Grating-based monochromators

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This chapter describes narrow-bandwidth filtering of soft X-rays by diffraction gratings in optical systems known as monochromators for the purpose of performing spectroscopic measurements. The X-ray sources considered are confined to broadband sources generated by synchrotron storage-ring facilities and beamlines at these facilities, which consist of monochromators and associated optics to collect the source radiation and focus it at the sample position. A brief history of soft X-ray synchrotron beamlines, from the 1970s to today, is provided, separated into three eras of beamline development that correspond to the three generations of synchrotron storage rings. The advantages and disadvantages of the principal types of beamlines from the three eras is provided, along with a more detailed description of the latest generation of soft X-ray beamlines. The dramatic improvements in flux (greater) and spot size (smaller) over the 50-year history of synchrotron beamlines are described.

1. Introduction

The predominant means of selecting a narrow-bandwidth source of soft X-rays for use in an absorption spectroscopy experiment is by filtering using a diffraction grating in an optical system known as a monochromator. Typically, monochromators include, or are accompanied by, optical elements for manipulating the X-ray source, such as collecting a solid angle of emission and focusing the beam onto apertures and/or the sample being investigated in the absorption experiment. While grating-based monochromators can be and are used for laboratory-type soft X-ray sources, the focus of this section will be on broadband soft X-ray sources such as those produced by synchrotron facilities. As for hard X-ray monochromators, the relevant parameters are the range of soft X-ray energies \( E \) that can be selected, the bandwidth \( \Delta E \) about the selected energy, the transmission efficiency \( (I/I_0) \) for photons within the bandwidth \( \Delta E \) about \( E \) and the ability to not transmit photons at other energies. Similar to hard X-ray monochromators, soft X-ray versions must maintain stability of \( E, \Delta E \) and the exit beam position and angle as \( E \) is scanned to perform an absorption experiment.

Over the relatively short (~50-year) history of synchrotron facilities, the requirements for stability and performance have become more stringent by at least two orders of magnitude, with the latest generation of monochromators delivering \( \Delta E/E \) values in the \( 10^{-5} \) range or less and maintaining the phase space of the photon beam (the product of spatial and angular dimensions) at or near diffraction-limited values. The range of photon energies \( E \) covered by grating-based monochromators has increased significantly over the history of synchrotron facilities by increasing the upper energy limit as the ability to fabricate high-quality soft X-ray optics, and soft X-ray gratings in particular, has improved by leaps and
bounds. Whereas grating-based monochromators struggled to compete above 1 keV photon energy in the 1970s and early 1980s, soft X-ray monochromators have evolved to operate up to ~2 keV routinely and are now competitive up to ~5 keV in the so-called tender X-ray regime.

2. Diffraction gratings

Diffraction gratings are one-dimensional dispersive optical elements that are routinely used to disperse the light produced by synchrotron facilities in the vacuum ultraviolet (VUV) and soft X-ray ranges and are pushing into the tender X-ray range.

A generic diagram depicting diffraction from a grating is shown in Fig. 1. The grating, shown in cross section as the blue-shaded region in Fig. 1, consists of a set of grooves ruled or etched in the surface of the grating substrate perpendicular to the diffraction plane defined by the incoming and outgoing beams. The angle between the incoming beam (‘incident wavefront’) and the normal to the surface of the grating substrate is defined as $\alpha$ and the angle between the normal and the outgoing beam (‘diffracted wavefront’) is $\beta$. For constructive interference, the path-length difference between the two beams, given by $d(\sin \alpha + \sin \beta)$, where $d$ is the groove spacing, must be an integral number ($m$) of wavelengths $\lambda$. The index $m$ is referred to as the diffraction order. This is the so-called grating equation, which determines the angles of the principal rays in diffraction from a simple grating:

$$\frac{m \lambda}{d} = (\sin \alpha + \sin \beta). \quad (1)$$

To determine the properties of a photon beam with finite angular divergence, as opposed to just the principal rays, a coordinate system such as that shown in Fig. 2 is used, where the principal incoming ray is $AO$ and the principal outgoing ray is $OB$. Photons comprising the beam strike the grating surface at generic points labelled $P$. The $(x, y, z)$ coordinates of $P$ are named $(\xi, \omega, \iota)$.

Owing to aberrations, incoming rays $AP$ are diffracted as rays $PC$, intersecting the image plane at a generic point $C$. To analyse the collective effect of the ensemble of rays $C$ centred about principal point $B$ in the image plane, we follow the original derivation by Noda et al. (1974), alternate formulations of which have been derived and published over the years (Howells, 1980c, 2001, 2010; Johnson, 1983; West & Padmore, 1987; Williams, 1992). The optical path function for the diffracted rays is

$$F = \langle AP \rangle + \langle PC \rangle + \frac{m \lambda}{d}. \quad (2)$$

The optical path lengths $\langle AP \rangle$ and $\langle PC \rangle$ can be expanded as

$$\langle AP \rangle = [(x - \xi)^2 + (y - \omega)^2 + l^2]^{1/2},$$
$$\langle PC \rangle = [(x' - \xi)^2 + (y' - \omega)^2 + (z' - l)^2]^{1/2}, \quad (3)$$

where $x'$, $y'$ and $z'$ are the Cartesian coordinates of the intersection of the outgoing ray with the image plane. By power-series expansion in the aperture coordinates, the optical path function $F$ can be written as

$$F = F_{00} + w F_{10} + \frac{1}{2} w^2 F_{20} + \frac{1}{2} l^2 F_{02} + \frac{1}{2} w^3 F_{30} + \frac{1}{2} w l^2 F_{22} + \frac{1}{8} w^4 F_{40} + \frac{1}{4} w^2 l^2 F_{24} + \frac{1}{8} l^4 F_{04} + \ldots. \quad (4)$$

where the indices $ij$ in $F_{ij}$ consist of grouped powers of $w$ and $l$ in order to associate them with recognizable types of aberrations. The first few terms that affect energy resolution are

$$F_{00} = r + r',$$
$$F_{10} = \frac{m \lambda}{d} - (\sin \alpha + \sin \beta),$$
$$F_{20} = \text{defocus},$$
$$F_{12} = \text{astigmatic coma},$$
$$F_{30} = \text{coma},$$
$$F_{40}, F_{22}, F_{04} = \text{spherical aberration terms}, \quad (5)$$

where $\alpha$ and $\beta$ are the angles of incidence and diffraction in the $xy$ plane. Note that in the sign convention used here, $\alpha$ is positive and $\beta$ is negative in Fig. 2.

Fermat’s principle holds that the path function $F$ should have a stationary value such that $\partial F/\partial w = 0$ in the dispersion plane. Applying this to the $w F_{10}$ term yields the grating equation (1). The remaining terms represent aberrations, as listed in equation (5). The wavelength spread associated with aberrations depends linearly on $\partial F/\partial w$ as

$$\Delta \lambda = \frac{d}{m} \frac{\partial dF}{\partial w}. \quad (6)$$

The first ($m = 1$) inside diffraction order (the diffracted beam that lies between the incident beam and the zero-order reflected beam) is the most-used order in soft X-ray grating monochromator designs. Using the expansion for the optical path function $F$ in equation (4), the aberration-limited wavelength resolution is given by

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\[ \Delta \lambda = \frac{d}{m} \left( w F_{20} + \frac{3}{2} w^2 F_{30} + \frac{1}{2} w^2 F_{12} + \frac{1}{2} w^3 F_{40} + \ldots \right), \]  

(7)

where the contribution from the \( F_{10} \) term is zero by the grating equation (1).

Organizing the aberration terms (defocus, coma, astigmatic coma and spherical aberrations) as shown in equation (5) is useful because the types of monochromator designs used in synchrotron-radiation beamlines are distinguished by the ways in which they deal with minimizing aberrations. Descriptions of the principal types of monochromators used in synchrotron beamlines, including their dominant aberrations, are provided in Section 3.

The advantages of using diffraction gratings as dispersive elements include (i) relatively large wavelength coverage (a factor of \( \sim 3-10 \) per grating), (ii) selectable dispersion (wavelength range per unit angle in the dispersion plane) and (iii) adequate diffraction efficiency (up to 30\% or higher in the first order). The main disadvantage associated with diffraction gratings is the presence of unwanted diffraction orders in the diffraction plane. For continuum sources such as synchrotrons, a selected angular slice that selects energy \( E \) in the first diffraction order \( (m = 1) \) will also necessarily select energies \( m^*E \) in the \( m \)th diffraction orders \( (m = 2, 3, \ldots) \). Mitigation measures include (i) the selection of grating parameters that maximize the efficiency of the first \((m = 1)\) diffracted order, (ii) other means of filtering the source spectrum to reduce its intensity in the energy range of the unwanted orders (for example additional mirror reflections and/or selectable mirror coatings) and (iii) specialized sources such as quasi-periodic elliptically polarized undulators (QP-EPUs; Hashimoto & Sasaki, 1995; Schmidt et al., 2002) that shift the energies of harmonics away from multiples of the fundamental so that they do not fall into the small angular slice in the diffraction plane that is selected by the beamline.

The type of grating described so far in this section has uniform groove spacing \( d \) along a tangent to the grating surface in the diffraction plane. These constant-line-spacing gratings are known as Rowland gratings (Rowland, 1883). A variant of this type of grating with variable line spacing (VLS; Harada & Kita, 1980; Hettrick, 1984; Harada et al., 1986) is able to provide focusing in the dispersion plane as well as the diffraction properties described above. Monochromators based on both constant-line-density and variable-line-spacing gratings are described in Section 3.

Gratings used in soft X-ray beamlines can be fabricated via a number of methods, with the principal two being mechanical ruling and holographic recording; see Rowland (1883) and Pieuchard & Flamand (1972). In the 1980s and earlier, the typical substrate material of choice was fused silica or variants such as Zerodur (Viens, 1990), which offers low thermal expansion near room temperature. Later, single-crystal silicon became the substrate material of choice when it was demonstrated that silicon could be ground and polished to state-of-the-art figure \((\lesssim 0.1 \text{ rad r.m.s.})\) and finish \((\lesssim 0.2 \text{ nm r.m.s.})\) values. Along the timeline, attempts were made to use metal-alloy substrates in order to be easily compatible with liquid-cooling schemes, but these were largely abandoned because these materials were not able to be polished to mirror-quality finish over sufficiently large areas.

Diffraction efficiency is a key performance metric which drives the overall throughput of the monochromator and thereby the entire beamline. For a given geometry (angles of incoming and diffracted beams) and a chosen groove spacing (line density), grating-diffraction efficiency depends on two factors: groove shape and surface material.

Figure 2
Coordinate system for diffraction from a grating. Principal rays \( AO \) and \( OB \) are shown, along with generic rays \( AP \) and \( PC \), where the location of \( C \) is the intersection of the outgoing generic ray with the image plane. Reprinted from West & Padmore (1987).
The three main choices for groove shape are laminar (rectangular), blazed (triangular) and sinusoidal, where laminar and blazed types are those most commonly used on soft X-ray beamlines. Laminar groove shape is usually realized by lithographic recording and etching techniques in the substrate material. These gratings, therefore, are masters and can be stripped and recoated if the overcoating layer becomes contaminated. Blazed gratings can also be fabricated lithographically via the use of asymmetric etching techniques (Matsui et al., 1982; Ju et al., 2005) or they can be directly ruled in the coating material (Gleason et al., 2017). For any type of groove shape, the smoothness of the groove facets (any portion illuminated by the incoming beam) is an important quality. Rough surfaces contribute to unusable grating output referred to as scattered light because this emission is rather spread out (‘smeared’) in angle and wavelength, thereby not contributing in a useful way to the first-order diffracted beam and, more importantly, sending intensity of the wrong wavelength co-propagating with the outgoing first-order diffracted beam.

The advantage of blazed gratings is the freedom to choose the so-called ‘blaze angle’, which is the angle between the grating facets and the substrate plane. The blaze angle can be selected such that the incoming and diffracted beams are in close-to-specular geometry with respect to the facets for a portion of the photon energy range covered by a grating, thereby enhancing the diffraction efficiency in that range. The advantage of laminar gratings is a superior degree of fabrication perfection (groove-placement accuracy, groove shape and groove smoothness), at least to date; multiple efforts are under way to produce blaze gratings at a level of perfection presently realized only with laminar grating-fabrication technology. The differences in performance between achievable laminar and blazed grating types become greater as the line density increases. For this reason, laminar gratings presently dominate over the blazed type for the highest resolution applications.

In order to select the optimal grating parameters for a given application, algorithms and codes for the calculation of grating efficiency as a function of grating geometry (the angles of the incoming and outgoing beams), groove spacing, groove shape and coating material are indispensable. One of the earliest such codes was written by Névière et al. (1974, 1978) and many others have followed (see, for example, Roumiguieres et al., 1976; Petit, 1980; Valdes et al., 1994). Embedding these calculators into optimization scripts permits the determination of the best choice of grating parameters within a chosen parameter space (Padmore et al., 1994).

The overall process for the design of grating-based monochromators involves the calculation and optimization of (i) geometric parameters to determine and optimize the wavelength range, resolution and throughput and (ii) grating parameters to optimize the diffraction efficiency. Section 3 describes the variety of types of grating-based monochromators and associated beamlines that have been developed over the history of synchrotron radiation, grouped into three approximate time phases.

All of the beamline designs described in this chapter diffract in the vertical plane in order to take advantage of the smaller source size of synchrotron sources in the vertical plane compared with the horizontal plane. This is true of all of the generations of synchrotron sources developed to date (first through fourth). Some beamlines designed to maximize the degree of spatial coherence, which is generally greater in the vertical than in the horizontal, have chosen to diffract in the horizontal plane; these designs are not described in this chapter and are generally not very relevant for absorption spectroscopy applications.

3. Monochromator and beamline designs

The variations in grating-based beamline designs have to do with the different ways that optical elements such as mirrors (Howells, 1986) and diffraction gratings (Namioka, 1998) can be combined to produce a beam with the desired properties at the sample position: selectable, stable energy $E$, small bandwidth $\Delta E$ and high flux in a small spot size. Other photon properties such as polarization can also be important, depending on experimental requirements, and affect beamline design; however, these will not be described further in this chapter.

This section will concentrate on soft X-ray beamline designs, in part because this class of beamlines has seen the greatest degree of evolution over the past five decades. The other common type of grating-based beamline design is based on normal incidence monochromators (NIMs), which typically operate in the VUV photon energy range and below (less than $\sim 40$ eV photon energy). While the same diffraction principles apply to NIMs and soft X-ray monochromators, the near-normal angles of incidence on the gratings in the NIM design place reduced technical demands on the grating properties. Similarly, the means of handling focal properties in NIM designs are simpler than in soft X-ray designs. Examples of NIM-based synchrotron beamlines include beamline 5-4 at
SSRL (https://www-ssrl.slac.stanford.edu/content/beamlines/BL5-4) and the Bloch beamline at MAX-IV (https://www.maxiv.lu.se/accelerators-beamlines/beamlines/bloch/bloch-beamline-optics/), as well as the ESM beamline at NSLS-II described in Section 3.3. In fact, the Bloch and ESM beamlines are hybrid designs featuring both NIM and soft X-ray design aspects in order to cover both the VUV and soft X-ray photon energy ranges.

3.1. Prior to the mid-1980s

Soft X-ray beamline designs during the time period from the beginning of synchrotron-radiation (SR) usage to the mid-1980s, known as the first generation, generally fall into three general types.

3.1.1. Beamlines based on toroidal grating monochromators (TGMs). The toroidal grating monochromator (TGM) design (Lepere, 1975) takes advantage of the combined dispersion and focusing provided by the toroidal grating to yield a simple optical layout: just the toroidal grating is located between the source (usually the entrance slit) and image (usually the exit slit). Optical matching of the synchrotron-radiation source to the TGM entrance slit and of the image at the TGM exit slit to the sample position is usually provided by toroidal or ellipsoidal mirrors.

The advantages of the TGM design are (i) optical and operational simplicity and (ii) insensitivity of $E$ and $\Delta E$ to source motion.

The disadvantages of the TGM design are (i) a relatively large $\Delta E$ ($i.e.$ poor resolution) resulting from optical aberrations inherent to the toroidal grating shape, dominated by the astigmatic coma aberration, (ii) energy-dependent focal properties in both the meridional plane (limiting the energy resolution) and the sagittal plane (limiting the sagittal beam size at the exit slit), and (iii) reduced throughput resulting from losses at the exit slit arising from the defocus, astigmatic coma and coma aberrations.

The TGM-based beamline design (see, for example, Stockbauer & Madden, 1982; Himpsel et al., 1984) was a good match to the properties of SR sources of the time, in which the source (the electron beam) position was considerably less stable than subsequent-generation machines. The use of a (stable) entrance slit in the TGM design was therefore a necessary choice to maintain photon-energy stability. This consideration, plus optical and operational simplicity, made TGM-based beamline designs quite popular. Similarly, the achievable figure error of grazing-incidence optics was considerably behind current capabilities and these errors usually dominated the energy resolution, outweighing the contribution of the inherent optical aberrations associated with the toroidal surface shape.

3.1.2. Beamlines based on Rowland-circle spherical grating monochromators (SGMs). Compared with the TGM, the optical design philosophy of the spherical grating monochromator (SGM) is to eliminate the astigmatic coma aberration by having the grating not provide sagittal focusing, thereby improving (reducing) the energy resolution $\Delta E$. Most if not all of the SGMs constructed at SR facilities prior to the mid-1980s utilized spherical gratings in the Rowland-circle design (Rowland, 1883), thereby eliminating aberrations up to spherical aberration (defocus, astigmatic coma and coma are eliminated). This design choice necessitated sagittal focusing using an optic other than the grating; usually this function was integrated into the pre-monochromator collecting and focusing optics. For example, the Grasshopper (Brown et al., 1978) and Extended Range Grasshopper (Hulbert et al., 1983) beamline designs utilized a Kirkpatrick–Baez (KB; Kirkpatrick & Baez, 1948) pair of mirrors to match the source to the SGM entrance slit in the vertical and to the SGM exit slit in the horizontal independently (negligible horizontal–vertical coupling). This, combined with vertical focusing of the dispersed X-rays at the exit slit by the Rowland-circle geometry, results in a stigmatic image at the exit slit to serve as the source for post-monochromator refocusing optics.

The advantages of the SGM design are (i) quite good energy resolution, essentially not being limited by inherent optical aberrations, (ii) faithful line focusing of the SR source onto the SGM entrance slit in the vertical, independent of horizontal angular acceptance, thereby improving throughput (efficiency).

The disadvantages of the SGM design are (i) a larger number of optics (usually one or two more than the TGM design), thus reducing throughput, (ii) increased mechanical complexity in order to maintain the Rowland-circle condition as a function of photon energy and (iii) a fixed grazing angle of incidence on the grating, which is not an optimal match to the energy-dependent diffraction efficiency of soft X-ray gratings.

The nearly aberration-free property of Rowland-circle SGMs was counteracted by (i) the relatively poor figure error of grazing substrates during this era (10 $\mu$rad r.m.s. or greater was typical) and (ii) the relatively short arm lengths of these designs (resulting from mechanical and control limitations). While these factors set limits on the achievable resolution, the Rowland-circle SGM beamlines provided the highest photon energy resolution available from synchrotron beamlines during this time period. A side benefit of the Rowland-circle geometry as implemented in the Grasshopper optical layout was the presence of one deflection mirror that helped to reject high-order diffraction contamination; this filtering is provided more strongly at low photon energies, where it is needed most ($i.e.$ where higher harmonics are the most intense). This feature was absent in the other beamline designs of this time period.

3.1.3. Beamlines based on plane-grating monochromators (PGMs). The design basis of plane-grating monochromators (PGMs) during this era (see, for example, Howells, 1980b; Barth et al., 1983) is to utilize the grating only for dispersion (not focusing), requiring a perfectly collimated input beam and leaving the function of focusing of the output beam to other optical elements. In this geometry, with collimated (zero-divergence) illumination of a plane grating ($R = \rho = \infty$), the optical aberrations vanish, leaving only aberrations from the surface figure error of the grating. The minimum number of optical elements for a PGM beamline is three (one
paraboloidal mirror for collimation, the grating for dispersion and another paraboloidal mirror for focusing), which is comparable to other soft X-ray beamline designs.

The advantages of the collimated-light PGM design are (i) aberration-free optical design (other than aberrations resulting from figure errors) and (ii) elimination of the entrance slit in most implementations, thereby providing higher throughput than beamline designs such as the TGM and SGM described above.

The disadvantages of the PGM design of this era are (i) the figure errors of all three PGM optical elements (mirror, grating, mirror) contribute to the overall energy resolution, and the achievable figure error of paraboloidal mirrors is considerably worse than that of other figure types (especially flats and spheres), and (ii) the omission of an entrance slit means that any vertical motion of the source increases \( \Delta E \) (i.e. reduces the resolving power).

PGM-based beamlines (see, for example, Klaffky et al., 1982) were utilized successfully, especially in the lower end of their photon energy ranges, where the disadvantages listed above were relatively less important. The resolution problems experienced at higher photon energies, those in the heart of the soft X-ray range, led to less utilization of this type of PGM beamline design. A new PGM beamline design that did not suffer from these problems was developed in the early to mid-1980s and is described in the next section.

Howells (1980a) published a summary of the three types of soft X-ray monochromators and beamlines described in this section. The beamlines provided a photon energy resolving power in the range from a few hundred to approximately 1000. The improved designs described in the next section improved the resolving power by approximately a factor of ten.

### 3.2. Mid-1980s and 1990s

The beamline designs developed during the late 1980s and 1990s evolved from the earlier designs to match the improved source properties of second-generation synchrotron sources. These sources were smaller in cross section and more stable than first-generation sources, which opened up opportunities for higher throughput beamline designs.

The beamline designs of this period can be characterized as improved versions of the three types of designs already existing from the earlier era: TGMs, SGMs and PGMs.

#### 3.2.1. Beamlines based on improved toroidal grating monochromators (TGMs)

The principal uncorrected optical aberration plaguing the first-generation TGMs was defocus; the earlier designs typically focused only at two photon energies within the range covered by a given grating. In the late 1980s, beamline designs began to include a movable exit slit that was moved in coordination with the rotation of the grating to maintain focus versus photon energy (Chen et al., 1984). The absence of the defocus aberration over the entire wavelength range covered by a given grating was a major advance. The trade-off of this design was that the moving monochromator exit slit necessarily created a moving vertical source for the final refocusing optics; the benefit of improved resolution was usually found to outweigh the relatively small changes in focal spot at the sample. Not many beamlines of this type were constructed, owing to the emergence of the improved SGM-based beamline design described in Section 3.2.2, which offered considerable advantages compared with the TGM-based design.

#### 3.2.2. Beamlines based on improved spherical grating monochromators (SGMs)

The mechanical and control issues that plagued the Rowland-circle SGMs of the earlier era led to an SGM design that can be thought of as a hybrid between the earlier SGM design and the new TGM design described in Section 3.2.1. In the new SGM design (Chen, 1987; Hogrefe et al., 1986; Hettick & Underwood, 1986; Heimann et al., 1990; Padmore et al., 1998; Smith et al., 1994; Warwick et al., 1995; Song, Ma et al., 2001; Song, Tseng et al., 2001; Song et al., 2006; West, 1998; Lai et al., 2001), the toroidal grating in the movable-exit-slit TGM design described above is replaced with a spherical grating. This change required that horizontal collection and focusing be provided by a separate optical element, usually a first, horizontally focusing mirror, as was the case for the Rowland-circle SGMs described in Section 3.1.2 above. The advantages of the improved SGM design are (i) improved resolution from reduced inherent optical aberrations, with only coma and higher aberrations remaining, (ii) a simple mechanical design, requiring only two motions (rotation of the grating and translation of the exit slit), (iii) the ability to lengthen the SGM entrance and exit arms in order to increase the linear dispersion at the exit slit, thereby improving the resolution (lower \( \Delta E \)) for practically realizable exit-slit openings (as small as ~5 \( \mu \)m), and (iv) if a Kirkpatrick–Baez mirror pair is used for the first optical elements, the throughput advantages of independent vertical and horizontal focusing at the entrance (vertical focus) and exit (vertical and horizontal focus) slits are realized, as was the case for the Rowland-circle SGM design.

The disadvantages of the improved SGM design are the following. (i) The moving exit slit creates a variable source distance for the final focusing optics. The result is that either these optics need to be able to change their focal properties (for example via bending) or the focal spot size at the sample varies with photon energy. (ii) The grazing angle of incidence on the grating is constrained by the diffraction geometry and is not an optimal match to the energy-dependent diffraction efficiency of soft X-ray gratings. These disadvantages apply to TGM designs as well as SGMs.

The advent of the improved PGM designs described in Section 3.2.3 was able to address these disadvantages by providing the freedom to select the angle of incidence on the grating as a design parameter via the addition of another optic (plane mirror) upstream of the grating. Subsequently, it was pointed out that this design solution could also be applied to SGMs (Padmore, 1989), but by this time PGMs had become the dominant optical design choice for synchrotron beamlines.

In addition to the reduced inherent optical aberrations of the SGM design, the grating manufacturers were able to produce improved (lower figure error) gratings during this time period (those with 3 \( \mu \)rad r.m.s. or lower were available}
commercially). Furthermore, high-quality, low figure error, spherical grating substrates were much easier to fabricate compared with toroidal grating substrates. The ability to fabricate superior-quality spherical gratings led to demonstrations by SGM-based beamlines of record energy resolution in the soft X-ray range (Chen & Sette, 1989). These records stood until the 2000s, when the improved PGM designs described in Section 3.2.3 were able to surpass them.

3.2.3. Beamlines based on improved plane-grating monochromators (PGMs). In the late 1970s and early 1980s, Petersen developed a type of PGM, known as the SX700 (Petersen & Baumgärtel, 1980; Petersen, 1982), that was able to address the limitations of the source parameters at that time (relatively large beam size and not very good stability) while using plane gratings, which could be fabricated with higher precision than either spherical or toroidal gratings. The SX700 optical design added a mirror just upstream of the grating which rotated around an axis near the grating rotation axis (Riemer & Torge, 1983) and, owing to the geometrical properties of a plane grating illuminated by divergent light (Murty, 1962), served to create a virtual source that was many times further from the grating than the real source. Having the virtual source located further from the grating led to smaller angular contributions to the SX700 PGM resolution from either a larger source size or, equivalently, from an unstable vertical source position. This advantage was accompanied by a geometrical constraint: in order to maintain a fixed virtual source position, the SX700 design required that the ratio be held constant. Later variants of the SX700, described below, collimated the light incident on the grating in order to be relieved of this constraint. The divergent illumination of the grating in the SX700 design imposed the requirement to focus the dispersed light onto the monochromator exit slit. In the original SX700 design (Petersen & Baumgärtel, 1980; Petersen, 1982) this focusing was provided by an ellipsoidal mirror located downstream of the grating. This mirror also focused in the horizontal plane at a point downstream of the vertical focus since the distance from the virtual source to the grating is many times greater in the vertical plane than in the horizontal plane. The trade-offs resulting from the inclusion of a mirror as a resolution-determining optic are described below. A number of SX700-type beamline designs were proposed; see, for example, Jark et al. (1983) and Brown & Hulbert (1984). A variant of the SX700 in which the focusing mirror is a plane elliptical mirror focusing only in the vertical was proposed by Nyholm et al. (1986).

The advantages of the SX700 PGM design are (i) no defocus, reduced astigmatic coma and partial removal of coma aberration (Murty, 1962), (ii) a smaller source-size contribution to resolution, (iii) the use of superior (lowest) figure error plane gratings and (iv) maintaining focus at a fixed exit slit (via a vertical focusing mirror downstream of the grating), providing a fixed effective source for downstream focusing optics. The other advantages of the improved SGM design described above also apply to the SX700, including the long entrance and exit arm lengths to improve linear dispersion and the possibility of separating horizontal and vertical focusing to minimize image distortion and maximize throughput. Another advantage of the mirror–grating combination in the SX700 PGM design is the ability to cover a large photon energy range (approximately a factor of ten in wavelength) with a single grating. This advantage is particularly important for spectroscopy beamlines, for which the ability to cover a large photon energy range, for example from just below to far above a particular absorption edge, or to measure multiple absorption edges without switching gratings is important.

The disadvantages of the SX700 PGM design include the following. (i) A vertical focusing mirror is required downstream of the grating to focus vertically at the exit slit. Figure errors in the surface of this mirror are resolution-determining, in a similar way to the earlier PGMs described in Section 3.1.3. In the SX700 case an elliptical figure was needed [point-to-point focusing in the diffraction (vertical) plane], but ellipsoidal mirrors could not be fabricated with low figure error in this time period (~10 µrad r.m.s. was the best meridional surface figure error achievable for ellipsoids), thereby limiting the achievable energy resolution; in addition, this mirror needed to provide greatly different magnification in the vertical and horizontal planes, owing to the virtual source in the vertical plane being much further from the grating than the real horizontal source. (ii) The dual-rotation mirror-grating mechanism in the SX700 PGM is relatively mechanically complex compared with the single grating rotation required by TGMs and SGMs; however, this incremental engineering challenge was addressed successfully by the manufacturers. (iii) The SX700 PGM design includes two extra (compared with the SGM and TGM designs) reflections within the monochromator: the plane mirror upstream of the grating and a vertical focusing mirror downstream of the grating, which costs flux (efficiency).

In 1989–1990, an improvement to the original SX700 design in which the in-monochromator elliptical mirror was replaced with a lower-figure-error spherical mirror was proposed (Padmore, 1989; Reininger & Saile, 1990). Another version (Calcott et al., 1992) used a translating plane mirror downstream of the grating. Later, in the 1990s, Follath & Senf (1997) published a breakthrough variant of the SX700 design in which the grating is illuminated by a horizontally deflecting/focusing toroidal mirror which collimated sagittally (vertically, the diffraction plane) and the diffracted light, which is necessarily also vertically collimated, is focused vertically at the exit slit by a horizontally deflecting sagittally focusing cylindrical mirror. The sagittal collimating and focusing geometries of these two mirrors significantly reduced the effect of mirror surface-slope errors via the so-called forgiveness factor (DiGennaro et al., 1988; de Castro & Reininger, 1991; Shi et al., 2014). It is worth noting that the collimated-light SX700-type PGM was a hybrid of the earlier PGM designs (Howells, 1980b) and the Petersen SX700 design (Petersen, 1982), with an overall performance that exceeded any other designs of this time period. In addition to the advantages of the SX700 design listed above, the Follath/Senf improved version provided the ability, within geometrical constraints, to adjust the angle of incidence on the grating as a
function of photon energy, thereby enabling the grating to operate close to its greatest diffraction efficiency in the first order and, thereby, with less higher order contamination.

The beamline designs described in this section provided photon-energy resolving power in the range from a few thousand to approximately 10 000. For a review of VLS PGM design principles, see Underwood (1998). The improved designs described in the next section improved the resolving power by another factor of ~10.

3.3. 2000s and 2010s

The time period since 2000 coincides roughly with the third generation of synchrotron storage rings, which provided significantly smaller emittance than second-generation sources and were designed to optimize insertion-device sources (undulators and wigglers). This generation of synchrotron sources produce much brighter photon beams, achieving nearly diffraction-limited performance in the soft X-ray range and below.

During the 2000s and 2010s, soft X-ray monochromator design has coalesced around the plane-grating designs, as will be described below. There are some exceptions, however; one of these is a variant of the SGM in which the radius of the grating can be changed using a bendable grating substrate, referred to as an adaptive grating. Being able to adjust the grating radius to the ideal value at each photon energy serves to minimize both the defect and coma aberrations at a fixed exit-slit position, thereby mitigating the disadvantages of the SGM design described in Section 3.2.2. Development of adaptive gratings was performed successfully at the Taiwan Photon Source and applied to a soft X-ray beamline that features adaptive gratings in both the monochromator (an adaptive grating monochromator; AGM) and in a matched emission spectrometer (an adaptive grating spectrometer; AGS) (Lai et al., 2014).

The majority of soft X-ray beamlines developed in the last decade or so have been based on plane-grating monochromators of the SX700 design and the improved variants of this design which have evolved during this time period. The remainder of this section is devoted to a description of these PGM-based beamlines.

3.3.1. Variable-line-spacing plane-grating monochromators (VLS-PGMs).

As early as the mid- to late 1980s, Harada proposed a variant of the SX700 that used variable-line-space (VLS) gratings to provide in-monochromator vertical focusing instead of a mirror (Harada et al., 1986; Harada, 1990). A beamline based on this optical concept was developed at the Photon Factory, using a cam mechanism to adjust the angle of the plane mirror upstream of the grating instead of the patented Riemer–Torge mechanism (Riemer & Torge, 1983). This beamline design is the earliest variant of what is called the VLS-PGM. Another VLS-PGM design variant replaces the plane mirror upstream of the grating with a spherical mirror to provide converging light on the VLS grating, rather than diverging light when a plane mirror is used (Hettrick et al., 1988; Amemiya et al., 1996; Hu et al., 2007).

In the early 2000s, Reininger & de Castro (2005) developed a VLS-PGM design that combined the advantages of the SX700 mirror/mechanical arrangement (Riemer & Torge, 1983) and the vertical diffraction plus focusing of VLS gratings to create a VLS-PGM design that forms the basis of almost all soft X-ray beamlines constructed since that time. This development, the focusing VLS-PGM (FVLS-PGM), thereby represents a gamechanger in the history of soft X-ray beamline development. The FVLS-PGM design evolved from all of the earlier SX700-based designs and took advantage of the relatively well developed technology for fabricating VLS-grating rulings. By not needing to include mirror(s) to provide vertical focusing, the FVLS-PGM design is able to include a horizontal focusing mirror that acts only in the horizontal plane and, owing to the so-called forgiveness factor (DiGennaro et al., 1988; de Castro & Reininger, 1991; Shi et al., 2014), does not degrade optical performance in the vertical plane.

The advantages of the FVLS-PGM design over earlier SX700-type PGMs include (i) higher throughput via saving one mirror reflection and (ii) the ability to change the location of the vertical focus over a significant distance (of the order of metres) via programming of the available parameters. The second advantage is useful in two ways. (i) By adjusting the available parameters, the diffracted beam can be focused vertically over a significant range of distances along the axis of the diffracted beam. This feature can be used to focus vertically at multiple exit-slit positions along this axis, which can be used to serve multiple endstations without introducing extra optics. (ii) This design can compensate for unwanted thermal distortions of optical surfaces, principally of the grating and upstream mirror(s); these distortions are typically spherical over the optical footprint and can be compensated by suitable adjustment of available parameters, thereby maintaining vertical focus at the exit slit (Reininger et al., 2008).

3.3.2. Performance of beamlines based on VLS-PGMs.

A large number of beamlines based on VLS-PGM and FVLS-PGM monochromators have been constructed and put into operation since the early 2000s at synchrotron facilities worldwide, including PETRA III/DESY (Viehhaus et al., 2013), ESRF (Brookes et al., 2018), Shanghai Light Source (Xue et al., 2014; Gong et al., 2016), Canadian Light Source (Hu et al., 2007), Synchrotron Radiation Center, Wisconsin, USA (Severson et al., 2011), ALS/LBNL (Warwick & Reininger, 2010; Shapiro et al., 2013), APS/ANL (McChesney et al., 2014) and NSLS-II/BNL (Reininger et al., 2010, 2011, 2012; Reininger, 2011; Jarrige et al., 2018).

For illustration purposes, the VLS-PGM implementation at the Electron Spectro-Microscopy (ESM) beamline (21-ID) at NSLS-II, Brookhaven National Laboratory will be described here.

3.3.3. ESM beamline optical design.

The optical layout of the ESM beamline (Reininger et al., 2012) is shown in Fig. 3. The elliptically polarized undulator source is first deflected horizontally by a plane mirror (M1) that is internally water-cooled to absorb unwanted source power, primarily in the hard X-ray portion of the source-power spectrum that is
outside the soft X-ray energy range covered by ESM. The next optical element is the FVLS-PGM, which consists of a vertically deflecting (upward) plane pre-mirror (M2) followed by one of three selectable vertically deflecting (downward) diffraction gratings (G). As described in Section 3.3, focusing in the dispersion (vertical) plane at the vertical slit (‘v. slt.’ in the side view shown in Fig. 3) is provided by the varied-line-space gratings (DiGennaro et al., 1988; de Castro & Reininger, 1991; Shi et al., 2014).

The monochromatic beam emerging from the vertical/horizontal slits is further demagnified in both the vertical and horizontal planes by a KB pair (Kirkpatrick & Baez, 1948) of elliptical cylinder mirrors (M4A and M4B) which form a stigmatic focus at the sample position. The two-stage demagnification, in both the vertical and horizontal planes, provided by the ESM optical design is able to produce a considerably smaller spot size at the sample location than could be provided by a single-stage design. Other variants of the focusing FVLS-PGM beamline design optimize other quantities such as coherent flux (the CSX beamline at NSLS-II; Reininger et al., 2010) and energy resolution (Dreamline at SSRF; Xue et al., 2014; Gong et al., 2016). The soft resonant inelastic X-ray scattering (RIXS) FVLS-PGM beamline (SIX; Jarrige et al., 2018) at NSLS-II, in its quest for superior overall energy resolution (beamline plus spectrometer), optimizes both energy resolution and spot size, since the vertical spot on the sample forms the source for the RIXS emission spectrometer and a small spot size is needed for high energy resolution spectrometer performance.

3.3.4. ESM beamline calculated energy resolution, flux and focused spot size. The energy resolution and flux calculated for the four gratings in the ESM beamline are shown in Fig. 4 in overlapping photon-energy ranges covering 10–1000 eV. The energy resolving power ($E / \Delta E$) is in the $2 \times 10^3$ range. Flux values (lower panel in Fig. 4) range from $10^{11}$ to $10^{13}$ photons s$^{-1}$ at the resolution values shown in the middle panel of Fig. 4. These flux values are some of the highest delivered by SR beamlines; in the typical units of flux per 0.1% bandwidth (i.e. $E / \Delta E = 10^3$), the flux values shown in Fig. 4 are in the $10^{12}$–$10^{14}$ photons s$^{-1}$ range.

The calculated focused spot size at the sample in the $\mu$ARPES endstation is of the order of 1 $\mu$m (horizontal) $\times$ 1 $\mu$m (vertical), with 1$\sigma$ values in the 0.2–0.4 $\mu$m range, depending on photon energy and resolution.

3.3.5. ESM beamline measured energy resolution, flux and focused spot size. The measured energy resolution and flux of the ESM beamline are in good agreement with the calculated values described above. Two measured energy resolution

![Figure 3](image.png)

**Figure 3**
Schematic optical layout of the FVLS-PGM beamline named ESM (Electron Spectro-Microscopy) located at sector 21-ID of the NSLS-II synchrotron facility at Brookhaven National Laboratory. Plan (top) and side (elevation) views are shown. PM, plane mirror. Elp. Cyl., elliptical cylinder; h. defl., horizontal deflection; v. slt., vertical slit; h. slt., horizontal slit; v. f., vertical focus; h. f., horizontal focus. Reproduced from Reininger et al. (2012), with the permission of AIP Publishing.
values are shown by the symbols in Fig. 4: the measurement at ~65 eV is described below and in Fig. 5, while the measurement at ~400 eV has been extracted from N K-edge absorption measurements of N₂ gas. These measurements, as yet unpublished, were provided by E. Vescovo, K. Kaznatcheev, Y. Zhu and the rest of the ESM team at NSLS-II, Brookhaven.

An example measurement of ESM photon energy resolution is provided in Fig. 5, which displays the measured He(2p, nd) double-excitation Rydberg absorption series of helium gas at ~65 eV photon energy. Taken using the 800 lines mm⁻¹ grating, the extracted instrumental resolution, ~1.35 meV FWHM, is in good agreement with the calculated value shown in Fig. 4 and is well described by wavefront-propagation simulations (Canestrari et al., 2014).

The best (smallest) focused spot size measured at the ESM µARPES endstation to date is ~4 × 4 µm, compared with the calculated value of ~1 × 1 µm. It is clear that vibration is a major cause of the discrepancy between the calculated and measured values; as of early 2020, efforts to achieve the target spot size are ongoing.

3.4. Evolution of soft X-ray beamline performance

3.4.1. Evolution of photon energy resolution. The VLS-PGM design described in this section provides photon-energy resolving power in the multiple tens of thousands range, pushing upwards towards 100 000. This capability represents a factor of ~10² increase in resolving power since the early days of SR beamlines described in Section 3.1.

3.4.2. Evolution of soft X-ray beamline focused spot size. The focused beam-spot size on the sample has decreased by at least three orders of magnitude since the early days of synchrotron beamlines, from ~1 mm in the 1980s to ~1 µm today. Credit for this improvement goes both to large reductions in source phase space (i.e. much brighter sources) and to the improvements in optic figure error and overall source and beamline stability that were required to maintain (i.e. not destroy) this phase space.

3.4.3. Evolution of soft X-ray beamline flux. Photon flux values on the sample have increased steadily over the history of SR sources. In the early days, soft X-ray beamline flux values were in the 10¹⁰ photons s⁻¹ per 0.1% bandwidth range, compared with 10¹³ photons s⁻¹ per 0.1% bandwidth or higher today. These increases are due only mildly to increases in electron beam current (factors of 2–5). The principal drivers of the dramatic increases in beamline flux during these 50 years were (i) the introduction of undulator sources, which defined the onset of the second generation of synchrotron sources, and (ii) improvements in optical efficiency resulting from improvements in optical quality (mirrors and gratings). The high brightness (small phase space volume) of undulator sources has reduced flux losses associated with overfilling of optics and, similarly, has reduced the impact of optical aberrations, which depend on a power series in the angular divergence of the beam (see equation 7). Improvements in the surface figure of beamline optical elements have also led to significant reductions in optical aberrations; in addition, the more ideal photon beams suffer fewer losses at apertures and slits. The combined impact of the factors described here have improved flux values on the samples in beamline endstations by 2–3 orders of magnitude compared with the first-generation synchrotron facilities.

3.5. Thermal considerations

Synchrotron source power, even that produced by the earliest-generation sources, is sufficient to distort materials that intercept the beam, and thermal management is required to minimize unwanted thermal distortions and/or movements. Soft X-ray mirrors typically experience higher thermal engineering issues than hard X-ray beamlines because the typical grazing angle of incidence on mirrors used in the soft X-ray range is an order of magnitude larger than that of hard X-ray mirrors, owing to the energy-dependent dielectric properties of any mirror substrate material. The situation is reversed for dispersing elements, with the crystals used in hard X-ray beamlines generally operated at much larger grazing angles than those used for gratings in soft X-ray beamlines.

In the early days of SR facilities, the source-power values were relatively low and beamline performance was limited by many factors, such as poor optical surface figures, in addition to thermally induced problems. In these early days (see Section 3.1) most beamlines did not actively cool the optical elements, instead choosing low-thermal-expansion materials such as Zerodur (Viens, 1990). That is, the first mirrors in these beamlines became rather warm, but did not distort to the...
point of breakage (usually) and the optics, their holders, and their supports and vacuum chambers eventually reached some sort of thermal equilibrium.

As sources became more powerful and concentrated that power into narrower angular beams (see Section 3.2), the need to actively cool the beamline optical elements grew dramatically. At the same time, the figure quality of these optics improved, setting tighter requirements on thermally induced distortions. In addition, the mirror substrate material of choice became single-crystal silicon owing to its superior achievable surface figure and finish performance. Silicon is a better thermal material than glass, with the relevant metric (ratio of thermal conductivity to thermal expansion) for silicon being many times greater than for glass materials. The thermal properties of silicon also readily lend themselves to benefiting from active cooling to limit temperature changes and, thereby, to limit thermal expansion. Therefore, this period of synchrotron history (1980s and 1990s) saw the advent of water-cooled silicon mirrors using either indirect (Khounsary et al., 1998) or direct (DiGennaro et al., 1988) schemes in most beamline designs. Later, the power density levels absorbed by gratings grew to values that also needed to be actively cooled (DiGennaro & Swain, 1990).

The current generation of synchrotron sources (see Section 3.3) are bright enough to generate nearly diffraction-limited soft X-ray beams. To preserve the exquisite properties of these sources, the design goal of the latest generation of soft X-ray beamlines is to maintain an aberration-free (as much as possible) wavefront shape as the beam propagates down the beamline and is focused and dispersed by the beamline optics (mirrors and gratings in the soft X-ray case). This requirement contrasts strongly with the those of earlier, less bright, sources, which were relatively tolerant to figure errors in the horizontal plane owing to the relatively large source size in that plane. Put another way, the current and future synchrotron sources are generating closer and closer to round beams, thereby demanding optical perfection in the horizontal as well as vertical planes. The goal of maintaining diffraction-limited beam quality along the entire length of the beamline places extremely tight requirements on thermal management of these optics. Direct water-cooling schemes are giving way in many cases to cryogenic cooling schemes (Freund et al., 1990), either indirect or direct. Even the best thermal engineering performance achievable today is not sufficient to avoid distortion of the wavefront of the beam incident on the sample beyond the diffraction-limited performance that is desired. Unless or until thermal engineering improvements can be devised, the principal mitigating measures are measurement of the wavefront downstream of optical elements (Mercère et al., 2010) and adaptive optics feedback schemes that utilize measured surface-distortion data to correct the optical surface figure (Mimura et al., 2011).

4. Conclusion

The designs and performance of soft X-ray synchrotron beamlines over the past 40+ years has improved dramatically, staying in step with improvements in source properties over this period. As a result, the energy resolution has improved by approximately two orders of magnitude and the flux and spot size on the sample have improved by approximately three orders of magnitude. Combined with the improved mechanical stability required to generate and maintain this improved performance and the wide energy coverage possible without changing configurations, synchrotron beamlines are ideal sources to perform state-of-the-art absorption spectroscopic techniques.

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