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Optimization strategies for XUV monochromators

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The techniques of monochromator optimization are reviewed, and it is shown that until recently only a few of the available parameters were used at the same time. Efficient optimization can be performed numerically. The computation method developed at LURE is explained and an example is given. Extension and development of the method are outlined.

Keywords: XUV; monochromators; monochromator optimization.

1. Introduction

As for any optical instrument, the performances of XUV monochromators depend on two factors, the quality of the optical design itself in terms of reduction of aberrations and diffraction limit when applicable, and the quality of realization. This last term is not always under the control of the designer, because the extreme conditions under which these instruments have to work always require the manufacturing and construction limits to be pushed forward. However, in this paper, without neglecting this last aspect, we will concentrate on optical optimization. First we will show that tolerances in terms of slope errors can be included in the computation. Second, there has been so much progress in the manufacturing accuracy of synchrotron optics and in their control during recent years, that one can expect that the 0.5 µrad slope-error level, which yesterday was only dreamed of, will be tomorrow routinely achieved or even surpassed.

For this accuracy reason and also for throughput, one of the constraints of short-wavelength optical design is to minimize the number of elements. The designer has therefore only a few free parameters at his disposal, and should not waste them. It is enlightening to look at the evolution of the concepts and see that progressively these parameters are more efficiently used and for more useful tasks. This naturally leads to the concept of global optimization in the numerical sense, on which the optics group of LURE has been working in recent years, mainly for PGMs (plane-grating monochromators) and fixed-deviation monochromators. We will describe how numerical optimization was implemented and give an example of a monochromator. We will then attempt to prospect for new degrees of freedom which could extend the possibilities of the method.

2. Review of monochromators designs and concepts

The first XUV monochromators used with synchrotron radiation were derived from VUV and therefore based on spherical gratings on the Rowland circle. Due to the grazing incidence, they suffered from astigmatism and from defocusing along an energy scan, an effect we will hereafter refer to as axial chromatism, and their aperture collection was quite small.

2.1. *Stigmatic monochromators*

The first improvement was soon made by the TGM (toroidal-grating monochromator), a simple one-surface fixed-deviation monochromator. In 1975, Lepère showed how, by drawing an holographic grating on a toroidal surface, one could correct most of the above problems (Lepère, 1975). For a fixed-deviation grating the chromatic defocus almost follows a second-degree variation law *versus* wavelength. When the grating is drawn with a linear variation of line spacing it gives the grating a small convergence which linearly varies with wavelength. Compensation, though not perfect, can be quite significant. In the same way a quadratic variation of spacing compensates for coma. Astigmatism was also corrected. Later on, the correction of grating aberrations with a variation of groove spacing became popular under the name of VLS (varied-line-spacing) gratings. But the fundamental ideas are already there in Lepère's 1975 paper. The only difference between ruled VLS and holographic gratings might be a wider range of variation; however, nearly all VLS can be made holographically with non-stigmatic wavefronts (Amemiya *et al.*, 1996).

Besides the optical quality of the toroidal surface, the main problem with the TGM is the radius of curvature of the grating. To avoid all chromatism there is one solution – to use a plane grating in parallel light, *i.e.* between two collimating mirrors. It is simpler, however, to use the grating in diverging light. Petersen and co-workers (Willmann *et al.*, 1991) showed that there is a simple relation to satisfy between incidence angle α and emergence angle β in order to keep a constant image distance, namely

$$\cos^2\alpha - c\cos^2\beta = 0, \tag{1}$$

where c is the ratio of the distances from the grating to the virtual image and to the object. By combining this focus condition with the grating equation, a special scanning law is found which associates a grating rotation and a variation of the included angle. This is the principle of the SX700 PGM. In order to keep a fixed-exit direction, the variable included angle is compensated by a flat mirror with no other optical role (a spherical mirror cannot do the job). There is also some uncompensated coma which limits the collection aperture (0.2 mrad for 10^4 resolution). As a real image of the entrance slit is required, refocusing on the exit slit has to be performed without adding aberrations. In the original monochromator a coma-free image was made with an elliptical mirror, but any optics in a coma-free condition, like a torus or at a magnification of unity, can be used. It should be noted that the astigmatism coming from the grating was not compensated in the first design and produced a small focal line slightly curved by the ellipsoid sagittal radius. This compensation was performed later (Jark, 1992). Later on, Padmore (1989) extended the zero defocus scanning law of the SX700 to gratings having a curvature along the dispersion direction. Still considering the plane grating in slightly diverging light, but at a fixed included angle, it can be observed that the axial chromatism [equation (1)], though not suppressed, can be made almost linear *versus* wavelength for an equal arm length ratio c = 1. Then, as was performed in the TGM, a holographic grating cancels the linear chromatic term, and the first remaining term, of third degree of the wavelength, is small enough that the image of the entrance slit is almost fixed in a large wavelength range. The coma is also compensated by the spacing variation and, in the original holographic PGM design of P. Thiry (unpublished), astigmatism was completely suppressed by a particular choice of the hologram construction points. A toroidal mirror at a magnification of unity was used to image the entrance slit on the exit slit.

2.2. *Astigmatic monochromators*

A new generation of monochromators was initiated by Chen with the SGM design (spherical-grating monochromator) he named DRAGON (Chen, 1987; Chen & Sette, 1989). Chen started from the point that most of the previous designs suffered more from surface defects of the optical elements (mainly from the aspheres) than from aberrations. Therefore he advised the use of the only surfaces that can be manufactured at the highest optical quality, namely flats and spheres, and the use of the minimum number of them. Chen also remarked that a complete (two-dimensional) stigmatism is not required for a monochromator. A one-dimensional stigmatism only is required in the grating dispersion plane. Of course, a point image of the source at the sample position is desirable but it can be performed with optical elements outside the monochromator slits. Also, large spheres in grazing incidence can be considered as quasi cylindrical, which means that optical calculations also can be performed in the vertical plane (two-dimensional computations).

These ideas lead to a very simple and efficient design: one spherical grating in fixed deviation. The radius is chosen to cancel the coma in the centre of the spectral range. Axial chromatism is not compensated and one slit is translated to track the focus condition. As it is oriented to minimize surface-error effects, the design still achieves its best performances at higher energy in the soft X-ray region.

Following this demonstration, most of the designs of the previous generation were converted into astigmatic designs simply by changing the aspherical internal surface for a sphere, improving their resolution. This was also performed on LURE holographic PGMs and we were able to attain the 6000–8000 limit expected from computations.

3. Optimization

The monochromators of these two first generations are characterized by the fact that the grating is computed first, in order to fulfil prescribed criteria on chromatism and aberrations at chosen wavelengths. Then, if required, a focusing element is added in such a way that it does not change the aberration budget. The result is then checked by ray tracing and spot diagrams. If needed, the criteria are modified and the procedure iterated.

The procedure is time consuming. One can expect a computer to be better and quicker. Moreover, there is no reason to restrict computation to the grating alone; mirror parameters and slit distances are useful extra degrees of freedom for the optimization. Though common in conventional optical design, optimization procedures have been only recently described for grazing-incidence monochromators. While McKinney and co-workers simply proposed to evaluate the width of the geometric image from discrete ray traces (Wheeler *et al.*, 1996), we have elaborated an optimization procedure which is completely deterministic and hence robust (Delcamp *et al.*, 1996). Let us briefly outline its principles.

3.1. *Merit function*

Optimization first requires one to define a merit function to be minimized. It has to be related to the spectral bandwidth or to the monochromatic point spread function (PSF) to which it is linked by dispersion. This PSF is the result of several factors: aberrations of course, slit widths, slope errors and diffraction widening. In the first approach, the r.m.s. width of the PSF seems like a good criterion. It is true when the PSF is defined by geometric effects, but one should mind that the r.m.s. width of a diffraction-defined PSF is not finite (a reason for using the Rayleigh criterion). However, in the present case we want to optimize the design geometry and it is reasonable to take care of aberrations only and use the aberration-limited PSF. This choice will be discussed later. In practice, the resolution has to be optimized for a range of wavelengths. The actual merit function is the mean value in the wanted spectral range of the relative r.m.s. bandwidth as

$$F(\text{parameters}) = \int_{\lambda_2}^{\lambda_1} \langle y^2 \rangle \frac{\mathrm{d}\lambda}{\mathrm{d}y} \frac{1}{\lambda}\, \mathrm{d}\lambda. \qquad (2)$$

3.2. *Computation method*

Quite generally, any ray from a pencil of light can be deduced from a generating function known as the eikonal. When the pencil is issued from one point, the eikonal simply reduces to the wavefront. Close to an image, the transverse displacement of a ray with respect to its ideal position is simply related to the optical path difference (OPD), Δ, between the real wavefront and the ideal one (*i.e.* a sphere centred on the ideal image) as

$$y = \mathrm{d}\Delta(u)/\mathrm{d}u, \qquad (3)$$

where u is the image aperture angle. As with grazing-incidence optics, aperture angles are always small, the OPD can always be approximated by a polynomial of low degree. Moreover, taking into account the lessons learned from DRAGON, we know that we can reduce the problem to cylindrical optics. Δ is thus a fourth-order polynomial of a single variable. Then, taking into account the intensity distribution of radiation, $I(u)$, on the optics, the r.m.s. width of the PSF is computed as

$$\langle y^2 \rangle = \int \frac{I(u)}{I_0} \left(\frac{\mathrm{d}\Delta}{\mathrm{d}u} \right)^2 \mathrm{d}u. \qquad (4)$$

The parameters which define a monochromator are few. Some of them can be reasonably selected at the same time by a designer for optimization, while the others are kept fixed. Therefore, any good method of minimization converges rapidly.

3.3. *Example of optimization*

As an example we give the results of a computation of a PGM which has been optimized by the above-described method, for the SU8 beamline of Super-ACO (Delcamp *et al.*, 1997). It is, for slope-error reasons, a two-surfaces monochromator with fixed slits. The plane grating is holographic and we compute directly the construction parameters rather than the VLS parameters. It is used in fixed-deviation conditions and slit-to-slit focusing is made by a spherical mirror. There are six gratings to cover the range from 15 to 900 eV, which are grouped by pairs working at the same included angle. Therefore, there are in fact three spherical mirrors of different radii, one for each included angle ($D/2$ = 80, 85, 87°).

Fig. 1 presents the aberration-limited resolution as it comes out of the optimization computations, while Fig. 2 takes into account a 10 μm slit width and 1 μrad r.m.s. slope errors on each surface. The aperture angle, indicated on the figures, differs from one grating to another in such a way that resolution is not limited by diffraction effects. It is obvious from Fig. 2 that slope errors of the surfaces are the main resolution-limiting factor in the high-energy range, while at low energy the aberrations still play a significant role in limiting the grating tuning range. In optimizing the 87° gratings it has been found useful to increase the line density of 1600 mm^{-1} in order to obtain almost the same resolution as the other grating of the pair. The merit function, however, is lower. This shows the limits of a merit function which does not take into account all the resolution factors. In the same order of ideas, it is not obvious that the relative bandwidth $\delta\lambda/\lambda = \delta E/E$, rather than δE, is the criterion most adapted to the user's demands.

4. Improving the resolution and the grating tuning range

How can resolution be improved? First, it is important to try to produce (and control) optical elements with lower slope errors: 0.5 μrad seems to be an achievable goal for spheres, an even better accuracy could be reached with flats. In any case the high-energy range will remain very sensitive to figure errors, due to the extreme grazing conditions, and will benefit by reducing the number of optical elements. In the low-energy range there is more freedom to improve the resolution by better designs. Actually, a very high resolution can be obtained with most of the designs but in a limited wavelength range because the aberrations increase rapidly apart from the correction wavelength. This behaviour can also be observed for the first gratings of the previously described PGM in Figs. 1 and 2, and it comes from the fact that the chromatic dependence of aberration is not linear with wavelength as that of the hologram.

It has already been mentioned that chromatic effects vanish when a linear plane grating is used in parallel beam, and high theoretical resolution is obtained from fixed-deviation configurations where the grating is preceded and followed by collimating mirrors. However, the slope-error-limited resolution of such a design with tangentially focusing mirrors is usually less than that of a single-focusing-mirror design, because one of the mirrors has to be placed on the low angular dispersion side of the grating. It is questionable whether sagittal focusing could better solve the problem, and at present the attainable level of sagittal slope errors has not been measured or evaluated.

We are missing parameters to progress in the optimization of single-focusing-element monochromators. However, in all the designs we have considered here, one parameter, the included angle, was defined somewhat arbitrarily. Fixed deviation is only a convenience to limit the number of surfaces and scanning movements. The SX 700 law of scanning or others are linked to some *a priori* assumptions on the grating shape. Let us now assume that $\sin\alpha$ has been defined as a power expansion of the wavelength; the coefficients of this expansion can be used as free parameters for the optimization process. The drawback is again an extra mirror, but this mirror is flat and can be put on the same high-dispersion side as the spherical mirror, and an extra movement whose accuracy has to be controlled.

It should not be forgotten that the usable scanning range of a grating is also fundamentally limited by the efficiency curve, which depends on the incidence angle and the groove profile. Attempts to define the scanning law to keep the grating 'on blaze' do not appear satisfactory in terms of resolution, and conflict with the philosophy of keeping a maximum number of degrees of freedom for optimization. However, the efficiency of laminar gratings, which are most commonly used at short wavelengths, is mainly determined by the groove depth. On recent monochromators with astigmatic design, the footprint of radiation on the grating is usually quite narrow, a few mm in width, so that it is rather easy to adapt the groove depth to the wavelength by using a variable-groove-depth (VGD) grating. VGD gratings can be either continuous or stepwise and their production only requires a small change of the etching process of a single grating mask. Efficiency is then adjusted by translating the grating sideways on the interchange slide. Finally, let us recall that the simple efficiency law deduced from the thin-grating model completely fails to predict the cutoff which occurs when one of the angles α or β is almost grazing (Mirone *et al.*, 1998). Slope-error-limited monochromators have their best performances in these extreme cases where exact calculations of efficiency by electromagnetic codes are required.

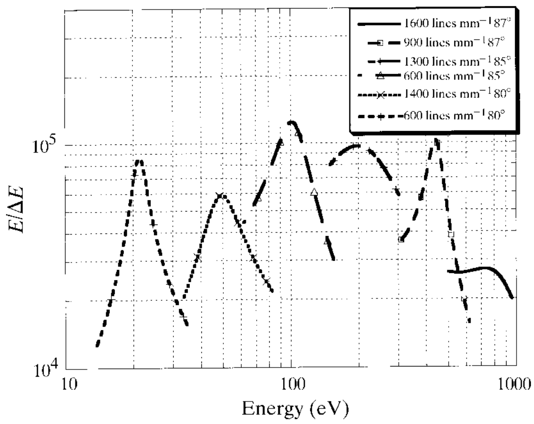

Figure 1
Aberration optimization of the SU8 beamline. The aperture angles are 3 mrad for 600 lines mm^{-1} at 80°, 2 mrad for 1400 lines mm^{-1} at 80°, 1.3 mrad for 600 lines mm^{-1} at 85° and 0.8 mrad for the other gratings.

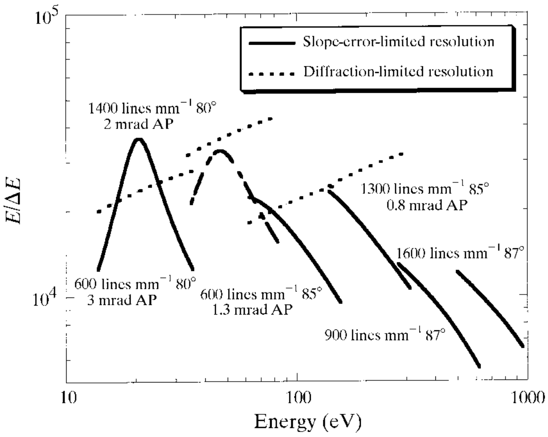

Figure 2
Geometrical resolution of the SU8 monochromator including effects of aberrations, slit width (entrance slit 10 μm, matched exit slit) and slope errors (1 μrad r.m.s. on each optical surface), and diffraction-limited resolution for low-energy gratings (AP is the aperture angle).

5. Conclusions

The design of XUV monochromators must be performed on a small set of free parameters which have to be used as efficiently as possible. It is therefore well suited to a numerical optimization. A merit function based on the width of the geometrically defined PSF, though it could be improved, is well adapted for building an efficient optimization code, and computation stability is achieved by deriving the computation from the wavefront aberrations. VLS-based monochromators can be designed with a high degree of aberration correction. Slope-error reduction will be essential to improve the resolution. Further improvement of monochromator design should be mainly directed to widen the grating tuning range. VGD gratings can preserve a high efficiency on a wide range. More degrees of freedom are required to widen the resolution curve; they could be found in a variable deviation of the grating or in the use of focusing elements on both grating sides.

References

Amemiya, K., Kitajima, Y., Ohta, T. & Ito, K. (1996). *J. Synchrotron Rad.* **3**, 282–288.

Chen, C. T. (1987). *Nucl. Instrum. Methods*, A**256**, 595–604.

Chen, C. T. & Sette, F. (1989). *Rev. Sci. Instrum.* **60**, 1616–1621.

Delcamp, E., Lagarde, B. & Polack, F. (1997). *Proc. SPIE*, **3150**, 48–57.

Delcamp, E., Lagarde, B., Polack, F. & Susini, J. (1996). *Proc. SPIE*, **2856**, 120–128.

Jark, W. (1992). *Rev. Sci. Instrum.* **63**, 1241–1246.

Lepère, D. (1975). *Nouv. Rev. Opt.* **6**, 173.

Mirone, A., Delcamp, E., Idir, M., Cauchon, G., Bizeuil, C., Polack, F. & Dhez, P. (1998). *Appl. Opt.* Accepted.

Padmore, H. A. (1989). *Rev. Sci. Instrum.* **60**, 1608.

Wheeler, B. S., McKinney, W. R., Hossain, Z. & Padmore, H. (1996). *Proc. SPIE*, **2856**, 331.

Willmann, M., Petersen, H., Schäfers, F., Mast, M., Müller, Br. & Gudat, W. (1991). *BESSY Annual Report 1991*, pp. 466–470. BESSY, Berlin, Germany.