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High acceptance high resolution soft X-ray grating spectrometer: Choice of optical design

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ABSTRACT

Elementary excitations in correlated electron systems produce low intensity spectral features that may be observed by resonant inelastic X-ray scattering (RIXS). In the soft X-ray region, ruled gratings are used to obtain optimum energy dispersion. Gratings have to operate at small grazing incidence so that in practice the angular acceptance is small. Schemes have been proposed using varied line spacing plane gratings combined with large focusing mirrors to increase acceptance. Here we analyze the relative performance of spherical and elliptical mirrors by means of numerical calculations of the light path function. We show that the use of an elliptical mirror provides higher resolving power over an extended energy range. Thus the 50–1000 eV energy range can be covered by two gratings only and the resolving power can be adapted to the experimental conditions.

1. Introduction

Synchrotron SOLEIL, the French storage ring, focuses on serving the national scientific community to the highest international standards. In the case of resonant inelastic X-ray scattering (RIXS) there is a demand for state of the art experimental stations both at high energies and in the soft X-ray region. The former will be catered for by a crystal spectrometer at the GALAXIES beamline [1] and the latter by a grating spectrometer AERHA (adjustable energy resolution – high acceptance) at the SEXTANTS beamline [2]. A detailed description of AERHA itself will be presented elsewhere; here we place the emphasis on the reasons which brought us to choose a novel design to fulfill the scientific objectives.

A major part of the soft X-ray RIXS activity is centered on elementary low energy excitations that occur in correlated-electron materials in particular those involving first period transition metals (TM) (see [3] for instance and [4] for a recent review). Vibrational states in gases or liquids are another promising field of research [5]. Mostly, these excitations are in the tenths of an eV range which means that a resolving power better than 5000 is a basic requirement. It is also advantageous to cover the energy range of the TM M edges (3p-3d resonances) where resolution can more easily reach hundredths of an eV [6]. Ideally the instrument should cover 50–1000 eV unless beamline resources can be made available for more than one spectrometer.

The prospect of applying high-resolution RIXS to further classes of material such as nanostructures or buried interfaces implies an additional requirement: the instrument should also provide a large angular aperture and large throughput so as to keep data collection times within manageable limits. In fact this parameter is crucial also for reducing exposure times for fragile samples. Put trivially, even an increase in angular acceptance by a factor of two can halve the exposure time.

The resolving power that can be attained depends to a certain extent on the length of the instrument. High resolution also means mechanical stability of the same order as that of the storage ring itself. Thus permanently allocated space is needed, the dimensions of which will put a limit on the attainable resolution. Another requirement arises from the need to adjust the scattering geometry, especially as it can serve in X-ray magnetic dichroism experiments [7] or q-dependent studies [8] when the parameters of the unit cell allow. Thus the instruments footprint will be given by its length rotated about the entrance slit over the required scattering angle range. In our case, at SEXTANTS, the instrument had to comply with an all inclusive length of 3.5 m over the 45–135° scattering angle range.

To date the highest resolving power has been obtained at the ADRESS beamline at the Swiss Light Source with SAXES [9] and

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further progress is planned [10]. It operates with a varied line spacing spherical grating (VLS-SG) at a small angular aperture. Recently another instrument based on a similar optical scheme and with a comparable resolution has been installed at SPring-8 [11]. The same form of numerical analysis that we use here has fully vindicated this choice [12]. The VLS-SG design is valid if high resolving power is the main objective and if the instrument can be made long enough. A short instrument favors acceptance, given the same size optical elements, but increases aberrations owing to contributions from rays that are further from paraxial.

Recently some designs have adopted the use of a spherical mirror and a VLS plane grating (SM/VLS-PG). The purpose is to separate the focusing and energy dispersing functions as originally proposed by Hettrick and Underwood [13]. The model described by Hague et al. [14] has probably the highest acceptance for a relatively extended energy range. It uses an additional bendable mirror in the non-dispersive plane to increase the collecting angles as proposed by Underwood and Koch [15]. Other instruments (see [16] for instance) operate at low energies only, and do without the additional collecting mirror. There, the acceptance can be favored by using large grazing angles because reflectivity is higher at low energies. In all cases the trade-off between increased acceptance by using large additional optical elements and reduced throughput because of angle-dependent reflectivity must be taken into account.

A preliminary study was made using the ray tracing simulation package SHADOW to see if the SM/VLS-PG scheme described in [14] could be scaled up to meet the required resolving power while maintaining the same angular acceptance. Several difficulties were encountered. In particular it was found that four gratings would be needed to cover the required energy range and fabrication by the holographic method had to be ruled out because of the strongly non linear VLS parameters needed to correct for the concave spherical mirror.

For decades it has been largely accepted that the advantages of elliptical mirrors are counterbalanced by their modest quality in terms of shape definition and surface slope errors. At present, however, several manufacturers master the production of large elliptical surfaces. This is accompanied by progress in metrology able to measure the parameters with sufficient precision and even provide feedback to correct for fabrication defects [17].

It is straightforward to demonstrate the superiority of an elliptically shaped mirror using SHADOW, but it does not provide a straightforward means of comparing performance of a spherical mirror over an extended energy range. Yet it appeared timely to compare EM/VLS-PG and SM/VLS-PG schemes to achieve both high resolving power and high angular acceptance. The only way to approach this is by means of a full numerical analysis of the light-path function so as to obtain a sufficiently accurate representation of what may be attained in each case. In particular it should be noted that closed-form formulas [18] to calculate the VLS parameters cannot be used in the case of large angular apertures because they are valid close to the paraxial ray only. The numerical analysis is described in the next section.

2. Numerical approach

In principle the use of an elliptical concave mirror adds the immediate advantage of point-to-point focusing. Thus there is no need to vary the grating groove density to correct for the optical aberrations as is the case for a spherical mirror. The VLS dependence becomes almost linear and the production of the grating by holographic methods is eased.

It is clear that using mirrors for high angular acceptance is a valid approach provided the mirror can be placed sufficiently close to the source. This simple condition imposes that the mirror exit arm, r'_m, be made substantially longer than the mirror input arm, r_m. This drives the mirror into magnification $M = r'_m/r_m$ greater than one. In the case of spherical mirrors this gives rise to large high order optical aberrations. On the other hand slope errors tend to be larger for elliptical mirrors because of the more complex fabrication technique.

In order to quantify the performance of each type of mirror for large acceptance we calculate the light path function, F, which gives the distance traveled by the light through the system from the source to the detector. The layouts displayed in Fig. 1 share several common features. The light arising from the source S is reflected by a concave mirror to a point V. We denote by M and G the centers of the mirror and grating, respectively. Spherical mirrors deliver an astigmatic image, the tangential focus being described by:

$$\frac{1}{\langle SM\rangle} + \frac{1}{\langle MV\rangle} = \frac{2}{R\sin\varphi}$$

where R is the radius of the spherical mirror and φ is the incidence angle. In the case of an elliptical mirror the surface is defined such that S and V are situated at the foci of the ellipse. Considering an arbitrarily point M' on the mirror surface, we can write:

$$\langle SM\rangle + \langle MV\rangle = \langle SM'\rangle + \langle M'V\rangle$$

In either case the VLS grating in placed in a convergent beam as close as possible to the mirror and is operated in negative (outside) diffraction order ($m = -1$). That is $\alpha < |\beta|$ where the incidence angle measured from the normal to the grating surface is taken to be positive ($\alpha > 0$) and the diffraction angle negative ($\beta < 0$). The choice of negative diffraction order is justified by the ratio between usable lengths of the mirror and grating: to collect all rays reflected by a long mirror, a shorter grating can be used if $\alpha < |\beta|$. The virtual image of the mirror, V, is the effective source of the grating. The ruling density of the grating, $a(w)$, is taken to have a polynomial dependence on the width w with the coefficients a_i: $a(w) = a_0 + a_1(w) + a_2w^2 + a_3w^3 + \cdots$. The groves of the grating serve to diffract the light and to correct the optical aberrations of the concave mirror. The detector is placed at a distance $\langle GD\rangle$ from the grating. We denote the entrance arm of the grating $r = -\langle GV\rangle$ and the grating exit arm $r' = -\langle GD\rangle$. For the optimization of the instruments we adopt the strategy described by Underwood and Koch [14]: r and r' can be chosen independently in such a way that the ratio $-r'/r$ is given by two wavelength/incidence-angle pairs (λ_1, α_1) and (λ_2, α_2) at which the instrument is in focus. This condition delivers [15]:

$$\frac{-r'}{r} = \frac{\lambda_1\cos^2\beta_2 - \lambda_2\cos^2\beta_1}{\lambda_1\cos^2\alpha_2 - \lambda_2\cos^2\alpha_1}$$

The incidence and diffraction angles are linked by the grating equation:

$$\sin\alpha + \sin\beta = a(w)m\lambda$$

The a_i parameters of the VLS dependence are calculated *numerically* by evaluating the optical light path function, F, for all rays contained in the meridional plane.

The central ray is given as $F(0) = \langle SM\rangle + \langle MG\rangle + \langle GD\rangle$. An arbitrary ray hitting the mirror in M' will be reflected and arrive at the grating at $G'(w)$, where the line density is $a(w)$. If the system focuses perfectly, the diffracted ray will reach D on the detector, the corresponding light path function being $F(w) = \langle SM'\rangle + \langle M'G'\rangle + \langle G'D\rangle + n(w)m\lambda$, i.e. a jump of $m\lambda$ triggered by each grove. According to Fermat's principle, a perfect image of the point source S is obtained when F remains constant independently of the light trajectory through the spectrometer. This approach enables the a_i parameters to be calculated for a reference