. It is clear that a diffraction pattern will look smeared out above a certain size of the radiation source. Such an analysis allows us to estimate the efficiency of ZP in various constructions in order to “see” a diffraction pattern and understand the effect of the lens position with respect to an incident X-ray beam and the motor-drive stage used. The DS Software performs raster calculations and representations, allowing us to calculate the change of the complex amplitude during the passage of radiation through a few pixels of the ZP to the plane of calculation. Numerical calculations of the Fresnel integral are performed using Fast Fourier Transform (FFT). The calculations take into account the ZP thickness profile, whereas the source profile is given analytically. This enables us to simulate the source image using a convolution of a point source image from a bitmap file and source profile. The program package can be used in combination with the Nanomaker software (Interface Ltd) to prepare data for ion and e-beam surface modifications and corrections.

As an example in figure 1 is shown a structure of RZP, working with grazing angle of 0.34º. This is an elliptical ZP with size 10x0.35 mm for 2D focusing of 8800 eV radiation. Also shown is a fragment of a hologram which dedicated to create 10x10 μm uniformly illuminated area at 2.4 nm wavelength.

The RZP is capable of nanofocusing because the focusing size is defined by the small effective zone size [12]. It is difficult to achieve hard X-ray nanofocusing (< 100 nm) using conventional ZP optics, since X-ray propagation through a structure with very high aspect ratio (> 20) is inhibited by an effect based on rigorous diffraction theory. In this case a zone profile in depth must be not more rectangular but following elliptical shape of isophase surfaces which makes its fabrication almost impossible. For more details see [13].

For demonstration of our software capabilities in figure 2 are shown calculated diffraction patterns for elliptical lens (see figure 1,a) at the focal plane: (a) ideal lens alignment, (b) 18º azimuthal angle
misalignment, (c) 18” incident angle misalignment. Figure 3 demonstrates a structure of ZP with ribs (a) and calculated efficiency of such element with ribs and without ribs (b). Software allows change the number of ribs, calculate the focus quality modifying in the presence of ribs and the intensity logarithm at the focus of the ZP with ribs and without ribs.

Figure 1. Fabricated on silicon surface RZP with minimum zone of 50 nm (a) and fragment of a calculated hologram with minimum feature of 50 nm and diameter of 1.8 mm (b).

Figure 2. Calculated diffraction patterns for elliptical lens (see figure 1,a) at the focal plane: (a) ideal lens alignment, (b) 18” azimuthal angle misalignment, (c) 18” incident angle misalignment.

Figure 3. 1\textsuperscript{st} plus 3\textsuperscript{rd} diffraction orders transmission ZP with ribs (a) and calculated efficiency of this ZP with ribs and without ribs (b).

A great advantage of these RZPs is their ease of fabrication. It is very simple to produce reflective zones on a flat substrate. In addition, this device has much less rigid size and aspect ratios for the zone pattern than for an FZP or a Laue lens. Some RZP should have a variable profile depth along the propagation of radiation. That is, in fact, we have to calculate and fabricate 3\textsuperscript{D} DOE. The state-of-the-art 3\textsuperscript{D} DOE elements can be efficiently used for X-ray monochromatization and beam focusing at photon energies from 20 eV to 20 keV. Such 3\textsuperscript{D} DOE can be used in beamlines with specific beam conditions, such as very high thermal and radiation load. This is of particular interest for the European
X-ray Free Electron Laser project. It is recommended to place 3D RZP off-axis to provide the best energy and spatial resolution in the diffraction (vertical) plane [10].

Energy recovery linacs (ERLs) and FELs will require 3D DOE (spatially variable) with a depth profile accuracy of ~0.5 nm for the soft and hard x-ray energy range. The surface-metrology techniques and instrumentation allow one to trace changes in the surface structure within a fraction of an angstrom. The profile depth of these 3D DOE will range from 5 to 30 nm, depending on the focusing energy, and it will vary along the structure. The accuracy and reproducibility of the profile depth should be no worse than 0.5 nm on a plane of 100 mm in diameter.

3. Conclusions

The Institute for Nanometre Optics and Technology of HZB develops, fabricates and uses different X-ray diffractive optical elements. In accordance with the requirements of modern physical experiments, particular attention is paid to the design and fabrication of DOE and gratings at total external reflection, with the linear size of the structure being up to one meter. This software package allows us to create a topology of these elements and simulate their behavior in real experimental conditions or analyze a possible result if technological errors occur during the manufacturing process.

3D DOE give the unique possibility for novel optical elements to achieve a step advance in existing ultra-high time resolution and fs-slicing beamlines, both now and in the future.

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References

[1] Mimura H, Yumoto H, Matsuyama S, Sano Y, Yamamura K, Mori Y, Yabashi M, Nishino Y, Tamasaku K, Ishikawa T and Yamauchi K 2007 Appl. Phys. Lett. 90 051903
[2] Suzuki Y, Takeuchi A, Takano H and Takenaka H 2005 Jpn. J. Appl. Phys. 44 1994
[3] Schroer C G, Kurapova O, Patommel J, Boye P, Feldkamp J, Lengeler B, Burghammer M, Riekel C, Vincze L, van der Hart A and Küchler M 2005 Appl. Phys. Lett. 87, 124103
[4] Kang H C, Maser J, Stephenson G B, Liu C, Conley R, Macrander A T and Vogt S 2006 Phys. Rev. Lett. 96 127401
[5] Rehbein S, Heim S, Guttmann P, Werner S and Schneider G 2009 Phys. Rev. Lett. 103 110801.
[6] Mimura H, Handa S, Kimura T, Yumoto H, Yamakawa D, Yokoyama H, Matsuyama S, Inagaki K, Yamamura K, Sano Y, Tamasaku K, Nishino Y, Yabashi M, Ishikawa T and Yamauchi K 2010 Nature Physics 6 122
[7] Bjeoumikhov A, Erko M, Bjeoumikhova S, Erko A, Snigireva I, Snigirev A, Wolff T, Mantouvalou I, Malzer W and Kanngießer B 2008 Nucl. Instrum. Met. Phys. Res. A 587 458
[8] Isakov A F, Stein A, Warren J B, Narayanan S, Sprung M, Sandy A R and Evans-Lutterodt K 2009 J. Synchrotron Rad. 16 8
[9] Erko A, Firsov and Holliday K AIP Conf. Proc. 2010 1234 177-180
[10] Erko A, Firsov A, Roshchoupkin D and Schelokov I 2008 Volume Modulated Diffraction X-Ray Optics Modern Developments in X-Ray and Neutron Optics (Springer Series in Optical Sciences vol 137) ed A Erko, M Idir, T Krist and A G Michette (Berlin/Heidelberg: Springer) pp 471-500
[11] Firsov A, Svitsov A, Firsova A, Chevallier P and Populus P 1997 Nuc. Instrum. Methods A 399 152-159
[12] Takano H, Tsuji T, Hashimoto T, Koyama T, Tsusaka Y and Kagoshima Y 2010 Appl. Phys. Express 3 076702
[13] Erko A, Aristov V and Vidal B 1996 Diffraction X-Ray Optics (Bristol/Philadelphia: IOP Publishing Ltd) P 98