Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research, A

journal homepage: www.elsevier.com/locate/nima

Advances in X-ray optics: From metrology characterization to wavefront sensing-based optimization of active optics

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ARTICLE INFO

Keywords:
X-ray optics
Optical metrology
Active optics
Synchrotron optics
FEL optics
Wavefront propagation

ABSTRACT

Experiments using high brightness X-rays are on the forefront of science due to the vast variety of knowledge they can provide. New Synchrotron Radiation (SR) and Free Electron Laser (FEL) light sources provide unique tools for advanced studies using X-rays. Top-level scientists from around the world are attracted to these beamlines to perform unprecedented experiments. High brightness, low emittance light sources allow beamline scientists the possibility to dream up cutting-edge experimental stations. X-ray optics play a key role in bringing the beam from the source to the experimental stations.

This article explores the recent developments in X-ray optics. It touches on simulations, diagnostics, metrology and adaptive optics, giving an overview of the role X-ray optics have played in the recent past. It will also touch on future developments for one of the most active field in the X-ray science.

Contents

0. Introduction

One of the key developments that has pushed Synchrotron Radiation (SR) and Free Electron Laser (FEL) science is the ability to manipulate the photon beam, preserve the source quality, and adapt the X-ray beam to the needs of the experiments. Often taken for granted by the beamline scientists, X-ray optics played a major role in making the 2nd and 3rd generation SR sources and FELs useful for X-ray experiments like microscopy, inelastic scattering, high resolution photoelectron spectroscopy, diffraction experiments and many more.

The development of new optics, dispersive and diffractive elements, coatings, cooling schemes, simulation tools and new methods of beam characterization, is usually fostered in small laboratories or by small groups and then adopted by the entire community. Some of the noteworthy developments that have had major impacts in this field include: Zone Plates, which have seen higher and higher spatial resolution [1,2] and, more recently, higher and higher aspect ratio [3]; the Long Trace Profiler [4] which boosted metrology and impacted mirror quality in the nineties; the multilayer deposition techniques, recently used for nano-focusing applications [5]; crystal monochromators. With the advent of the 3rd generation light source, many facilities recognized the need to invest human capital in the development of tools for X-ray optics and for optimizing the performance of the beamlines. This effort produced new optical designs, with higher resolution, higher flux and overall better performances. The once feared variable line space grating is

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https://doi.org/10.1016/j.nima.2018.03.026
Received 29 December 2017; Received in revised form 6 March 2018; Accepted 6 March 2018

Please cite this article in press as: D. Cocco, et al., Advances in X-ray optics: From metrology characterization to wavefront sensing-based optimization of active optics, Nuclear Inst. and Methods in Physics Research, A (2018), https://doi.org/10.1016/j.nima.2018.03.026.

now commonly used, producing more flexible and compact optical systems [6–8].

As the 3rd generation light sources boosted the first big step in X-ray optics, the Free Electron Laser (FEL) and upcoming Diffraction Limited Storage Rings (DLSR) is unleashing a new one. With coherent sources, the need to preserve the wavefront and, produce diffraction-limited focused spots, seeded the realization of new polishing techniques for optics [9].

The improvements in optical manufacturing have been possible thanks to the simultaneous improvements in optical metrology. Both in- and ex-situ metrology have been receiving more significant investments in recent years than in the previous ones. Ex-situ metrology is still evolving toward sub-nm and nrad precision on assembled mirrors. In-situ metrology is becoming more and more popular, pushing the potential of the new beamlines to their limits.

Moreover, thanks to the improvements in mirror polishing and metrology (dedicated to assembled mirror), it has been possible to produce for the first time an almost perfect out of focus wavefront in an X-ray facility. At LCLS, the development of a stress-free mirror holder coupled with the use of ultra-polished mirror has lead to a remarkable improvement of the quality of the beam, in and out of focus (see Fig. 1), in agreement with the expected performances [10].

Along with hardware developments, software used to model and simulate beamline performance has seen significant growth. The first Ray Tracing Program widely used by the X-ray community was developed by Franco Cerrina and his team at Madison in the Eighties [11]. It has subsequently been adopted worldwide and adapted to different platforms and equipped with user interface. Very recently, advanced programs handling coherent sources and representing a major upgrade to ray tracing, have been realized thanks to collaborative work from different laboratories. Programs like WISE [12,13], Hybrid Shadow [14] and Synchrotron Radiation Workshop (SRW) [15], are friendly, permitting the design of advanced beamlines and the possibility to test novel optical schemes and giving a deeper understanding of their performance.

Hybrid Shadow is an evolution of the well-known Shadow, described earlier. It is based on a “hybrid method” calculating the diffraction effects from an optical element by means of wavefront propagation, and combining the results with ray tracing. In this way, diffraction effects due to clipping or apertures as well as shape errors are taken into account, and can be handled in far and near field. SRW computes the synchrotron radiation from relativistic electrons in the near and far field range. X-ray (as well as longer wavelengths) 2D propagation is implemented by using Fourier Optics and can handle both, partial, and fully coherent radiation.

WISE is a physical optics simulation package used to compute the complex electromagnetic field downstream of one or more optical elements. Originally developed for simulating astronomical telescopes, as many other programs, it has been recently included in the OrAnge SYnchrotron Suite (OASYS) [16], a new graphical environment gathering most of the simulation tools that have been developed and used within the synchrotron and free electron laser community. WISE is designed for use in the operating range from extreme ultraviolet to hard X-rays, at grazing angles of incidence, using spatial and temporal fully coherent sources. At grazing incidence, where the reflection in the XUV range is higher, diffraction is more effective in the incidence plane than in the transverse direction, usually by a factor of 100–1000. This allows the user to neglect the mirror’s sagittal error and to consider only the longitudinal profile. The computation of the intensity distribution in the focal plane, or Point Spread Function (PSF), is performed using Kirchhoff’s scalar diffraction formula over a 1D domain:

$$PSF(x) = \frac{\Delta R}{E_0^2 \lambda f L^2} \left| \int_{f-L}^{f} E\left(r_h, 0, z_h\right) e^{-i \frac{2\pi}{\lambda} \sqrt{\left\{(x-r_h)^2 + z_h^2\right\}},} dz_h \right|^2$$

where f is the nominal focal distance, $L \ll f$ is the mirror length, ΔR is the maximum–minimum radius, λ is the wavelength of the focused beam and E is the diffracted field on the second mirror at the x–z plane. It is possible to include mirror defects in terms of figure error (measured or calculated) and micro-roughness (though there is no physical distinction between the two, a practical one may exist). Except where explicitly stated, all the simulation shown in this paper has been performed using WISE.

In the following sections, this article will focus on the development in X-ray optics fields that have seen major investments in recent years. Ex- and in-situ metrology and adaptive optics will be discussed including the current achievements and ongoing projects. This is not intended to be an exhaustive lists but an overview biased by the authors involvement and knowledge of how the particular needs have been addressed and solved.

1. Optical metrology

During the past decades, optical metrology has played a major role on the development of synchrotron optics. X-ray mirrors quality has evolved rapidly, accelerated by the development of extremely brilliant 3rd/4th generation synchrotron and Free Electrons Laser (FEL) radiation sources. These X-ray mirrors, planes or off-axis ellipses with lengths of up to 1 m, must preserve the incoming wavefront so they are mainly characterized by residual slope errors in the range of 50 nrad rms or sub nm rms height errors, and 0.3 nm rms or less for micro-roughness [17].

In-situ, at wavelength, metrology became essential for assessing the beamline performances and ex-situ metrology plays the role of achieving the ultimate performance. In the next two sections, these two complementary aspects of mirror and beamline performance characterization will be described.

1.1. *Ex-situ metrology*

In the field of optical metrology, there are many possible metrology technology solutions with different benefits and shortcomings. Interferometers typically have sub wavelength accuracy but require dedicated designed null optics when the surface under test is not spherical. For measuring grazing incidence optics, those typically used in SR and FEL facilities, the Long Trace Profiler (LTP) is the most commonly used instrument, also the one that started the modern optical metrology technology boom. This is a direct slope measurement device, able to detect slope variations of the order of 0.1 μrad. The Long Trace Profiler (LTP) is based on the principle of the pencil-beam interferometer developed by Von Bieren [18]. The concept of the LTP, very similar to an autocollimator, is simple. A narrow collimated laser beam is sent to the Surface Under Test (SUT) and the variation of the SUT-reflected beam angle is measured by means of a high quality long focal lens and a CCD detector. In this way, by moving the laser beam on the mirror surface, one can reconstruct its slope. In some cases mirrors are specified using height error also, it can be useful for the mirror manufacturer to know the height error when making corrections. This information can be derived from the slope data simply by integration. The first generation surface profiler (or profilometer), referred to above as the LTP, [19–21] was originally developed at Brookhaven National Laboratory (USA) in 1989 to test large plane, spherical and aspherical mirrors. Since its conception the LTP has been adopted by many laboratories around the world and several custom modifications have been implemented. By construction, the system does not need a reference surface, provided the direction of the probe beam is perfectly preserved during the scan. The best translation stages (air-bearing, for example) can have parasitic motion below 10 μrad for a 1 m long translation. This is not sufficient compared to the desired slope resolution. To tackle this problem, the first improvement was made by tracking the optical head tilt with an extra reference beam path. Currently most instruments stabilize their probe beam by scanning only a pentaprism as was first proposed by Qian [22]. The pentaprism maintains a constant angle between the incoming beam, parallel to the translation and the reflected beam directed to the SUT even if the penta-prism is tilted. With the scanning

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