Metrology, Mirrors and Gratings – Advances and Challenges in Synchrotron Optics

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Abstract. Ultra-precise reflective and diffractive optical elements like blazed diffraction gratings or ultra-precise mirrors of flat, elliptic, parabolic, or other shapes have become key components in today's synchrotron optics. These optical components feature nanometre accuracy on a macroscopic length scale. Beamlines with extreme lengths of 100m to 1km or more (as planned for the European XFEL) will require plane mirrors characterized by a residual slope error of 50nrad rms and a curvature radius of > 1000km on a length of 800mm or even more. Diffraction limited focusing mirrors for hard X-ray application show residual slope deviations of 50nrad rms on a length of 350mm. The current slope limit for focusing mirrors in VUV-application lies at around 0.5µrad rms, one order of magnitude inferior compared to hard X-ray focusing optics, and it can still not be exceeded due to technological restrictions. The requirements for diffraction gratings are even more challenging. In addition to the challenges posed by perfect substrate quality, special attention is needed to guaranty a precise positioning of the grooves along the full aperture length. A positioning accuracy of about 20nm for the carriage system of a ruling engine is mandatory to meet the Marechal tolerance for gratings. For the manufacture of blazed and laminar gratings, we are currently establishing a new technological laboratory at the Helmholtz Zentrum Berlin (HZB), including instrumentation from Carl Zeiss. Besides the present Zeiss technology, we are also developing an advanced technology line, including a new ultra-precise ruling machine, ion etching technology as well as laser holography.

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1. Introduction

The quality requirements for reflective synchrotron optics like mirrors have increased significantly over the last ten to fifteen years. Today, grating blanks of 0.1µrad rms residual slope error, 150mm length and a curvature radius larger than 200km are state of the art. It is being discussed to install plane mirrors with a length of 800mm, 50nrad rms slope error, respectively 2nm pv figure error and a curvature radius larger than 1000km in beamlines at the European XFEL. Dedicated metrology instrumentation of comparable accuracy has been developed to characterize such optical element. 2nd generation slope measuring profilers like the Nanometer Optical component measuring Machine (NOM) [1] enable the inspection of reflective optics up to a length of 1.5 meter [2] with an accuracy better than 0.05µrad rms. It will supersede the well known Long Trace Profiler-II (LTP) [3] as a fundamental tool for the inspection of optics. Gratings are of essential importance in the low energy range to provide a monochromatic beam with high flux and high spectral resolution. After closing the grating production at Carl Zeiss in Oberkochen a new facility will be gradually established at the Helmholtz Zentrum Berlin (HZB) until the end of 2013. This facility will provide gratings mainly but not only to the synchrotron community. The Zeiss ruling machine GTM-6 has been recently re-commissioned and a new ruling machine providing a much larger ruling area than the GTM-6 will become operational until the end of 2013.

2. Metrology – a subject of continuous improvement

Ultra-precise metrology is a key diagnostics tool to characterize X-ray optical components. It provides essential information for the manufacture and handling of optical components like mirrors or gratings. Whereas commercially available instruments like white light interferometer (WLI) or atomic force microscopes (AFM) can be used to measure the mid (1mm^{-1} - $1\mu\text{m}^{-1}$) and high ($1\mu\text{m}^{-1}$ – 10nm^{-1}) spatial frequency roughness with excellent accuracy, the slope error of synchrotron optics ($>1\text{mm}^{-1}$) is usually measured by dedicated instruments like LTP or NOM. Since the first NOM-system at BESSY came to operation [4] further labs have followed this way [2, 5, 6] in order to improve the measuring accuracy for optics. Slope measuring profilers like the NOM are based on a high resolution autocollimator used in a scanning penta prism configuration [1]. Usually, the penta-prism configuration is realized in a 45° double mirror set-up to avoid the measuring beam to be influenced by inhomogeneigty of the bulk-glass. The BESSY-NOM is equipped with two λ/100 quality mirrors. This design has shown <20nrad rms accuracy for plane or slightly curved mirrors as characteristic for hard-X-ray application [1]. 0.2µrad rms accuracy was achieved for strongly curved optics showing a local curvature of r=10m and below. Key factors in achieving such accuracy are the careful characterization and calibration of the instrument [7; 8]. A Vertical Angle Comparator (VAC) [7] could be successfully used to identify error sources, improve the NOM and demonstrate an rms accuracy of 50nrad up to a length of 1000mm in principle [7], which is a requirement to measure upcoming plane mirrors for the European XFEL [9]. Figure 1 shows an example for a state-of-the-art plane grating blank (for the coherent soft X-ray beamline at the NSLS-II) measured with the BESSY-NOM. The residual slope error was found with 97nrad rms.

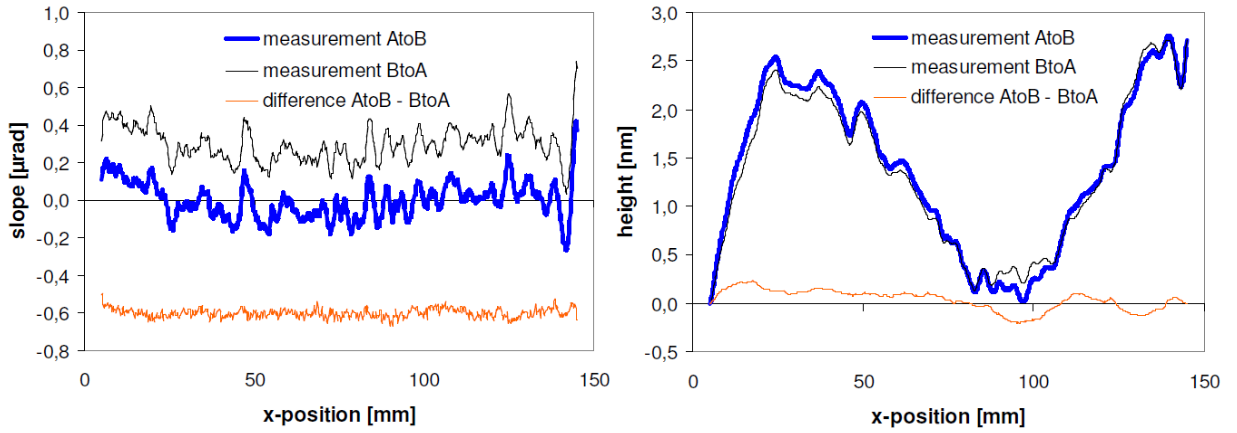

Figure 1. Left: profiles of residual slope measured under different alignment conditions. Right: corresponding profiles of height achieved by integration of the slope data.

In order to verify the measuring accuracy, the substrate was measured first from side A (x_0=0mm) to side B (AB) and than after a 180° rotation from side B to side A (BA). The subsequent comparison of both measurements showed an agreement of 20nrad rms respectively 1Å rms. This value can be taken for the estimated accuracy in case of this measurement. Note: this method is very useful for characterizing the performance of a slope measuring profiler. It allows identifying aberration effects of the detector optics or pixel errors on the CCD array. However, it can of course not identify the spherical (linear) part of the error budget but this is irrelevant if we look at the residual slope only. When measuring plane optics, the angular range of the detector used is very small (± 0.25µrad – see e.g. figure 1). For spherical and aspherical optics as needed for application in the VUV-range a much larger angular range (up to 5mrad and more) is needed to measure the curvature of the optics. In case of very long or strongly curved optics, stitching technique [10] can be applied to measure the mirror. Another improvement in metrology is to measure optics face-side, required where optics are used to reflect in horizontal direction [11]. A slope measuring profiler is usually applied to measure a line scan along the optics in meridional or sagittal direction. This is sufficient for a quality check but not to provide a three-dimensional data-set, as required to optimize the shape of a mirror by deterministic surface finishing. In case of the BESSY-NOM, a dedicated mapping technique was developed to provide such information on the mirror topography [4]. Based on NOM-data, several plane substrates and two-dimensional elliptical focusing mirrors were figured by use of Ion Beam Figuring (IBF) [12].

3. Towards “Picometry”? – ultra-precise mirrors for synchrotron application

Compared to transmission zone plates, wave guides or compound refractive lenses mirrors are the most efficient option to guide and focus synchrotron light to a defined position. The quality of synchrotron mirrors has been improved by a factor of 5 over the last 10 years. It will need further improvement to fulfil the requirements for future light sources like FEL or ultimate storage rings. Taking the Maréchal criterion [13], which describes an acceptable rms wavefront distortion as $\sigma_{rms} < \lambda/14$, than to meet the acceptable residual surface errors of a reflective optical element, can be described by h_{rms}.

$$\Delta h_{rms} \le \frac{\lambda}{14\sqrt{N}\,2\theta} \qquad (1)$$

where N is the number of reflecting surfaces in the system, θ is the angle of incidence of the beam being reflected off this surface and λ the wavelength [13]. Clearly, the requirements on surface quality become linearly more difficult to achieve with decreasing X-ray wavelength, hence the challenge lies in making such high quality X-ray reflective optics. The proposed plane mirrors for the European XFEL will require a residual figure error of 2nm pv over 800mm aperture length [14]. In addition, such mirrors need an excellent micro-roughness, not only to avoid a loss of photons by scatter but also to prevent the mirror from being heated up and finally damaged. Thus, the required micro-roughness lies in the range of 0.1nm rms. Mirrors of the above described quality have never been manufactured so far. Such mirrors need to be finished by deterministic surface finishing technology like ion beam figuring (IBF) 15], elastic emission machining (EEM) [16], computer-aided-polishing (CAP) or magneto rheological jet polishing (MRJP). IBF-technology is a well established technique to optimize the mirror shape up to a length of 1500mm and EEM-Osaka-mirror technology has been recently improved to a length of 1000mm [16]. However, conventional polishing is applied for three dimensional aspheres like toroids, rotational ellipsoidal or parabola mirrors, as well as mirrors of extreme length or steep sagittal curvature with radii of a few ten millimeters only. Depending on the applied technology, a typical “fingerprint-like” residual is often present on the mirror – corresponding to e.g. the polishing tool size (in case of IBF, EEM, CAP and MRJP), typical textures on the polishing tool or guiding errors of a conventional polishing tool. A comparison of different finishing technologies is given in Figure 2, showing the PSD for a conventional polished and an IBF finished mirror. Table 1 gives an overview on the quality of different mirrors, as measured at the BESSY-Optics Lab. It shows that the finishing of plane, spherical and two-dimensional aspherical mirrors allows a significantly better residual slope error compared to three-dimensional aspheres.

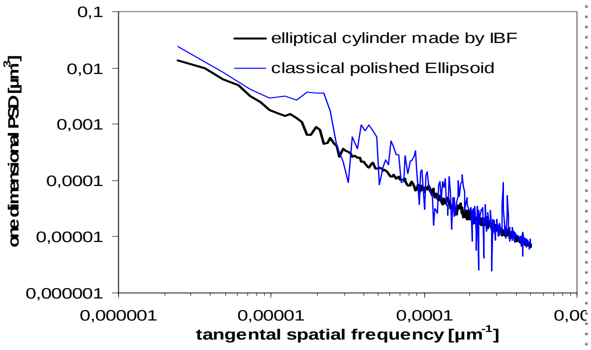

Figure 2. one-dimensional PSD - comparison of classical polishing and deterministic (IBF) finishing technology

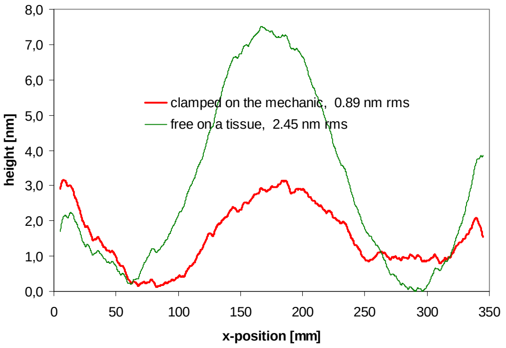

Figure 3. profile of residual height of a elliptical cylindrical focusing mirror in the free and clamped state

Table 1. Quality of X-ray mirrors of different shape – inspected at the BESSY-II Optics-Laboratory.

shape	Energy range	Length [mm]	Average merid. radius	Residual slope[a] [µrad rms]	Residual figure error [nm rms]	Micro-roughness[b] [nm rms]
Plane grating blank [1]	VUV at NSLS-II	150	>200 km	0.09	0.7	0.1
Plane mirror [1]	VUV at BESSY-II	290	>100 km	0.1	0.8	<0.2
Plane mirror [1]	Hard X-ray at PETRA-III	800	>200 km	0.28	11.3	<0.1
Spherical [1]	Calibration sphere	120	9.312 m	0.17	0.8	<0.2
Cylindrical [2]	Hard X-ray at PETRA-III	750	>100 km	0.21	8.2	0.1
Toroid [2]	VUV at BESSY-II	100	49,4 m	0.6	3.8	0.1
Elliptical cylinder [1]	VUV at FLASH	110	9.5 m	0.67	2.2	<0.6
Elliptical cylinder [1]	VUV at BESSY-II	120	15.1 m	0.5	2.8	<0.2
Elliptical cylinder [1]	VUV at PETRA-III	430	354 m	0.33	7.6	<0.3
Elliptical cylinder [3]	Hard X-ray at PETRA-III	90	261 m	0.038	<0.1	0.1
Elliptical cylinder [3]	Hard X-ray at LCLS	350	348 m	0.056	0.9	0.1
Rotational elliptic [4]	VUV at BESSY-II	185	33.4 m	2.5	26	0.3
Paraboloid [2]	Hard X-ray at BESSY-II	1300	6.1 km	4.6	108.8	<0.2

applied finishing technology: [1] IBF, [2] conventional polishing , [3] EEM, [4] CAP

[a] as measured by use of the BESSY-NOM,

[b] as measured by use of a White Light Interferometer, magnification 20x and 50x, usually a slightly higher value for the roughness is found applying magnification 1.25x or 2.5x – to cover the mid-spatial figure error

In case of elliptical cylindrical focussing mirrors made by EEM, both figure error and micro-roughness are at the same order of magnitude. Some exclusive mirrors show an rms 1Å-accuracy on a macroscopic length scale. In this sense, the quality of the optics as well as the accuracy of the metrology approaches the ten pico-meter range. If such excellent optics are available, the mounting becomes critical. Figure 3 shows an example of a vertical focusing mirror for the CXI-beamline at LCLS [17]. The mirror was finished by EEM to a dedicated shape which compensates the gravitational impact when placing the optics at the supporting points on the mechanic. In general mirror and mechanic have to be taken as one unit!

However, mirrors like those at the XFEL will sustain a change of shape related to significant head-load [18]. It is proposed to compensate this by use of active optics. Bimorph-mirrors are proposed to compensate the wave-front distortions. A recent investigation on the performance of bimorph-mirrors has shown it`s usability for a hard X-ray-beamline of the EMBL at PETRA-III [19], illustrating, however, a strong need for further development to meet the requirements for the XFEL. A promising solution for such a mirror was shown at SPring-8 [20] and recently, a first study has been started at the XFEL in Hamburg.

4. The Grating Project at the HZB

Gratings are essential components to provide monochromatic light for applications in the IR-, UV, VUV- energy range. To close the current gap for the availability of blazed gratings, HZB has started to establish a grating laboratory in Berlin. We intend to apply mechanical ruling, holographic recording, anisotropic etching [21] and ion beam etching technique for the production of gratings. The old Carl Zeiss ruling machine GTM-6 (Gitter-Teil-Maschine, designed to rule gratings up to a length of 6”) was transferred to the HZB and re-commissioned. First test rulings on an aperture of 45x20mm^2 were done for a groove-density of 650 and 1000l/mm – see fig. 4. The achieved micro-roughness on the grooves after ruling is of 0.4nm rms, comparable to the quality of the former production at Carl Zeiss. Equipment like an ion-etching machine, a groove-density measurement set-up as well as a system for laser interference lithography is installed and operational. In addition, the development of a new ruling machine is in progress. While the GTM-6 has a ruling area of 150x100mm^2, the new ruling machine (GTM-24) is designed to enable ruling on an area of 600x300mm^2. The GTM-24 is designed to manufacture gratings with groove-densities from 50l/mm up to 5000l/mm (homogeneous or with density variation) with a blaze angle between 1 – 20°. A challenge for the ruling machine is the position accuracy of 20nm along the full travel range of 600mm, required to meet the Marechal tolerance for gratings. This will be realized by a dedicated Laser-position measuring system to control the ruling. Note: due to limitations in the ruling speed (of max.10mms^{-1}), it is not planned to ever make gratings with high groove density on very large apertures. This would easily end up in production times of several years! However, it will be possible to manufacture long gratings with 50 to 150l/mm up to a length of 600mm, as required for beamlines at the XFEL [9].

The ruling of such gratings is performed on a gold-film by soft plastic deformation with a boat bottom shaped diamond. Taking advance from the different etching rates of gold and silicon for different etch-gases like Ar or Xe, the final blaze angle is realized by ion-etching [22]. This technique allows transferring the blaze profile into the Si-substrate and enables an effective blaze angle reduction by a factor up to 10. A first study showed a final blaze angle of 0.4°, achieved with initially 5° after ruling. Finally, a dedicated single- or multi-layer coating will be deposited on the grating.

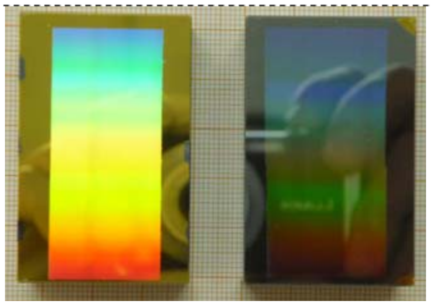

Figure 4. test gratings of 650l/mm left: after ruling into gold (5°), right: after ion beam etching (0.9°) – blank size: 50x25 mm^2

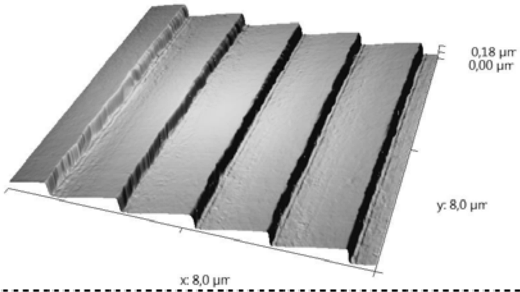

Figure 5. ruled blaze profile 650l/mm, blaze angle 5°, micro-roughness: 0.4 nm rms – AFM measurement on 8x8 µm^2

The GTM-24 with an expected weight of 15t will be installed on a separated basement in a dedicated laboratory, providing optimal environmental conditions. Our concept for the grating production includes a complete monitoring of the production by different type of metrology, ex-situ metrology (at the BESSY-II-Optics Lab.) and finally an at-wavelength acceptance test. This can be performed at the BESSY-II-Optics beamline. As part of the project, a new optics beamline, including a larger sized reflectometer, will come into operation at the end of 2013. The new reflectometer will cover the energy range from 10 to 1500eV (with a moderate resolution of 10.000 at 400eV). Samples of 300x60mm^2 (up to 4kg weight) can be investigated with linear and elliptical polarized light

5. Conclusions

Metrology and finishing technology for synchrotron optics have recently made significant improvement. In case of reflective optics, figure error and roughness are at the same order of magnitude in the rms 1Å-range. In this sense the development of synchrotron optics approaches "Picometry"- level. For three-dimensional aspheres, surface finishing and metrology are at the limit. Mounting of optics will be a critical topic for future high end applications. Thus, the final acceptance test of optics has to be performed in mounted state as designed to be used at the beamline (face-side or face-up). In general, mirror and mechanic have to be treated as one unit. In addition, it is proposed here to improve the options of online diagnostics, useful to tune a X-ray optical system to its desired performance.

Promising first results on the production of blazed gratings has been achieved. Dedicated instrumentation is under development to establish an efficient and qualitative supply of gratings, not only to the synchrotron community. A regular production of such diffractive elements is to be expected for the future within 2013 /2014.

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