Final Draft

Design of soft x-ray gratings for free electron lasers: from specification to characterization.

Maurizio Vannoni*[a], Daniele La Civita[a], Rolf Follath[c],
Liubov Samoylova[a], Frank Siewert[b], Harald Sinn[a]

[a] European XFEL Gmbh, Albert-Einstein-Ring 19,22761 Hamburg, Germany;
[b] Helmholtz Zentrum Berlin, BESSY-II, Institute for Nanometre Optics and Technology, Albert-Einstein-Str. 15, 12489 Berlin, Germany
[c] Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen-PSI, Switzerland

ABSTRACT

The European XFEL is a large facility under construction in Hamburg, Germany. It will provide a transversally fully coherent X-ray radiation with outstanding characteristics: high repetition rate (up to 2700 pulses with a 0.6 milliseconds long pulse train at 10Hz), short wavelength (down to 0.05 nm), short pulse (in the femtoseconds scale) and high average brilliance ($1.6\cdot10^{25}$ photons / s / mm^2 / $mrad^2$/ 0.1% bandwidth). Due to the very short wavelength and very high pulse energy, mirrors have to present high quality surface, to be very long, and at the same time to implement an effective cooling system. Matching these tight specifications and assessing them with high precision optical measurements is very challenging. One of the three foreseen beamlines operates in the soft X-ray range and it is equipped with a diffractive monochromator. The monochromator is using a variable line spacing grating that covers the wavelength range from 4.6 nm to 0.41 nm (energies from 270eV to 3000eV). The grating profile is blazed, and due to the small angle and relatively few lines/mm, it is also very challenging to realize and to be characterized. In this contribution we discuss about the requirements of the optics involved in the soft X-ray monochromator. We describe mirror and grating specifications and the tests that could be carried out during and after the manufacturing in order to ensure the specification match.

Keywords: X-Rays Optics, grating, optical testing

1. INTRODUCTION

The European XFEL[1] is a new Free Electron Laser, currently under construction in Hamburg, with the characteristics outlined in the abstract. The capability that sets the European XFEL facility apart from all other hard X-ray lasers or third generation synchrotron sources is the Megahertz repetition rate of FEL pulses in trains of up to 2 700 pulses and the high average brilliance of each pulse. That means up to several 10 Kilowatt heat load per mm^2 on some optical elements for the duration of a pulse train, while the average heat load is comparable or lower than other synchrotron sources. Considering this tremendous heat load, partially transferred to the various optical elements inside the beamlines, local surface deformations are expected and therefore the beam quality will be deteriorated, especially its spatial coherence that is one of the most desired key feature. To solve this issue, additional steady-state and transitory analyses through finite element calculations have been used to predict thermal effects and a proper cooling system will be provided.[2] However, to minimize the problem, the x-ray beam is also spread out over a large footprint in the grazing incidence reflections, resulting in very long optical elements. The desired optical requirements of these long elements are comparable with the “standard” but shorter ones already under operation in synchrotron facilities: in our case they range from 500 mm long gratings up to 1 meter long flat mirrors, with required peak-to-valley errors of few nanometers on their full aperture. Reaching this accuracy level becomes challenging on the desired length dimensions. In addition, another problem is to characterize these optical elements to ensure that the required surface quality has been reached and, for the gratings, that the ruling has been properly done. Correct metrology and characterization is also a challenging task: using a deterministic polishing to achieve the best surface, the manufacturing and characterization processes are connected together and an incorrect metrology could result in an out of specifications optical element.

*maurizio.vannoni@xfel.eu; phone +49 040 89985456; fax +49 040 89981905; www.xfel.eu
Among the different European XFEL beamlines, we are now considering just the soft x-rays one, called SASE3 beamline. Three different energies will be provided for the electron beam injected in this beamline: 10.5 GeV, 14.0 GeV and 17.5 GeV. Produced x-rays energies will span from 4.6 nm (=270 eV) to 0.41 nm (=3 keV), with a single pulse duration ranging from 2 to 100 femtoseconds. The typical spectral bandwidth expected is $5{\cdot}10^{-3}$,[1] and for some particular applications it is required to reduce the bandwidth even more. For that reason a monochromator have to be inserted on the beam path, in order to have a spectral bandwidth up to $5{\cdot}10^{-5}$, depending on the particular wavelength used and the alignment conditions. The expected pulse length will be stretched up to 100 femtoseconds, but it will be still short enough to allow a high repetition rate and time-resolved experiments. The monochromator can also be bypassed: moving out of the beam path the monochromator first optical elements allows the unfiltered beam ("pink beam") to go directly to the experimental hall. A schematic view of the beam transport optical setup is depicted in Fig. 1.

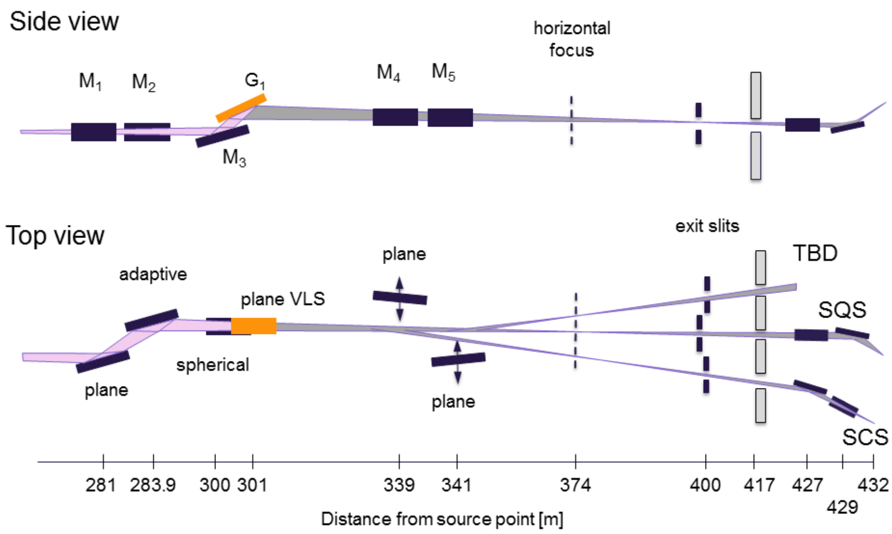

Figure 1. European XFEL SASE3 beamline: optical setup. M_1 and M_2 are two flat offset mirrors mainly used for radiation safety reasons. The first has fix shape, whereas the second has the possibility to change the surface through an adaptive piezoelectric system. M_3 is a focusing mirror; G_1 is the monochromator grating while M_4 and M_5 are used to distribute the beam to the selected experimental station.

In this setup every optical element is challenging, in particular the monochromator grating and the associated mirrors. In order to ensure the correct setup of the system and to achieve the desired x-rays beam characteristics, a careful engineering of each part is needed and a correct metrology approach must be provided. We will focus in particular on the grating element of the monochromator and on the linked M_3 mirror. Two exchangeable mirrors and two gratings with line densities of 50 lines/mm and 150 lines/mm, to cover the full energy range, will be provided. In the next sections, we will show the design and specifications of these gratings and mirrors, together with the required characterization.

2. MONOCHROMATOR DESIGN AND SPECIFICATIONS

The SASE3 soft x-ray monochromator, as depicted in Fig. 1, employs a Variable Line Spacing Plane Grating Monochromator (VLS-PGM) with the plane grating positioned in a converging beam. In the vertical (dispersive) plane, the focus distance is determined by the spherical mirror M_3 and the magnification ratio of the grating. In the horizontal plane, the focus position is determined by the adaptive M_2 mirror while the plane mirrors M_4 and M_5 are used to distribute the beam to three different experimental stations. To keep the beamline in focus for all photon energies, two different mirrors M_3 are used alternatively.

In the low photon energy range (270 eV – 1.2 keV), a spherical pre-mirror M_3B with a radius of curvature of 7.5 km and a grazing incidence angle of 20 milliradians is used. In the high photon energy range (1.2 keV to 3 keV) a pre-mirror M_3A with a radius of curvature of 16.7 km and a grazing incidence angle of 9 milliradians is instead used. Both gratings can be operated with each mirror. The grating G_1, with a line density of 50 lines/mm and a nominal resolution up to 14700, is intended for low spectral resolution experiments with a ultrashort pulse length. The grating

G_2, with line density 150 lines/mm, is more suitable for high spectral resolution applications and still a not so long pulse length. In any case, the pulse length stays below 100 femtoseconds. Both gratings will have blazed profiles. The blazed profile has been chosen to enhance the diffraction efficiency and to have higher damaging threshold levels. It has been shown that laminar profiles are more sensitive to high power beams and therefore more susceptible to beam damage[3]. The pre-mirrors have fixed positions and grazing incidence angles, to keep the setup simple, while the two gratings are interchangeable and can be rotated to select the photon energy.

The gratings have been designed to keep the distance to the exit slit constant at l=99 m. This can be accomplished by using a variable line separation $d(x)$ according to

$$d(x) = d_0(1 + \nu_1 x + \nu_2 x^2 + \cdots). \tag{1}$$

where d_0 is the central line spacing and ν_1 and ν_2 are free parameters. From the literature[4] we know that ν_1 parameter can be calculated as

$$\nu_1 = \frac{d_0}{n\lambda l}(\cos^2\alpha - \cos^2\beta) \tag{2}$$

where n is the diffraction order number (=1 in our case), λ is a selected wavelength, α and β are respectively the incidence and diffraction angle respect to the normal of the grating. The equation can be approximated as

$$\nu_1 \cong \frac{2d_0}{n\lambda l}(\sin\alpha - \sin\beta) \tag{3}$$

being α and β very near to $\pi/2$. From the grating equation we have

$$\frac{n\lambda}{d_0} = \sin\alpha - \sin\beta \tag{4}$$

so, combining Eq. 3 and Eq. 4, we have

$$\nu_1 \cong \frac{2}{l} \tag{5}$$

that in our case means $\nu_1 \cong 0.02020\ m^{-1}$. Using Eq. 1, this parameter creates a maximum line displacement of 0.5 %, corresponding to 0.1 micron for the 50 l/mm grating and 0.03 micron for the 150 l/mm grating, measured from the center to the edge. Further calculations[5] give a ν_2 estimation of $1\cdot10^{-4}\ m^{-2}$: in this case we have a negligible effect, about $6\cdot10^{-4}$ %, so we can neglect it safely.

The surface quality of both the pre-mirrors and the gratings substrates must be really good, to avoid any wavefront deteriorations that would spoil the properties of the beam at the experiment. To have a comparison, standard optics is generally used with visible light and normal angle incidence, and in that case a "standard quality" optical surface has normally a Peak-to-Valley maximum deviation from ideal surface that is around $\lambda/4$, a "good quality" surface is around $\lambda/10$ and a "very good quality" surface is better than $\lambda/20$. In our case, the λ parameter is really small, but the incidence angle is also very far from the normal: for a given deviation Δh and a grazing incidence, the wavefront distortion Δz can be roughly calculated with the following formula:[6]

$$\Delta z \cong 2\Delta h \sin\theta \tag{6}$$

As an order of magnitude, having a θ=20 mrad of grazing incidence angle and a Peak-to-Valley deviation of 3 nm, we calculate a wavefront aberration of $\Delta z = 2\Delta h \sin\theta = 0.12$ nm: if we consider λ=1 nm, this situation is comparable to an optical mirror with $\lambda/20$ quality. Following these guidelines, the final specifications have been decided and they are reported in Tab.1. With these specifications, full wavefront simulation have been carried out and the calculated beam quality is in the worst case better than $\lambda/8$, and in some cases it is better than $\lambda/20$.

	M3a pre-mirror	M3b pre-mirror	G1 grating	G2 grating
Substrate size (LxWxH) mm^3	600x100x70	600x100x70	530x100x70	530x100x70
Optical surface (LxW) mm^2	580x25	580x30	500x30	500x30
Figure	Spherical	Spherical	Flat	Flat
Incidence angle (milliradians)	9 (fixed)	20 (fixed)	max. 19.1 (1.5 keV) min. 5.7 (1 keV)	max. 17 (1.5keV) min. 1.8 (1 keV)
Radius of curvature (meters)	16700	7480	>300.000	>300.000
Line density			50 1/mm	150 1/mm
VLS parameter			2.0202e-5 1/mm	2.0202e-5 1/mm
Groove profile Angle			Blazed 0.1°	Blazed 0.3°
RMS slope error (nanoradians)	50	50	50	50
Residual height error (P-V) (nanometers)	3	3	3	3

Table 1. VLS-plane monochromator optical components specifications.

3. OPTICAL ELEMENTS CHARACTERIZATION

As reported in Tab. 1, designed specifications for monochromator optical elements are challenging and difficult to achieve even with state-of-the-art technology. A proper characterization must be planned and carried out. Now we will examine the main characteristics of the pre-mirrors and gratings, working out the way to perform characterization measurements for every parameter, with particular attention to the final accuracy. When possible, we will consider different methods to measure the same characteristic, examining the different information that we could gather from each one.

3.1 Pre-Mirror and Gratings surface figure

Two different methods are generally used to measure the optical surfaces figure: interferometry and deflectometry. Each one has its advantages and disadvantages.

For interferometry, a large aperture Fizeau instrument can be used,[7,8] but usually the maximum measurable diameter will be limited by the interferometer beam expander. To overcome this limitation, a grazing incidence setup[9] or a stitching method[10] can be used. Advantages of interferometric methods are: data acquisition speed, one-shot measurement in all the field of view, and usage of a standard instrument. Disadvantages for the grazing incidence setup are a reduced sampling interval and smaller height accuracy. Using a stitching method through a translation stage , the accuracy and sampling interval are maintained, but some “stitching errors” can be found between sub-apertures connections due to the mathematical algorithm and translation stage errors. In both the methods we still have to calibrate the reference surface attached on the interferometer with accuracy comparable or even better than desired results accuracy. Expected performances for a Fizeau interferometer setup with 300 mm beam-aperture diameter are reported in

Tab. 2. Basically, a Large Beam Aperture Fizeau interferometer is equipped with a 1Kx1K pixels CCD camera, and the accuracy is on a nanometric level if an absolute calibration is carried out, using three-flat test methods[11-13].

For deflectometry, typical instruments use a laser beam reflected over the test mirror surface: depending on the local topography of the surface, the beam is reflected in a different way on a position sensitive detector inside the instrument sensor head.[14] The position measurement is directly related to the local slope on the mirror surface. In contrast to interferometry this method does not rely on external references, but it is linked to its internal construction. One of these instruments is the Nanometer-Optical component measuring Machine (NOM):[15-17] it has been already used extensively to characterize other synchrotron optical elements and, by averaging a large number of scans, the random error budget can be minimized to values below 50 nanoradians (rms) over a sampling length of 0.7 mm. The performances details are also reported in Tab. 2.

	300mm Fizeau	NOM
Test mirror measurable size	300 mm diameter	1200x300 mm^2
Angle accuracy on 1 mm sample length	150 nanoradians	50 nanoradians
Maximum measurable angle	263 microradians	± 6.6 milliradians
Minimum measurable radius of curvature	1 km (without additional optics)	1 meter
Height accuracy	1 nm (absolute calibration)	1 nm
Time for a measurement	302 milliseconds	half an hour

Table 2. Comparison between two different methods to measure surface figure.

Analyzing the surface specification for pre-mirrors and grating substrates, we can see that the desired maximum slope error (Tab. 1) is in the same range of NOM accuracy. Even the maximum residual height error should be measurable within the Fizeau interferometer specifications. Basically, the two approaches are quite complementary. With deflectometry, we measure the slope error profile and the height profile is derived with numerical integrations; with interferometry, we measure the height profile and we calculate the slope profile with numerical derivation.

We analyze now the maximum radius of curvature admitted for these optical elements. Considering perfectly spherical profiles, the radius of curvature R and the maximum out-of-plane distance h are linked with optics diameter D through the formula:

$$h = \frac{D^2}{8R} \tag{7}$$

while the maximum slope angle $\propto$ is

$$\tan \propto = \frac{D/2}{R-h} \tag{8}$$

From these formulas, we calculate a maximum h =5.62 microns for the M3b pre-mirror, corresponding to a maximum slope error of $\propto$=38.8 microradians, and a minimum h =104 nm (corresponding $\propto$=833 nanoradians) for the gratings. However, with normal incidence interferometry only a limited portion of the mirror is observed at the same time, so for a 300 mm beam diameter Fizeau system the above value is scaled to h =1.5 microns maximum and h =37.5 nm, minimum.

3.2 Surface roughness and Power Spectral Density

The roughness of optical surfaces can be measured with a white-light interferometric microscope.[18] These instruments use an interferometric setup within their microscope objectives and they have typically sub-nanometer accuracy, but again the main limitation is the influence of the reference surface, that it is included inside the microscope objective. The output is a bi-dimensional profile, and the root-mean-square (rms) roughness value can be easily calculated. Following Ref. 19, the rms roughness of the test (σ_{test}) and of the reference surface (σ_{ref}) are connected with the measured profile with the formula:

$$\sigma^2{}_{meas} = \sigma^2{}_{test} + \sigma^2{}_{ref} \tag{9}$$

Two methods can be used to achieve 0.1 nm accuracy for the roughness measurement. We can perform two measurements in two different parts of the sample, then we calculate the difference profile between them ($Diff$) to cancel the reference influence, and the result is processed with a scaling factor of $\sqrt{2}$:

$$\sigma_{test} = \frac{1}{\sqrt{2}} \sigma_{Diff} \tag{10}$$

Another method is to use an almost perfectly polished optical surface, doing several measurements in different parts of this surface, and then averaging the results: the resulting profile is an estimation of the reference profile inside the interferometric microscope objective, and it can be removed from any other further measurement. The estimated reference rms roughness is connected to the "real" one, depending from the surface quality of the mirror used and the number of measurements *N*:

$$\sigma_{estimated} = \sqrt{\left(\frac{\sigma_{mirror}}{\sqrt{N}}\right)^2 + \sigma_{reference}} \tag{11}$$

With a surface correction, other kind of calculation could be used, as Power Spectra Density estimations that are generally used to provide a full simulation of the x-ray beam after the monochromator. Typical height resolution for these instruments is 0.1 nm while lateral resolution is ranging from 0.64 to 11.8 microns, depending on the objective used.

3.3 Grating variable line spacing parameters

As we have seen (Tab. 1), the variable line spacing parameter required along the grating is quite small. The method proposed to characterize it is to measure the profile surface in a Littrow setup.[20] In this setup, the incidence and diffraction angle are coincident. Using Eq. 4, that means:

$$\frac{n\lambda}{2d} = \sin\alpha \tag{12}$$

where *d* is given by Eq. 1. If a λ=632.8 nm is used to measure the grating, this angle is 0.91 degrees for the 50 lines/mm and 2.72 degrees for the 150 lines/mm. The expected maximum variations for these angles along the grating, are ±80 microradians and ±240 microradians, respectively.

3.4 Grating blaze angle

White-light interferometric profilometry can be also used to measure the blazed angle on the grating, to ensure that the correct specifications are matching and to provide data for further simulations. Using a 50x microscope objective we have a lateral resolution of 0.64 microns and a field of view of 140x110 microns^2. In both gratings, the maximum height for the blazed profile is designed to be 35 nm, with a tolerance of few nanometers. To have a reliable measurement of this variable, a calibration with a comparison with known steps of the same order of magnitude should be carried out.

4. CONCLUSIONS

The specifications of the European XFEL SASE3 monochromator optical elements have been showed and some basic considerations about the necessary characterization measurements have been carried out. From the analysis, the requirements result really challenging for present measurements technology. However, we have presented two methods, deflectometry and interferometry, with performances near to the accuracy requested. The approaches are quite complementary, starting from a slope error measurement in the case of deflectometry, while measuring the height error in the case of interferometry. Prototypes manufacturing is on the way and preliminary measurements will be carried out in the next future following the presented guidelines.

REFERENCES

[1] M. Altarelli, et al. (Eds.) XFEL, “The European X-ray Free-Electron Laser”, Technical Design Report, (2006), DESY 2006-097

[2] H. Sinn, M. Dommach, X. Dong, D. La Civita, L. Samoylova, R. Villanueva, and F. Yang, “X Ray Optics and Beam Transport”, Technical Design Report, (2012), XFEL.EU TR-2012-006

[3] J. Gaudin et al., “Investigating the interaction of x-ray free electron laser radiation with grating structure”, Optics Letters, Vol. 37, Issue 15, pp. 3033-3035 (2012)

[4] M. Hettrick and S. Bowyer, “Variable line-space gratings: new designs for use in grazing incidence spectrometers,” Appl. Opt. 22, 3921–3932 (1983).

[5] L. Poletto, G. Naletto, and G. Tondello, “Grazing-incidence flat-field spectrometer for high-order harmonic diagnostics,” Opt. Eng. **40,** 178–185 (2001)

[6] L. Samoylova, H. Sinn, F. Siewert, H. Mimura, K. Yamauchi, et al. “Requirements on hard x-ray grazing incidence optics for European XFEL: analysis and simulation of wavefront transformations”, Proc. SPIE 7360, EUV and X-Ray Optics: Synergy between Laboratory and Space, 73600E (2009)

[7] L. Rayleigh, “Interference bands and their application,” Nature 48, 212-214 (1893)

[8] R. Brünnagel, H.-A. Oehring, and K. Steiner, “Fizeau interferometer for measuring the flatness of optical surfaces,” Appl. Opt. 7, 331-335 (1967)

[9] P. Hariharan, "Interferometric testing of optical surfaces: absolute measurement of flatness", Optical Engineering Vol. 36(9), pp. 2478-2481 (1997)

[10] G. Forbes, P. Murphy, and J. Fleig, "Stitching subaperture data for testing aspheric surfaces," in *Frontiers in Optics*, OSA Technical Digest (CD) (Optical Society of America, 2004), paper OTuD5.

[11] M. Vannoni and G. Molesini, "Iterative algorithm for three flat test," Opt. Express 15, 6809-6816 (2007)

[12] M. Vannoni and G. Molesini, "Absolute planarity with three-flat test: an iterative approach with Zernike polynomials," Opt. Express 16, 340-354 (2008)

[13] Maurizio Vannoni and Giuseppe Molesini, "Three-flat test with plates in horizontal posture," Appl. Opt. 47, 2133-2145 (2008)

[14] R. D. Geckeler, “Optimal use of pentaprism in highly accurate deflectometric scanning,” Meas. Sci. Technol. 18, 115-125 (2007)

[15] F. Siewert, J. Buchheim, T. Zeschke, G. Brenner, S. Kapitzki, and K. Tiedtke, “Sub-nm accuracy metrology for ultra-precise reflective X-ray optics,” Nucl. Instrum. Methods Phys. Rev. A635, 552–557 (2010).

[16] F. Siewert, J. Buchheim, and T. Zeschke, “Characterization and calibration of 2nd generation slope measuring profiler,” Nucl. Instrum. Methods Phys. Rev. A616, 119–127 (2010)

[17] Frank Siewert, Jana Buchheim, Sébastien Boutet, Garth J. Williams, Paul A. Montanez, Jacek Krzywinski, and Riccardo Signorato, "Ultra-precise characterization of LCLS hard X-ray focusing mirrors by high resolution slope measuring deflectometry," Opt. Express 20, 4525-4536 (2012)

[18] Paul J. Caber, "Interferometric profiler for rough surfaces," Appl. Opt. 32, 3438-3441 (1993)

[19] Creath, K. and Wyant, J. C., “Absolute measurement of surface roughness,” Appl. Opt. 29, 3823-3827 (1990).

[20] D. Cocco, G. Sostero, and M. Zangrando, "Technique for measuring the groove density of diffraction gratings using the long trace profiler," Rev. Sci. Instrum. 74, 3544 (2003)