On the contribution of gratings with laterally graded groove depths to the design and performances of SOLEIL soft X-ray monochromators

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On the contribution of gratings with laterally graded groove depths to the design and performances of SOLEIL soft X-ray monochromators

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Abstract. The so called varied groove depth (VGD) etching technology, developed by Horiba-Jobin-Yvon, which consists in laterally grading the groove depth of a lamellar grating, is exploited in the monochromators of the seven soft x-ray beamlines of SOLEIL. With a VGD profile a single grating can perform in more than a decade wide energy band and some control is given over the harmonic content. It also requires a specific, but easily achieved design of the beamline optics to match the lateral footprint of the beam to the depth variation. Performances predicted by computation with electromagnetic propagation code are supported by flux measurements of the two first harmonics in the experimental chamber of a photoemission beamline, and by measurements of grating efficiencies on SOLEIL etrology beamline.

1. Introduction

Designing a monochromator for a soft x-ray beamline is at trade-off between achievable resolution, flux throughput and simplicity or cost effectiveness. Optical aberrations used to be a limitation to the achievable resolution. Grating with non uniform ruled grating, known as varied line spaced (VLS) gratings, have been for a long time used to apply the required wavefront correction, but the wavelength range in which such a correction is effective greatly depends of the aperture angle sustained by the grating. Nowadays, on an undulator beamline of a low emittance synchrotron source such as SOLEIL, the gap scan mode allows illuminating the grating under a quite small aperture angle, even without collimating. Therefore a simple VLS law easily achieves the aberration correction on a spectral range which can cover more than two decades.

The grating equation defines one relation between grazing angles of incidence α, and emergence β, but the designer is free to define a fix deviation angle $D=\alpha+\beta$, or if preferred, a given C_{ff} factor $C_{ff}=\sin\beta/\sin\alpha$. A constant C_{ff} is the condition for a fix focus with a plane grating in non parallel illumination. The choice of C_{ff} and average line density determines the grating angular dispersion and hence the balance between flux and resolution. However this analysis doesn't take into account that the diffraction efficiency also depends on the angles α and β, and is maximal when the blaze law is fulfilled. In case of a lamellar grating it expresses as $\sin\alpha+\sin\beta= \lambda/2h$, h being the groove depth of the grating, which obviously cannot be satisfied at all wavelengths.

This incompatibility between fix deviation or fix focus scan law and blaze law has been long acknowledged and some attempts were made to etch several tracks with different line depth from the same grating mask on a single substrate [1]. However the manufacturing of such grating was found difficult to control. Therefore, when the SOLEIL project was started, Soleil optics group and the Horiba Jobin-Yvon company, decided to try ion-etching lamellar gratings with a regularly varying depth along the lines from one side of the grating to the other. In reference to the VLS concept, these gratings were called varied grove depth (VGD) gratings. A 600l/mm prototype grating was made, and characterized at LURE SUPER-ACO in 2003 [2]. In view of this first result, all the seven soft x-ray beamlines of SOLEIL have been designed to make use of plane VGD gratings

2. VGD gratings properties

2.1. Design constraints

Some restrictions apply to the grating and monochromator design when a VGD profile is used. First the etch depth range should be limited to a factor about 4 to keep control on the profile duty cycle, i.e. the ratio of the groove width over the period, throughout the masking and etching process. We presently use 40 mm wide gratings which allow usable widths between 30 and 35 mm and so depth variations about 13%/mm. Hence obviously, the grating should be illuminated along a narrow line, the width of which should not exceed 1-2 mm. Soleil soft x-ray beamlines use astigmatic designs with an horizontal focus located nearly 0.5 m upstream or dowstream the grating, in order to limit the power density while keeping the requested small footprint [3]. These gratings are specified with a constant duty cycle over their surface. A target value of c/p=0.55 to 0.6 is typically chosen in order to achieve a proper second harmonic rejection while keeping the first harmonic efficiency near its maximum.

2.2. Expected performances

VGD grating are employed in the three classes of plane grating monochromators (PGM) of SOLEIL: fixed deviation with a spherical in tangential focusing mode (SM-PGM) on TEMPO and SEXTANTS beamlines; double rotation plane grating and plane mirror monochromators (PM-PGM), either in VLS self focusing mode (Cassiopée, Pléiades, Antarès), either with a sagittally refocusing cylinder (Deimos, Hermès)[3,4] . As an example, TEMPO's SM-PGM has 2 interchangeable spherical mirrors for 9 and 5 degrees total deviation. VGD profile allows the same grating being used at the two deviation angles in different energy ranges. The 800 l/mm grating, for instance, is used with a deviation angle of 9 degrees below 300 eV and 5 degrees over 300 eV. Figure 1 shows the maps of diffraction efficiencies of harmonics 1 and the second harmonic content of this 800 l/mm VGD grating, computed with our electromagnetic propagation code CARPEM [5] with the design parameters: groove depth on center line 22 nm, depth variation 0.87 nm/mm, duty cycle 0.6. Diffraction efficiencies are given in gray scale versus photon energy in abscissa and lateral position on the grating in ordinate, in the full spectral range. These maps show that a decent efficiency can be maintained over a wide range of energies and alternately a good harmonic rejection can be ensured at the expense of a moderate flux loss.

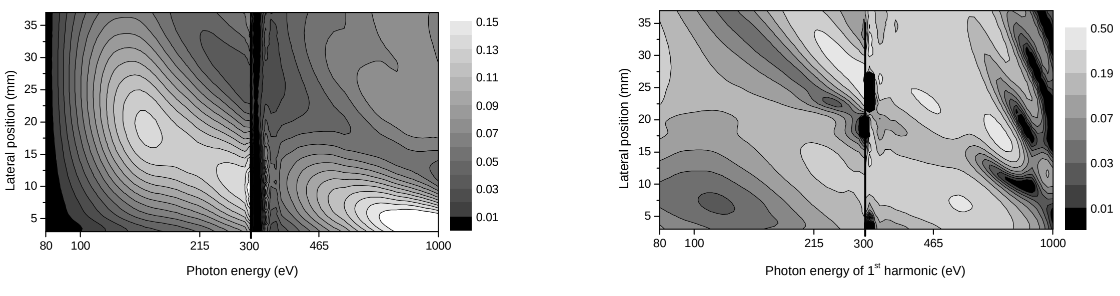

Figure 1. Computed efficiencies of the TEMPO 800l/ mm grating with the design parameters. Left map is the first harmonic efficiency, while right map shows the ratio of second to first harmonic. The grating is used with a fix deviation of 9 degrees below 300 eV and 5 degrees over 300 eV. The groove depth varies from 7.3 nm at 3 mm from the grating side to 36.7 nm at 37 mm.

In VLS self-focused PM-PGMs VGD profiles allow each grating to perform in an extended energy range. In the high dispersion mode (fixed $C_{ff} = 0.2$) the energy range covered by a single grating may exceed a factor 20. In classical sagittal mirror focused PM-PGMs, the C_{ff} factor can be actually varied without loss of efficiency, from 0.05, high dispersion mode to 0.8, low dispersion mode.

3. Characterization

3.1. AFM profile measurements

During and after manufacturing the groove profile is controlled with an AFM. It produces local maps of the groove profiles, typically 10 x 10 μm^2 wide, from which can be extracted the relevant parameters for computer modeling, groove depth, duty cycle, and roughnesses of the high and low lands of the lines. With a careful calibration, the absolute height accuracy is estimated around 0.2 nm. Jobin Yvon engages on ±10% depth uniformity along a longitudinal line and ±15% duty cycle uniformity on the whole surface, but AFM control measurements being rather tedious and risky are seldom made on more than 9 points on the surface by the manufacturer. This is not enough for being representative. On gratings etched in silicon substrates, we sometimes found large changes of profile from uncoated to coated gratings. It was especially noted that for some groove depths, platinum tends to deposit in excess on the edges of the grating lines. For these reasons we like to make our own control on more points whenever possible, but even so local defects may remain unnoticed.

3.2. Characteriztion at the beamline

The Metrology beamline was not available at the time the first soft x-ray beamlines that were mounted at SOLEIL, and therefore the grating efficiencies couldn't be measured beforehand. Characterizing the efficiency of a grating when it is mounted on the monochromator of an undulator beamline is quite difficult because the harmonic spectrum emitted by the undulator is far to be known with the desired accuracy. Throughput curves of the whole beamline can be easily measured but the harmonic content remains uncertain. Fortunately these first beamlines were photoemission beamlines. Electron spectrometry on a known clean metal surface allows separating the contributions of the different harmonics of the beamline since characteristic lines appear at shifted kinetic energies. Hence the flux in different harmonics can be evaluated, in the experimental chamber, within the precision at which photoemision cross sections are known. It gives a useful evaluation of the working position for higher flux or higher harmonic rejection, but cannot be compared to model computation in order to evaluate the quality of grating manufacturing. Figure 2 gives the results of such flux measurements made on the actual 800 l/mm grating of TEMPO in its low energy range (9 deg. deviation). Intensity have been normalized to the measured maximum of first harmonic. The design general trends of figure 1 are properly found, namely the position of the high efficiency ridge of harmonic 1 and the valley of low harmonic 2 content. This validated, at least partially, the VGD concept.

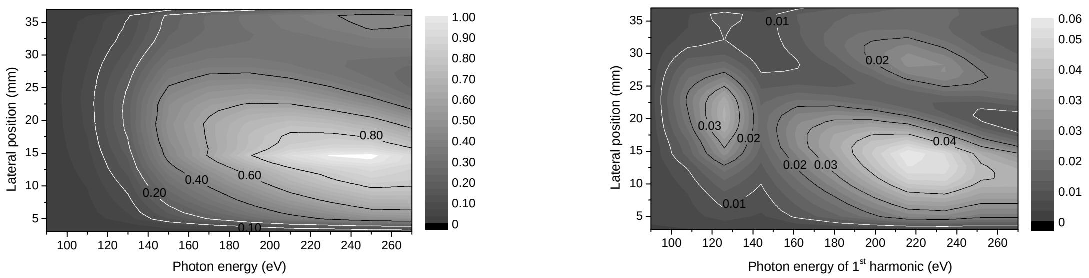

Figure 2. Flux at the experimental station of Tempo with the 800 l/mm grating in the 1st harmonic, left map, and 2nd harmonic right map, measured from photoemission yield. Intensities are normalized to the 1st harmonic maximum. Flux in harmonic 2 is plotted versus the energy of the 1st harmonic These flux maps show similar features but cannot be directly compared to computed efficiency maps of fig 2.

3.3. Diffraction efficiency measuremenst on Metrology beamline

Newly delivered gratings are now measured in the reflectometer of the Metrology beamline. Figure 3 compares the measurements made on a 450 l/mm grating, recently fabricated for Hermès beamline, to simulations with the CARPEM code. This grating has a groove depth varying from 7.5 nm, at -18 mm of the centerline, to 43.5 nm at 18 mm; the duty cycle is close to 0.55. Diffraction efficiencies are measured at incidence and exit angle corresponding to C_{ff}=0.5.in the 90 -800 ev spectral range. The photon energies available at Metrology beamline, which covers most of the 35 eV to1600 eV range, makes the complete measurement of harmonics 1 and 2 possible. The simulations shown together, use the depth and duty cycle measured with SOLEIL AFM as a starting point. Then a slight adjustment of these two parameters is done to best fit with the measured values, and so account for slight non uniformity along the beam footprint. Positions in energy of the maxima of harmonic 1 are most sensitive to the groove depth, while the shape of harmonic2 curves depends more on the duty cycle. A quite close agreement can be found in figure 3 between measured and simulated data.

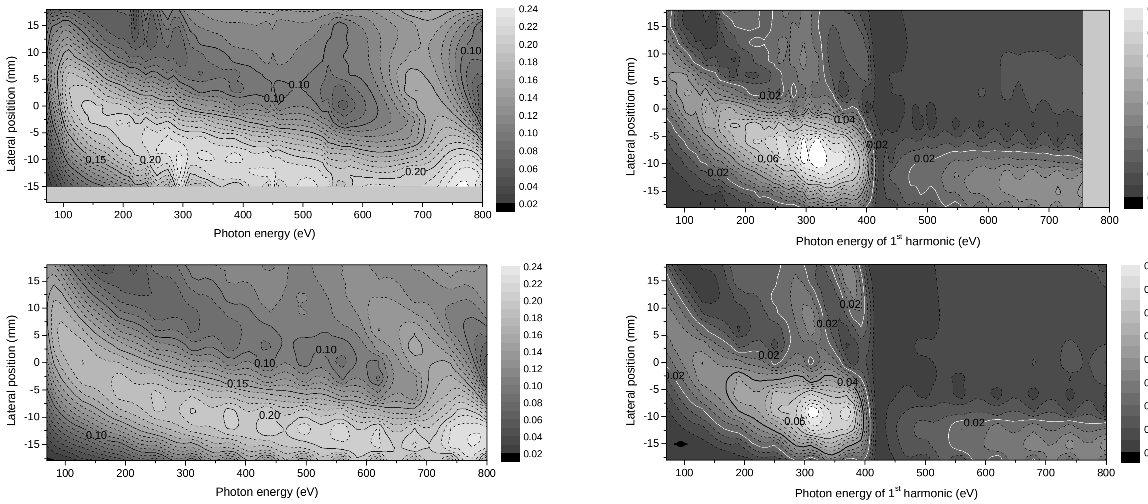

Figure 3. Measured and calculated efficiency maps of Hermès 450l/mm grating at C_{ff}=0.5, for the 1st (left column) and 2nd harmonics (right column). Measured values are in top row, CARPEM computed ones in the bottom row. Uniform grey rectangles are unmeasured areas.

4. Conclusion

The use of VGD gratings in soft x-ray monochromator is validated by the experience of the 6 soft x-ray beamlines presently in operation at SOLEIL, and by measurements. The measured efficiencies are close to calculated values and, as the manufacturing process is maturing, achieved profiles are getting more uniform and closer to the specifications. VGD profiles enable to trade-off between efficiency and harmonic content at almost any energy but mainly widen the working conditions of a single grating, thus reducing the number of gratings per monochromator.

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