

A new method to suppress high-order harmonics for a synchrotron radiation soft X-ray beamline^{*}

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Abstract: A feasible and convenient method is proposed to suppress higher-harmonics for a varied-line-spacing plane grating monochromator in the soft X-ray region. Related calculations and experiments demonstrate that decreasing the included angle slightly by changing the parameter of the exit arm length can significantly improve light purity. This method is suitable and has been used for experiments of detector calibration in beamline 4B7B at the Beijing Synchrotron Radiation Facility (BSRF).

Key words: soft X-ray, high-order harmonics, detector calibration, Monk-Gillieson monochromator, synchrotron radiation

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1 Introduction

The double crystal monochromator (DCM) and grating monochromator have been widely used in synchrotron radiation beamline, but both of them have a problem of high-order harmonics in monochromatic lights. For hard X-rays, the problem can be overcome by slightly detuning the second crystal of the DCM [1]. However, for soft X-rays it is difficult to suppress harmonics. So far, many efforts have been used to solve the problem. These can be classified into three kinds of methods based on their techniques: first, select appropriate materials to use as transmission filters [2, 3]. It works because the ratio of each harmonic in the transmitted light is changed by the absorption edge of a particular element. Second, use several pairs of total reflection mirrors as a suppressor [4, 5]. This method can cover a wider energy range, but it is more difficult to align the optical mirrors compared to the first method, and the light path may change slightly when switched to another set of mirrors. Third, change the modes of operation or replace the grating with a designated one. This method is often used in the SX-700 [6, 7] monochromator and varied-line-spacing plane grating monochromator (VSPG) in the soft X-ray range. SX-700-II [8] can operate in higher order suppression (HIOS) mode by changing the parameter of C_{ff} [9]. The VSPG monochroma-

tor can change another grating in order to get the high performance of spectral purity. However, these methods are expensive and not convenient enough, so we propose an easy method, which is similar to the DCM detuning method, to suppress the harmonics for the VSPG monochromator. Decreasing the included angle slightly by changing the parameter of the exit arm length can significantly improve light purity. This method has been used in beamline 4B7B at the Beijing Synchrotron Radiation Facility (BSRF) for detector calibration experiments.

4B7B is a soft X-ray beamline for detector calibration experiment and light element absorption spectroscopy, which uses a variable-included-angle Monk-Gillieson mounting monochromator with a varied-line-spacing plane grating covering the energy range of 50–1600 eV. The content of higher orders light varies with the X-ray energy. When the energy falls within 50–500 eV, the problem of harmonics is serious, especially between 50–150 eV. For detector calibration experiments the light purity is important so it is necessary to develop a new method to reduce the harmonics. With energy larger than 800 eV, it is pure enough because the optical mirrors offer high reflectivity for low energy X-rays. So the harmonic problem should be especially considered at the low energy range. Our novel method works well and related calculations are listed in the second section. The third section describes the relevant experiment

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which was used to verify our method. The discussion and conclusion are listed at the end of the article.

2 Analysis and calculation method

The content of each harmonic order and the corresponding suppression ratio are analyzed and calculated by the XOP software. These calculations are based on the optical components and the structures of 4B7B beamline which are shown in Fig. 1.

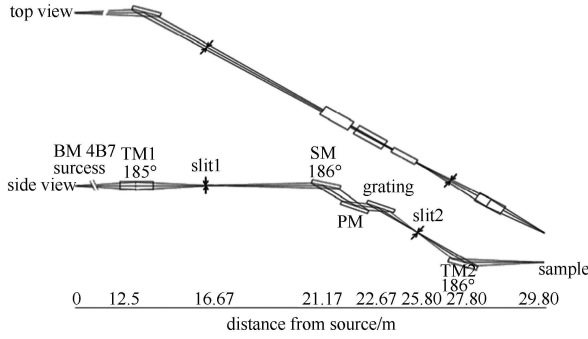


Fig. 1. The layout of the 4B7B beamline.

The flux of first, second and third harmonics at the sample can be given as follows:

$$\begin{aligned} Flux_{\text{sample}}(\lambda/n) &= \varepsilon \times Flux_{\text{source}}(\lambda/n) \\ \varepsilon &= c \cdot \varepsilon_{\text{TM1}}(\theta_{\text{TM1}}, \lambda/n) \times \varepsilon_{\text{SM}}(\theta_{\text{SM}}, \lambda/n) \\ &\quad \times \varepsilon_{\text{TM2}}(\theta_{\text{TM2}}, \lambda) \times \varepsilon_{\text{G}}(\alpha, \beta, \lambda) \\ &\quad \times \varepsilon_{\text{PM}}(\theta_{\text{PM}}, \lambda), \end{aligned} \quad (1)$$

where ε is the total transmission efficiency of the beamline. ε_{TM1} , ε_{PM} , ε_{TM2} are the reflectivity of the first toroid mirror, plane mirror and the second toroid mirror. ε_{G} is the diffraction efficiency of the laminar grating, and it depends on the incident angle α , the diffraction angle β and the wavelength of the X-ray if other parameters of the grating have been fixed. θ_{TM1} , θ_{TM2} , θ_{SM} are the incident angles of the first, second toroid mirror and the sphere mirror. The incident and diffraction angles of the grating depend on the working curve and vary with wavelength. θ_{PM} is the incidence angle of the plane mirror. λ/n is the wavelength of each harmonic order (first order $n=1$, second order $n=2 \dots$). Considering the acceptance efficiency of the beamline and the transmission efficiency of the slits, a constant factor c is introduced. The reflectivity of the mirror can be calculated with XOP 2.1 [10]. The results show that the reflectivity of second order light decreases rapidly when the energy is above 500 eV, while third order is 800 eV. The diffraction efficiency of the grating was calculated using the differential formalism of the exact electromagnetic theory [11]. The results are illustrated in Fig. 2, which demonstrates that the efficiency of the second order is higher in the range

of 70–120 eV and the third order is more serious in the long wavelength. According to the above formula, we obtained the suppression ratio with different energy in Fig. 3.

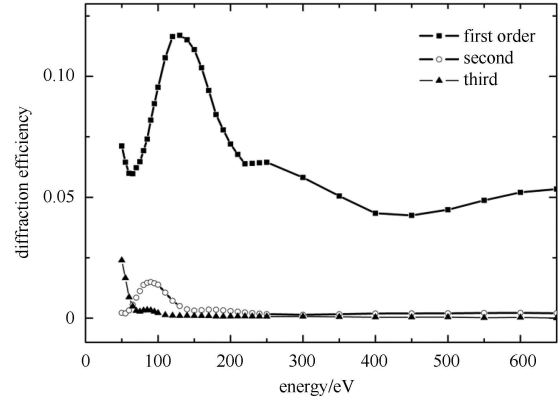


Fig. 2. The diffraction efficiency of the laminar grating of 800 l/mm.

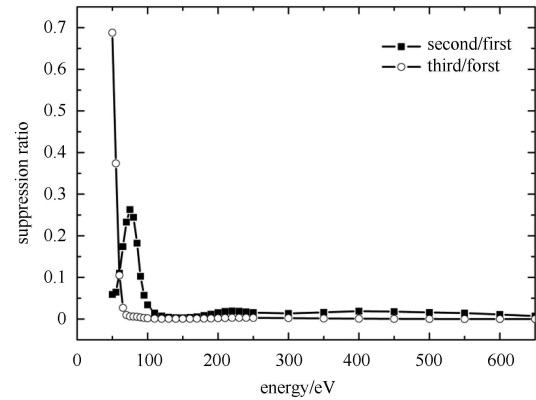


Fig. 3. The suppression ratio with different energy.

The grating equation and meridional focus equation [12] of this kind of beamline are:

$$d_0(\sin\alpha + \sin\beta) = m\lambda \left(\frac{\cos^2\alpha}{r} + \frac{\cos^2\beta}{r'} \right) + b_2 \frac{m\lambda}{d_0} = 0, \quad (2)$$

d_0 : The period in the middle of the grating; α : The incidence angle; β : The diffraction angle; m : Order of diffraction ($m = 0, \pm 1, \pm 2$); λ : Wavelength; r and r' : The distances from the entrance and exit slits to the grating centers; b_2 : The varied-line-spacing coefficients of the laminar grating.

By decreasing the exit arm parameter r' , we find the harmonic suppression ratio decreases. In other words, the spectral purity improves. This phenomenon can be explained by the decrease of the included angle $\alpha-\beta$ based on the above equation. The reflectivity of first order declined even faster than harmonics. In order to clearly demonstrate this change, we calculate how the suppression ratio changes with the r' at 170 eV. The result is

shown in Fig. 4. The suppression ratio will decrease from 0.54% to 0.25% if the parameter changes from 3165 mm to 3145 mm.

At different energies the curve is different more or less, but the trend is the same. So appropriate reduction of the value r' is beneficial for the harmonics suppression ratio. However the resolution and flux will be reduced accordingly. Since other methods sacrificed flux also and the resolution of the beamline is high enough for detector calibration experiments, we still believe it is a good method to suppress harmonics.

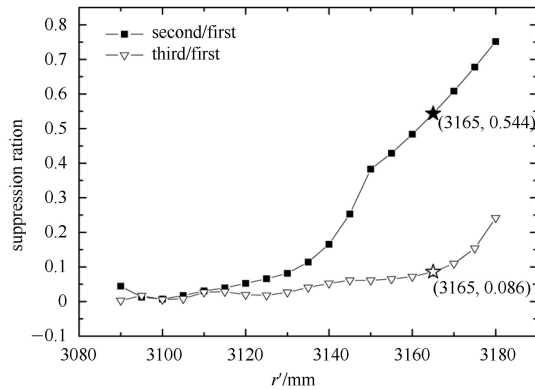


Fig. 4. Harmonics suppression ratio with parameter r' .

3 Experiments

The effect of this method was confirmed by the total electron yield (TEY) spectra. A similar experiment [9] has been done for SX-700 to verify the effect of HIOS. The absorb spectroscopy of CaSO_4 was collected at TEY mode on 4B7B beamline at BSRF. The electron energy was 2.5 GeV and the beam current was 150–250 mA. The resolution power ($E/\Delta E$) of the beamline is better than 7000 at 90 eV and 6000 at 250 eV. During data collection, the spectra signal is normalized by the TEY signal measured from a copper foil located under the second toroid mirror. The sample was measured at different values of r' . The linear extrapolation of the pre-edge has

been subtracted as background. The spectra have been normalized to the absorption peak of sulfur. As shown in Fig. 5, the $L_{2,3}$ edge of calcium appeared in the spectra because of the second order light and it showed significant changes with the parameter r' . The sharp peak of Ca became weaker and smaller, which demonstrates that the content of high order light is suppressed. This experiment result is consistent with the theoretical result in Fig. 4.

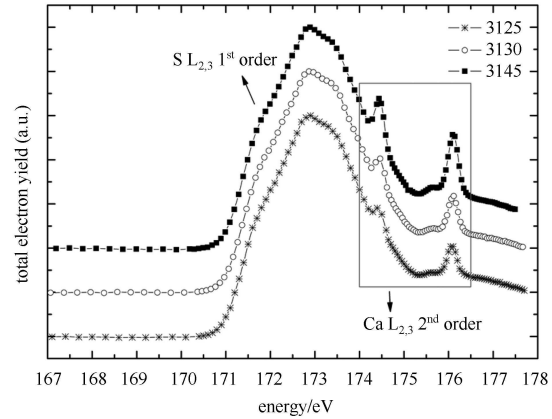


Fig. 5. Total electron yield spectra of CaSO_4 for the three different values of r' , and it shows that the optical purity is improved by decreasing the parameter r' .

4 Discussion and conclusion

The experimental and calculation results show that the introduced approach improves the light purity, and it shows feasibility and convenience and can be combined with other harmonic suppression methods in calibration experiments. The most appropriate parameter can be found for different photon energies if a compromise between the resolution and purity are taken into account. In addition, a quantitative measurement of the proportions of high-order harmonics [13] can make a further verification.

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