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Higher order harmonics suppression in extreme ultraviolet and soft x-ray*

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The extreme ultraviolet and soft x-ray sources are widely used in various domains. Suppressing higher order harmonics and improving spectral purity are significant. This paper describes a novel method of higher order harmonics suppression with single order diffraction gratings in extreme ultraviolet and soft x-ray. The principle of harmonic suppression with single order diffraction grating is described, and an extreme ultraviolet and soft x-ray non-harmonics grating monochromator is designed based on the single order diffraction grating. The performance is simulated by an optical design software. The emergent beams of a monochromator with different gratings are measured by a transmission grating spectrometer. The results show that the single order diffraction grating can suppress higher order harmonics effectively, and it is expected to be widely used in synchrotron radiation, diagnostics of laser induced plasma, and astrophysics.

Keywords: higher order harmonics suppression, extreme ultraviolet and soft x-ray, monochromator, single order diffraction grating

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1. Introduction

Synchrotron radiation and plasma light source are the most commonly used extreme ultraviolet and soft x-ray light sources. They are widely used in the fields of atomic and molecular physics, astrophysics, life science, micro-nano devices, and so on.[1–5] But because of the wide spectral range, we need a monochromator to gain a monochromatic light. In extreme ultraviolet and soft x-ray, most monochromators are grating monochromators. And the dispersive elements are usually laminar gratings and blaze gratings.[6–9] They disperse incident light into discrete orders as a function of wavelength (λ) and grating period (p). The diffracted beam directions or orders are given by the grating equation. However, higher order harmonics which diffract in the same direction cannot be avoided in monochromatic synchrotron beams, and it will lead to distortions in recorded spectra which are the main source of errors in spectral analysis. So, how to suppress higher order harmonics in a simple way is vital.

At present, synchrotron radiation often uses filters, suppression mirrors, and gas absorption cell to suppress higher order harmonics.[7–13] Absorber filters exploit the transmission cut-off at absorption edges. Using a couple of different materials, it can cover the energy range of 25 eV–200 eV. Absorption filters are easy to use and have a large 2nd order suppression capability, but not for higher orders and at the price of increased scattered radiation. The higher order suppression mirror system consists of a set of mirrors with different coatings. The high energy cut-off is freely selectable by the incidence angle chosen, due to drop of reflectivity above the critical angle. In this way, the energy range between 20 eV and 700 eV can be covered, but it needs to be aligned very accurately in order not to change beam direction. The gas absorption cell is an efficient differential pumping system and is most often used with noble gases such as Ar, Ne or even He. It can cover the energy range of 5 eV–21.6 eV, but it is a rather bulky installation and requires a powerful pumping system. Moreover, these methods should be used in combination to cover the total energy range of extreme ultraviolet and soft x ray. It will be accompanied by higher costs, larger space, and lower photon flux. Recently, Cao *et al.* proposed a new concept of x-ray dispersive element named as single order diffraction grating.[14–19] With optimal design of the structure, this grating can diffract x rays without higher order diffractions. It provides a new method to suppress any higher-order contamination in extreme ultraviolet and soft x ray. Using the single order diffraction grating, the monochromator will get rid of higher order harmonics in the total energy range without any other measures, and it will save a lot of cost and space.

This paper describes the principle of harmonic suppression with single order diffraction grating. Based on the single order diffraction grating, an ultraviolet and soft x-ray non-harmonics grating monochromator is designed. The perfor-

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mance is simulated by an optical design software. The emergent beams of monochromators with different gratings are measured by the transmission grating spectrometer. The results show that the single order diffraction grating can suppress higher order harmonic effectively.

2. Principle

It is known that laminar grating and blaze grating have higher order diffractions, but sinusoidal grating has only 0 order and ±1 order diffraction. Because of the special groove shape, the transmission/reflection function of sinusoidal grating is a sinusoidal function, and there are no higher-order diffractions. It is a kind of single order diffraction grating. However, soft x-ray sinusoidal gratings have not been developed so far due to the limitation of the fabrication technology. At present, soft x-ray gratings are often fabricated with steep and slope sidewalls, and it is almost impossible to fabricate a grating with perfect sinusoidal sidewalls.

Soft x-ray photon sieve is a single order diffraction grating based on the principle of sinusoidal grating.[15] Instead of sinusoidal sidewalls, the structure is randomly distributed dots with steep sidewalls. This greatly reduces the difficultly of fabrication. It can be fabricated easily by electron beam lithography and focused ion beam. Figure 1 shows the sketch of such a grating. The grating size is $Nd \times Nd$. The period is d, and the direction is along the horizontal. In a period, N mutually disjointed dots are randomly distributed. The dot is a circle of diameter $d/2$.

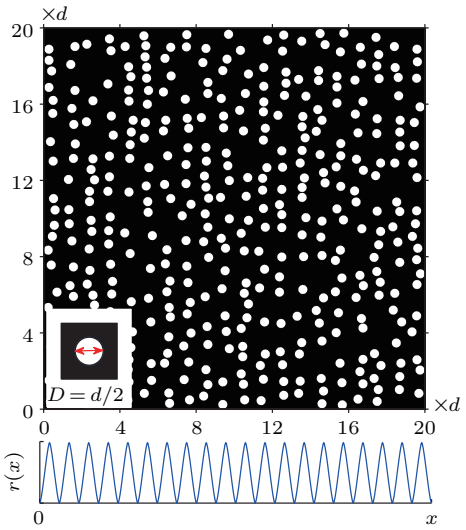


Fig. 1. (color online) Sketch map of soft x-ray photon sieves.

The reflection function of the grating can be written as

$$r(x)=\frac{\sum_i 2\sqrt{(d/4)^2-(x-x_i)^2}}{Nd}, \tag{1}$$

where x_i is the central location of the circle. If the grating is big enough, because of the random distribution, x_i will be randomly distributed in $[d/4, 3d/4]$, and N will be $d/2\Delta x_i$. Here Δx_i is the average distance between the dots. Consequently,

$$r(x)=\frac{4}{d^2}\int\sqrt{(d/4)^2-(x-x_i)^2}\,\mathrm{d}x_i. \tag{2}$$

After integration, the reflection function will be given by

$$r(x)=\begin{cases}\dfrac{\left[\dfrac{\pi}{2}-\sin^{-1}\left(1-\dfrac{4x}{d}\right)-\left(1-\dfrac{4x}{d}\right)\sqrt{1-\left(1-\dfrac{4x}{d}\right)^2}\right]}{8}, & x\in\left[0,\dfrac{d}{2}\right],\\[2ex] \dfrac{\left[\dfrac{\pi}{2}+\sin^{-1}\left(3-\dfrac{4x}{d}\right)-\left(3-\dfrac{4x}{d}\right)\sqrt{1-\left(3-\dfrac{4x}{d}\right)^2}\right]}{8}, & x\in\left[\dfrac{d}{2},d\right].\end{cases} \tag{3}$$

From Eq. (3), we can see that the reflection function of soft x-ray photo sieve is a quasi-sinusoidal function which is exactly symmetrical by line $x=d/2$. Equation (3) can be expanded into a Fourier series in infinite space

$$\begin{aligned} r(x) \;=\; & 0.1963-0.1804\cos\left(\frac{2\pi\cdot x}{d}\right)\\ & -0.009965\cos\left(\frac{2\pi\cdot 3x}{d}\right)\\ & -0.002693\cos\left(\frac{2\pi\cdot 5x}{d}\right)-\cdots \end{aligned} \tag{4}$$

It is similar to the condition of black-white transmission gratings that the items of the right of Eq. (4) correspond to the diffraction orders, respectively.[20] And the square coefficients correspond to absolute efficiencies of the diffraction orders. From Eq. (4), one can see that except the 0 order, there are no even order diffracions. Only ±1, ±3, $\pm5,\ldots$ orders exist. The contribution of the third order to the first order is about 0.3%, the contribution of the fifth order to the first order is about 0.02%, and the contributions of the higher orders to the first order are ignored. It indicates that the soft x-ray photon sieve can suppress higherorder diffraction effectively, and using it as the dispersive element of the monochromator, higher

harmonic radiation will be suppressed by a factor of 312. It is essential that there is no dependence on the photon energy, and the total energy range of extreme ultraviolet and soft x-ray will be covered. Compared with the methods that exploit the transmission cut-off at absorption edges and drop of reflectivity above the critical angle, the soft x-ray photon sieve is much easier, and saves a lot of costs and spaces.

3. Design of non-harmonic grating monochromator

Based on the soft x-ray photo sieves, we designed a small extreme ultraviolet and soft x-ray non-harmonics grating monochromator. The monochromator delivers soft x-ray radiation with the following parameters:

(i) photon energy range 10 eV–230 eV;

(ii) resolving power $E/\Delta E > 1000$;

(iii) angular acceptance 4 mrad (vertical)×15 mrad (horizontal).

The scientific profile of the monochromator is focused on higher order harmonics suppression of soft x-ray photo sieves.

The optical layout of the monochromator is shown in Fig. 2. The optical scheme adopts the concept of the Variable Angle Plane Grating Monochromator,[21] and it benefits from wide spectrum, high resolution, and operation at variable $C_{\rm ff}$ (focus constant) parameters. The source is a laser-produced Ar (or tin slab) plasma source. The entrance slit selects the center of radiation. Two spherical mirrors are arranged in the Kirkpatrick–Baez[22] configuration to focus both the horizontal and vertical x-rays on the exit slit. The monochromator situated downstream consists of a plane pre-mirror and selectable gratings, dispersing the beam in photon energies. Three photo sieves with constant groove densities N of 2000, 1000, and 250 lines/mm are used to provide even coverage of the monochromator resolution. A Laminar grating with constant groove densities N of 1000 lines/mm is used to compare with the soft x-ray photo sieves. Downstream from the monochromator is an exit slit, producing monochromatic light. Parameters of all optical elements are summarized in the following Table 1.

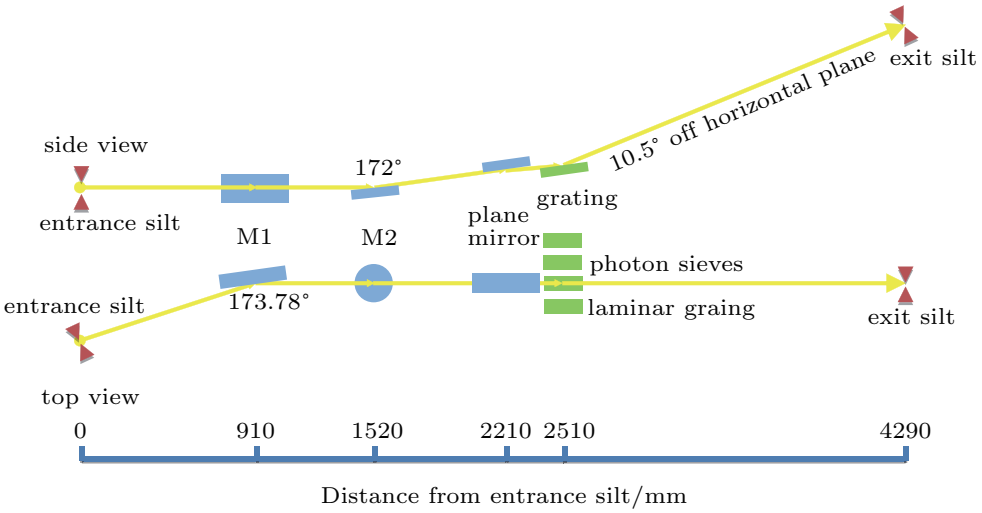


Fig. 2. (color online) Optical scheme of non-harmonics grating monochromator.

Table 1. Parameters of optical elements.

Optics	Type	Substrate/coating	Parameters	Incident angle/(°)	dimension/mm^2
M1	spherical	Si/C	$R = 2651.6$ cm	86.89	20×310
M2	spherical	Si/C	$R = 2186.7$ cm	86	$\phi 90$
Plane mirror	plane	Si/C		78.13∼84.67	20×280
Grating	photon sieves	Si/Au	2000 lp/mm	80.80∼85.36	20×60
	photon sieves		1000 lp/mm		
	photon sieves		250 lp/mm		
	laminar grating		1000 lp/mm		

Ray-tracing calculations were performed with a ray-tracing software X-Lab developed by ourselves.[23] Figure 3 presents the results of the 1st order diffracted rays of 10 eV, 40 eV, 120 eV, and 230 eV at the detector position. The left of the figure indicates the spot diagram, and the right indicates the statistical histogram along the y direction. The results show that the energy resolutions at 10 eV, 40 eV, 120 eV, and 230 eV are all larger than 1000.

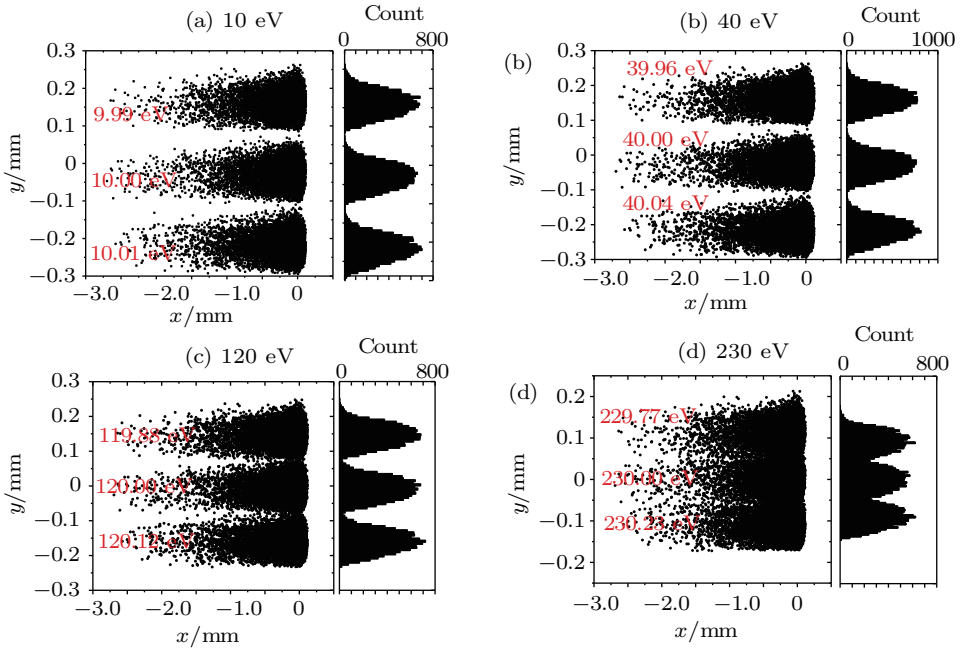


Fig. 3. (color online) Simulated results of different energies with X-Lab.

4. Experiments

In the experiment, a laser-produced Ar plasma source is fixed before the monochromator and a soft x-ray CCD is fixed at the location of the exit slit. Then, the energy resolution is obtained. The drive laser is an Nd:YAG laser, operating at a central wavelength of 532 nm, and generating 10-ns pulses with up to 700 mJ at 10 Hz. The CCD is PIXIS-XO CCD manufactured by Princeton Instruments Co., with 1024×1024 pixels (an etch pixel is 13.5 μm square).

Figure 4 shows the results of the monochromator resolution. The blue separated spectral lines are the x-ray spectra of laser-produced Ar plasmas. The coordinate graph is the intensity profiles of the output at different wavelengths. The energy resolution of the monochromator is about 1160 at 11.65 nm, and 1100 at 11.59 nm. It satisfies the design requirement.

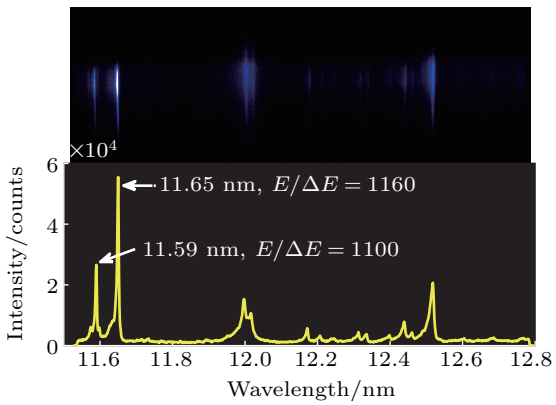


Fig. 4. (color online) Results of the monochromator resolution.

A transmission grating spectrometer[24,25] is mounted to test the output. It can verify the validity of harmonic suppression by the soft x-ray photon sieve. The period of transmission grating is 1000 nm, the size is about 100 μm×500 μm. In order to optimize the photon density and the illumination, the transmission grating is placed at the best focal point of the focusing mirrors instead of the exit slit. We used a laser-produced tin slab plasma source, because it has higher brightness than the laser Ar plasma source. After being dispersed by the monochromator, the soft x-ray produced by the laser tin slab plasma source would pass through the transmission grating. The diffraction patterns were acquired by the CCD. The intensities and positions of the zero and first order diffraction spectra could be read easily. Then, the output spectral component of the monochromator could be deduced. Experimental tests were made to compare the monochromator output with the soft x-ray photon sieve and laminar grating.

Figure 5(a) is the output of the monochromator with soft x-ray photon sieve at a working wavelength. The CCD got two light spots. The brighter one is the zero order diffraction of the transmission grating, and the other one is the first order. After unfolding the soft x-ray spectrum, we obtained the intensity diagram. The wavelength of the first order is 15.9 nm, and there are no distinguishable peaks at the other wavelength. It indicates that the transmission grating was only irradiated by the light of 15.9 nm. In other words, the output of the monochromator is a monochromatic light with wavelength of 15.9 nm, and there are no higher order harmonics. Figure 5(b) is the output of the monochromator with laminar grating at the same working wavelength. The CCD detected three light spots. According to the analysis of Fig. 5(a), the brightest one is the zero order diffraction of the transmission grating, and the other two are the first order diffractions at different wave-

lengths. The results of spectrum unfolding analysis show that the wavelengths of the first orders are 7.95 nm and 15.9 nm respectively. There are no distinguishable peaks at the other wavelength. This indicates that the transmission grating was irradiated by the lights of 15.9 nm and 7.95 nm, and the output of the monochromator is a polychromatic light. According to the results above, the 15.9-nm light is the fundamental component, the 7.95-nm one is the second-order harmonic contamination of the monochromatic light and it comes from the second order diffraction of laminar grating. So the laser-produced tin slab plasma source can generate the lights of 15.9 nm and 7.95 nm. And if laminar grating is used as the dispersive element, there will be the second-order harmonic contamination in the output of the monochromator, and it needs extra methods to suppress the second order harmonics. If the photon sieve is used, the output will be a monochromatic light, and the photons with twice the energy of the first order will be suppressed effectively by the photon sieve. It is more convenient and saves a lot. If we regard the intensity of photons with twice and triple the energy of the first order as the high order harmonics, the contribution of the higher orders to the fundamental component will be less than 0.5%.

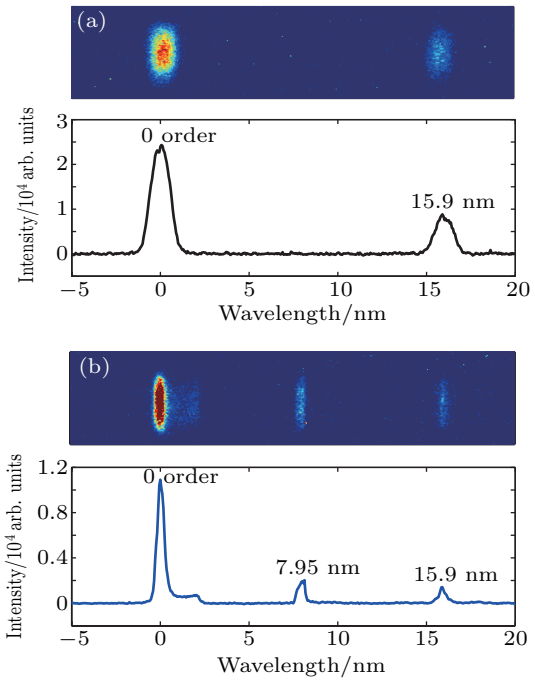


Fig. 5. (color online) Output of monochromator with (a) photon sieve and (b) laminar grating.

5. Conclusion

The principle of harmonic suppression with single order diffraction grating was described by the scalar diffraction. Based on the concept, an ultraviolet and soft x-ray non-harmonics grating monochromator is developed. The energy resolution is characterized, and the result is consistent with the theoretical simulation. The spectral purity of the monochromator output with soft x-ray photon sieve and laminar grating are measured by transmission grating spectrometer, respectively. The results show that the spectral purity is significantly improved to reduce the higher order harmonics contamination of the monochromatic light down to 0.5% by the single order diffraction grating. It can be predicted that there will be a broad perspective for the single order diffraction grating to be applied in the research fields of synchrotron radiation, diagnostics of laser induced plasma, astrophysics, and so on.

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