

# INFLUENCE OF THE GROOVE CURVATURE ON THE SPECTRAL RESOLUTION IN A VARIED-LINE-SPACING PLANE GRATING MONOCHROMATOR (VLS-PGM)\*

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## Abstract

Diffraction-limited synchrotron radiation (DLSR) light source with smaller source size and emittance makes ultra-high spectral resolution beamline possible. Here, we report an undulator-based beamline optical design with ultra-high spectral resolution using a varied-line-spacing plane grating monochromator (VLS-PGM), which is a well-proven design for achieving ultra-high resolution in the soft X-ray band. A VLS plane grating with a central groove density of 2400 l/mm is utilized to cover the photon energy region of 250 ~ 2000 eV. VLS gratings are generally fabricated using the holographic method, but the resulting grating grooves are two-dimensionally curved curves, which can affect the resolution of the monochromator. To analyse this effect, we first use a spherical wavefront and an aspherical wavefront to generate the fringes and optimized the recording parameters. We also present a method for calculating the grooves curvature of holographic plane VLS grating grooves. Furthermore, the influence of grating grooves curvature on beamline resolution is theoretically analysed based on the aberration theory of concave grating.

## INTRODUCTION

Diffraction limited synchrotron radiation (DLSR) has higher brightness and coherence. How to transmit the light from the storage ring to the experimental station with high quality is a challenge faced by beamline technology. Ultra-high spectral resolution beamlines are possible due to the smaller source size and emittance. The BL10 test beamline of Hefei Advanced Light Facility (HALF) proposed a design specification to achieve 100,000 resolving power at 400 eV photon energy. In this paper, a beamline optical design based on varied-line-spacing plane grating monochromator [1, 2] (VLS-PGM) is given, which uses a VLS plane grating with a central groove density of 2400 l/mm to cover the soft X-ray photon energy region of 250~2000 eV. And this beamline can achieve 100,000 resolving power at 1000 eV photon energy.

There are two methods for making varied-line-spacing plane gratings, mechanically ruling method and holographic exposure method. Compared with mechanically ruled gratings, holographic gratings are simple to fabricate, easy to change the shape of the grooves, and have the advantages of no ghost lines. However, the grating grooves fabricated by the holographic method are two-dimensionally curved curves. When calculating the beamline resolving power, it is not only necessary to analyse the effects of

aberration, entrance slit width, exit slit width, the slope error of optical elements, and diffraction limit of the grating on the monochromator spectrum broadening, but also to analyse the influence of grating grooves curvature on beamline resolution. We established a calculation model for the curvature of holographic VLS plane grating grooves. The curvature of the grating grooves is used as an important evaluation criterion when optimizing the parameters of the holographic recording system [3]. How to make the curvature of the optimized holographic grating grooves smaller is also a new challenge.

## OPTICAL DESIGN

The period length of the undulator is 40mm and the total length is 3920 mm. Figure 1 shows the layout of the optical system. The total length of the beamline is 72.41 m. The first mirror is a water-side-cooled plane mirror, coated with Au, deflecting the beam horizontally by 1.6°. The monochromator consists of a varied-line-spacing plane grating and a plane mirror, which is used to change the included angle of the grating while wavelength scanning. The nominal groove density of the grating is 2400 l/mm, covering the energy range of 250 ~ 2000 eV. The toroidal mirror downstream the exit slit has a grazing incidence angle of 0.8° and is used to focus vertically and horizontally to the experimental station.

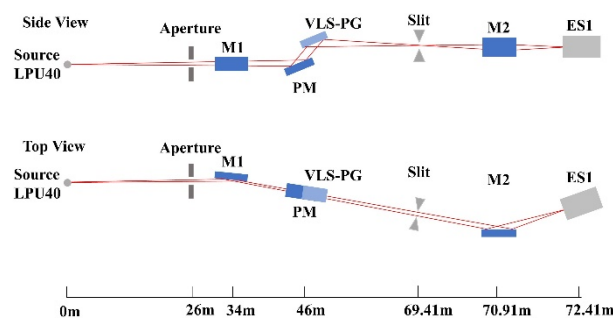


Figure 1: Layout of the optical system.

Due to the focusing characteristics of the VLS grating, a focusing mirror can be omitted upstream the exit slit, thereby improving the transmission efficiency of the beamline. The VLS grating parameters is expressed by equation  $n(w)=n_0(1+a_1w+a_2w^2+a_3w^3\dots)$ , where  $w$  is the position on the grating along the light propagation direction,  $n(w)$  is the grooves density,  $n_0$  is the grooves density at the center of the grating,  $a_i$  is the space variation parameters.

According to the concave grating aberration theory, the VLS coefficient  $a_2$  can be obtained by  $F20 = 0$ . Then,

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according to the grating including angle  $2K$  changes from  $174.904^\circ$  at 250 eV to  $178.223^\circ$  at 2000 eV, and eliminating coma and spherical aberration at 1000 eV photon energy, the grating parameters can be calculated. Table 1 shows the parameters of grating.

Table 1: Parameters of Grating

Optical elements	PG
Shape	Plane
Total surface size [mm]	$350 \times 30$
Material	Au
N0(1/mm)	2400
a1(1/mm <sup>2</sup> )	$-8.75357 \times 10^{-5}$
a2(1/mm <sup>3</sup> )	$5.51853 \times 10^{-9}$
a3(1/mm <sup>4</sup> )	$-3.14971 \times 10^{-13}$

## RESOLUTION

The main contributions to beamline spectral broadening are source width, exit slit width, optical system aberration, the slope error of optical elements, and grating diffraction limit. The tangential slope error of the grating is  $0.1 \mu\text{rad}$ , the tangential slope error of the plane mirror is  $0.2 \mu\text{rad}$ , and the sagittal slope error of the plane mirror M1 is  $3 \mu\text{rad}$ . Figure 2 shows the influence of various factors on the beamline resolution. It can be seen from the figure that the slope error of the grating, source width and the width of the exit slit are the main influencing factors.

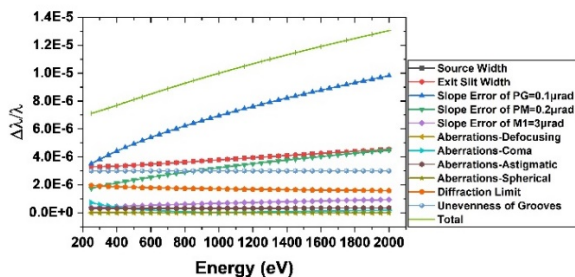


Figure 2: Contributions to the spectral broadening from different factors.

Figure 3 shows the ray tracing results of the beamline at the exit slit by SHADOW software. This beamline can achieve 100,000 resolving power at 1000 eV photon energy.

grating and the target VLS grating along the W (grating Length) axis under different L (grating Width) widths.

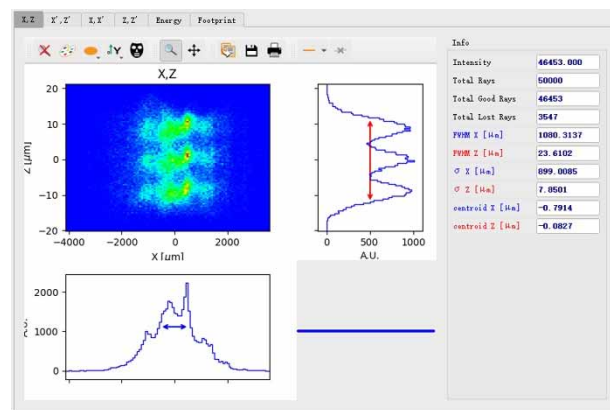


Figure 3: Ray-tracing result.

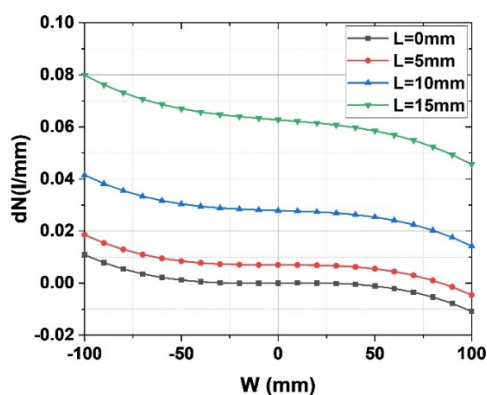


Figure 4: The dN error diagram between the optimized holographic grating and the target VLS grating.

## HOLOGRAPHIC GRATING

A spherical wavefront and an aspherical wavefront to generate the fringes and optimized the recording parameters. According to the VLS grating coefficients given in the design, the parameters of each component in the holographic grating recording system were optimized. The multiple sets of data obtained from the optimization were screened based on factors such as actual experimental conditions and the degree of curvature of the grating grooves. A more reasonable set of recording systems parameters was finally selected for grating fabrication. Figure 4 shows the dN error diagram between the optimized holographic

## GRATING GROOVE CURVATURE

The calculation method for the maximum curvature of the grooves at the edge of the holographic varied-line-spacing is: Under the same number of grooves, the focal positions of grating carving and W axis  $w_{l=0}$  and  $w_{l=L}$  are calculated by  $nh(w_{l=0},0)=nh(W,0)$  and  $nh(w_{l=L},0)=nh(W,0)$  at  $l=0$  and  $l=L$ , respectively. Then  $(w_{l=0}-w_{l=L})/L$  is the maximum curvature of the grooves at the edge of the grating, where W and L are the half length and half width of the grating respectively. It is calculated that the maximum curvature of the optimized holographic VLS grating grooves is 2.73 mrad, as shown in Fig. 5.

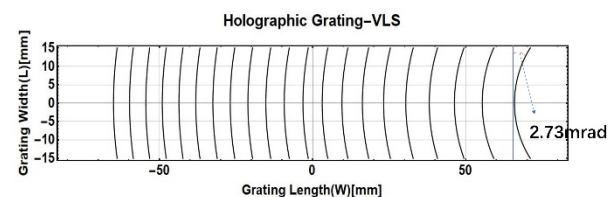


Figure 5: Grating grooves curvature diagram.

According to the concave grating aberration theory [4], the two-dimensional curvature of the grating grooves will increase the aberration term related to the L direction of the grating grooves, thereby reducing the resolution of the beamline. Figure 6 shows the variation of the beamline resolving power with photon energy using the varied-line-spacing grating fabricated by holographic method and using the target straight grooves grating.

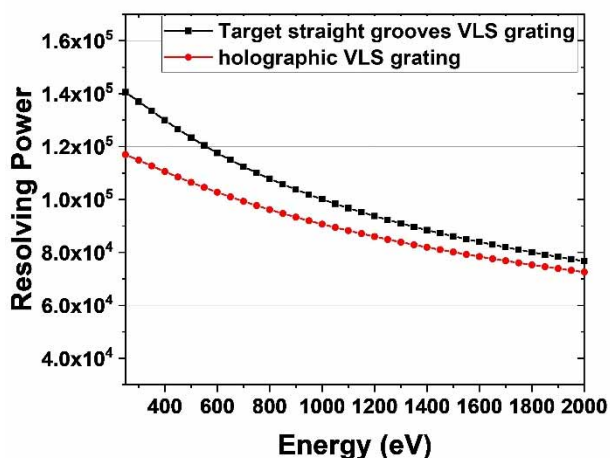


Figure 6: Variation of the beamline resolving power with photon energy.

It can be seen from the figure that the beamline resolving power of the grating fabricated by the holographic method is slightly lower than that of the target straight-line grating. Due to the current holographic VLS grating recording system parameter optimization range is limited to the actual

use of the optical element surface accuracy, the size of the optical platform and other factors. In order to further reduce the curvature of the holographic VLS grating, it is necessary to upgrade the various components used in the recording system and further optimize the calculation program of the recording system parameters.

## CONCLUSION

In this work, we introduce an ultra-high resolution beamline optical design and the optimized design of the VLS grating holographic recording system. We calculated the curvature of the grating grooves and the influence of holographic grating grooves curvature on the beamline resolving power through concave grating aberration theory. And theoretically analysed the factors that contribute to the spectral broadening of the grating monochromator from the perspective of grating fabrication process.

## REFERENCES

- [1] W. R. McKinney, "Varied line-space gratings and applications", *Rev. Sci. Instrum.*, vol. 63, no. 1, pp. 1410-1414, 1992. doi:10.1063/1.1143030
- [2] Jarrige, Ignace *et al.*, "Paving the way to ultra-high-resolution resonant inelastic x-ray scattering with the SIX beamline at NSLS-II", *Synchrotron Radiat. News*, vol. 31, no. 2, pp. 7-13, 2018. doi:10.1080/08940886.2018.1435949
- [3] T. Namioka, and M. Koike, "Aspheric wave-front recording optics for holographic gratings", *Appl. Opt.*, vol. 34, no. 13 pp. 2180-2186, 1995. doi:10.1364/AO.34.002180
- [4] H. G. Beutler, "The theory of the concave grating", *J. Opt. Soc. Am.*, vol. 35, no. 5, pp. 311-350, 1945. doi:10.1364/JOSA.35.000311