

2 Dimensional Variable Line Spacing Grating Based Optical Spectrometer

Cross-Reference To Related Application

This application claims the benefit of Singapore Patent Application No. 10201710659Q,
5 entitled "2D VLS Grating Based Optical Spectrometer" and filed on December 21, 2017,
which is expressly incorporated by reference herein in its entirety.

Field of the Invention

The present disclosure relates to a spectrometer that it able to obtain both lower
10 resolution over broad range (LRBR) and high resolution over narrow range (HRNR)
spectral information simultaneously in a single spectral information measurement.
Particularly, the present disclosure relates to a spectrometer having a 2 dimensional (2D)
gratings with variable line spacing.

15 Summary of the Prior Art

Spectrometers have vast applications over almost all industrial and scientific clusters.
With the assistance of spectrometers, spectral information obtained from the samples
play key roles in material characterization, structure inspection, chemistry analysis,
diseases diagnosis and pathological study. In most spectroscopy applications, broadband
20 spectral range and high spectral resolution are both required. The broadband spectral
range is necessary to identify all potential ingredients, whose spectral fingerprints may
loosely distributed over very broad spectral region. The high spectral resolution is
required for probing each ingredients' details such as orientation, phase, polarization,
energy status. However, in traditional spectrometer, there is a tight trade-off between
25 spectral resolution and spectral ranges due to the limited data sampling speed. Within a
single spectral measurement, spectral information is obtained with either a lower
resolution over broad range (LRBR) or a high resolution over narrow range (HRNR). It is
not possible to obtain spectral information for both LRBR and HRNR with a single
spectral measurement. As a result, multiple spectral measurements with single or even
30 multiple spectrometers have to be repeated in sequence to obtain full spectral information
of the samples.

The drawback of sequential spectral measurement is very obvious. First, it results in high
cost and tedious spectral measurement process. Secondly and more importantly, it is
35 difficult to obtain consistent reading between different the spectral measurements due to
multiple factors such as maintaining stability and repeatability of the source, preventing

system calibration error, measurement environment variation, ambient noise fluctuation, degradation of the samples or intrinsic transient dynamics of the targeted process. The above mentioned factors are difficult to control and are fatal to certain applications. One typical example is the measurement of coherent broadband EUV radiation generated through high order harmonic generation (HHG) as shown in Figure 1. Such broadband radiation has been used for micro-structure analysis of semiconductor material or single molecular. On one hand, scientist needs broadband HHG spectrum over hundreds to thousand eV (corresponding to thousands nm or Peta-Hertz bandwidth in terms of wavelength and frequency) to identify different absorption edge or bandgap structures. On the other hand, to obtain molecular information such as orientation, polarization or quantum trajectory, each individual harmonic orders (the tooth of comb spectrum shown in figure 1) is needed to be resolved and monitored in real time. However, the HHG process is carried out in vacuum and involves a lot of ultrafast dynamics with typical time constant varying from second to femto-seconds. The switch between different spectral instrumentation is not trivial and all dynamic information are inevitably lost during the sequential spectra measurement. Similar case can be found in many other applications. For example, in-vivo Raman and Fluorescence based imaging or spectroscopy, both narrow Raman peak and broad band fluorescence spectra are preferred to be resolved in real time or simultaneously to avoid the fluctuation of the signal and measurement errors.

Hence, those skilled in the art are always striving to provide a spectrometer that is capable of collecting both LRBR and HRNR spectral information simultaneously in a single spectral measurement.

Summary of the Invention

The above and other problems are solved and an advance in the state of the art is made by a spectrometer provided by embodiments in accordance with the disclosure. The first advantage of embodiments of the spectrometer in accordance with the disclosure is that spectrometer is capable of obtaining both lower resolution over broad range (LRBR) and high resolution over narrow range (HRNR) spectral information simultaneously. The second advantage of embodiments of the spectrometer in accordance with the disclosure is that the spectrometer fully utilises the capability of a 2D detector.

A first aspect of the disclosure relates to a spectrometer comprising a 2 dimensional detector that captures multiple spectra within a lower resolution broad range (LRBR) and a higher resolution broad range (HRBR) simultaneously; and a 2 dimensional grating

having grooves with variable groove density and period function, the groove density $G(z)$ and period function $d(y, z)$ are adaptable to focus incident EUV/X-ray source from a slit onto the 2 dimensional detector where z is a direction along the grooves and y is a direction across the grooves.

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In an embodiment of the first aspect of the disclosure, the groove density G is linearly increased from 300 to about 1500 along a positive z direction where the period function can be expressed as

$$d(y) = \frac{1}{G(z) \left(1 + \frac{2b_2(z)}{R} |y| \right)}$$

where $G(z) = 300 + 40.1z$, $b_2 = -19.5 - 0.003z$, $R = 5567\text{mm}$ and z ranges
10 between 0 and 30mm.

In an embodiment of the first aspect of the disclosure, the 2 dimensional grating is arranged such that the incident angle from the slit is 87° and at an incident distance of 237mm.

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In an embodiment of the first aspect of the disclosure, the 2 dimensional detector is apart from the 2 dimensional grating by a distance of 235mm from a center along the y direction of the 2 dimensional grating, between -3.5mm and 3.5mm of the z direction, and between 17 and 43mm in an x direction. The x direction is
20 perpendicular to the y direction.

In an embodiment of the first aspect of the disclosure, the spectrometer further comprises a cylindrical mirror and a spherical mirror. The cylindrical mirror and spherical mirror are arranged such that the cylindrical mirror is between the
25 spherical mirror and the slit.

In an embodiment of the first aspect of the disclosure, the spectrometer further comprises a concave mirror arranged between the slit and the 2 dimensional grating.

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In an embodiment of the first aspect of the disclosure, the 2 dimensional grating has a curved surface.

Brief Description of the Drawings

The above advantages and features in accordance with this invention are described in the following detailed description and are shown in the following drawings:

Figure 1 illustrates a measurement of coherent broadband EUV radiation
5 generated through high order harmonic generation (HHG);

Figure 2 illustrates a HHG spectral measurement using different grating;

Figure 3 illustrates a X-ray spectrometer;

Figure 4 illustrates a focus position on CCD imaging plane for (a) constant central
frequency with multiple spectral resolving power and (b) constant resolution;

10 Figure 5 illustrates a schematic of a 2D VSL grating in accordance with an
embodiment of this disclosure;

Figure 6 illustrates a groove pattern of the 2D VLS grating in accordance with an
embodiment of this disclosure;

Figure 7A illustrates an imaging plane of the incident light at low resolution
15 position when $G(z) = 300$;

Figure 7B illustrates the imaging plane of the incident light at high resolution
position when $G(z) = 1500$;

Figure 8 illustrates a schematic of grating illuminated by monochromatic light;

Figure 9 illustrates a flowchart of a process for designing a spectrometer;

20 Figure 10 illustrates a schematic of spherical VLS grating;

Figure 11 illustrates a flowchart of a process for selecting grating parameters
using genetic algorithms;

Figure 12A illustrates a change in the imaging plane by optimizing the grating
period function with groove density of 1200 lines/mm;

25 Figure 12B illustrates different imaging plane when b_2 is from -30 to -20 with
groove density of 1200 lines/mm;

Figure 13A illustrates a change in the imaging plane by optimizing the grating
period function with groove density of 300 lines/mm;

30 Figure 13B illustrates different imaging plane when b_2 is from -30 to -20 with
groove density of 300 lines/mm;

Figure 14A illustrates a change in the imaging plane by optimizing the grating
period function with groove density of 2400 lines/mm;

Figure 14B illustrates different imaging plane when b_2 is from -30 to -20 with
groove density of 2400 lines/mm;

35 Figure 15 illustrates a schematic of a 2D VLS grating with mounting parameters;

Figure 16 illustrates the calculation results of the mounting parameters for a grating with groove density 300 lines/mm, 1200 lines/mm and 2400 lines/mm;

Figure 17A illustrates a schematic of optical path for the EUV spectrometer;

Figure 17B illustrates a schematic of optical path for the EUV spectrometer with
5 concave mirror and curved 2D VLS grating;

Figure 18A illustrates a simulation result of the mirror mounting position as the function of the distance between HHG source and spherical mirror;

Figure 18B illustrates a focal distance of the spherical mirror and cylindrical mirror;

Figure 19A illustrates a width of the spotsize on the entrance slit (x-direction) and
10 the diffraction limit of the spherical mirror at 10 eV and 15 eV;

Figure 19B illustrates a height of the spotsize on the CCD screen (z-direction) and the diffraction limit of the cylindrical mirror at 10 eV and 15 eV;

Figure 20 illustrates the transmission of the entrance slit as the function of L at different slit openings;

15 Figure 21A illustrates a linear dispersion of gratings for different groove densities;

Figure 21B illustrates the spectral resolutions for different gratings when the slit opening is fixed at 80 μm ;

Figure 22A illustrates a spectral resolution determined by the CCD with pixel size of 13.5 micron and grating density of 300 lines/mm at different slit openings;

20 Figure 22B illustrates a spectral resolution determined by the CCD with pixel size of 13.5 micron and grating density of 2400 lines/mm at different slit openings;

Figure 23 illustrates the spectral resolution of the whole spectrometer system under grating groove density $G = 300$, $G = 1200$, $G = 2400$;

Figure 24A illustrates the reflection coefficient of gold mirror under different
25 incident angle;

Figure 24B illustrates the transmission coefficient of Al (Aluminium) filters with different thickness;

Figure 25A illustrates the measured diffraction coefficient of the first order for $G=1200$ grating and $G=2400$ grating

30 Figure 25B illustrates the total throughput of the spectrometer;

Figure 26 illustrates the deviation angle as the function of incident photon energy calculated using the parameters of a grating with groove density 1200 lines/mm;

Figure 27A illustrates a far field scattering pattern of 632-nm laser;

Figure 27B illustrates a scattering pattern from two different lasers with same
35 incident angle and incident position are detected by the CCD;

Figure 28 illustrates the normalized optical intensity as the function of pixel number along x direction; and

Figure 29 illustrates the measured spectra of 532-nm laser using proposed 2D VLS grating.

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Detailed Description

The present disclosure relates to a spectrometer that it able to obtain both lower resolution over broad range (LRBR) and high resolution over narrow range (HRNR) spectral information simultaneously in a single spectral information measurement.

10 Particularly, the present disclosure relates to a spectrometer having a 2 dimensional (2D) gratings with variable line spacing.

This disclosure discloses a novel optical spectrometer that it able to obtain both lower resolution over broad range (LRBR) and high resolution over narrow range (HRNR) spectral information simultaneously in a single spectral information measurement. The optical spectrometer is able to obtain the LRBR and HRNR through the design and fabrication of a novel 2 dimensional (2D) gratings, which can perfectly match with and fully release the potential of latest 2D photon detectors such as high-resolution CCD camera for spectrum measurement. The capability of optical spectrometer on simultaneously multiple spectra capturing with varied resolution and spectral ranges has been successfully demonstrated in visible region. Furthermore, variable line spacing (VLS) techniques are used on the developed 2D grating for the first time to extend spectral measurement region to EUV/ soft X-ray which has been verified by simulation. The results obtained from the simulation also can be extended to longer wavelength spectral measurements in infrared and Terahertz region due to the invariance of the fundamental principle.

The 2D grating design is used with a 2D photon detector such as flat-panel charge-coupled CCD for ultrafast spectral measurement over broadband spectrum range. The radiation diffracted by the 2D gratings are spectrally dispersed over two dimensions and focused on a large field of charge-coupled device (CCD). Furthermore, to extend the spectral cover range of the system from visible to EUV and soft-X-ray, a variable-line-space (VLS) design is applied on the 2D gratings. This can efficiently compensate the curvature of the diffracted radiation (especially for EUV/X-ray as the curvature increased with the photon energy) and make sure all diffracted radiation beams can be focused on a flat plane. The 2D VLS grating enables optical spectra with varied spectral resolutions,

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and spectral ranges can be collected by different pixel lines of the CCD camera. Therefore, the 2D VLS grating based spectrometer is able to simultaneously capture multiple spectra with varied resolution and spectral ranges. Both LRBE and HRNR information are captured in single shot measurement. Furthermore, compared with 1D fix-line-space (FLS) and 1D VLS gratings, the overall spectral detection range of the 2D VLS grating can cover much large bandwidth without much degradation on spectral resolution. By selectively choosing the pixel data reading path on the CCD imaging plane, special spectral measurement functions such as constant resolutions spectral measurement or constant central photon energy with multiple spectral resolving power (spectral magnification) can be realized in high speed without changing grating or mechanically moving the detector. Based on the 2D VLS grating in accordance with this disclosure, a comprehensive optical spectrometer design method contains all modules from grating design, pre-focus optics design, resolution and throughput optimization are developed. A software application is provided in accordance to a spectrometer with the 2D VLS grating to implement spectrometer system evaluation and optimization at both component level and system level are generated. The spectrometer with the 2D VLS grating is also ideal for other ultrahigh speed broadband spectroscopy applications in other optical region such as Mid-IR, IR even terahertz single-shot spectroscopy. It is also valuable for ultrafast spectrometer based imaging application such as lensless imaging, coherent interference imaging and ultra-high speed coherent tomography.

Briefly, a spectrometer is an apparatus to measure a spectrum. Generally, a spectrum is the intensity distribution with respect to wavelength, frequency, energy, momentum, or mass. Various types of optical spectrometers are developed. The most common spectrometer designs can be categorized into three major groups: refraction based spectrometer, diffraction based spectrometer and interference based spectrometer.

In diffraction and refraction based spectrometers, optical gratings are used to resolve different spectral components before it is projected on the photon detectors. Traditional optical gratings have period structure over single axis only. The optical spectrum is expanded over single dimension. Therefore, in principle, 1D photon detector such as line detector is good enough for spectral reading. With advance of photon detector technology, high resolution high sensitivity 2D photon detector such as CCD has been developed. It provides significantly improved huge information parallel capturing capability. Although those 2D photon detectors have been used for spectral measurement, they are only used to repeat the measurement and enhance the signal to noise ratio. 1D grating has become

the major bottleneck that limits the maximum spectral information flow in the 2D photon detector based spectrometer. Therefore, 2D grating perfectly matched with 2D photon detectors for high speed or high volume spectral information measurement is required.

Another bottle neck in spectrometers is the wavelength dependence of optics in different spectral region. Among, all above three spectrometer configurations, the diffraction based spectrometer can be used for almost full spectral regions from EUV to terahertz. Refraction based spectrometer only can be used for visible range and near-infrared region due to the lack of high performance refractive dispersion optics in other spectral region. Interference based spectrometer cannot be used for EUV and soft X-ray region due to the lack of optical splitter, collimator and broadband mirror at such short wavelength. In short, 1D gratings in traditional spectrometer cannot fully utilize the data capturing capability of 2D photon detectors (e.g. CCD). It induces bottle neck on information collection speed and results in tight trade-off between spectral resolution and spectral range.

The common problems in traditional spectrometers for all wavelength including X-ray, EUV, Visible, Infrared and Terahertz regions is the tradeoff between spectral resolution and spectral ranges. Increasing spectral resolution or spectral ranges will inevitably increase the total data points. In traditional 1D grating based on spectrometer design, the spectral information is diffracted along single axis. 1D line photon detector is enough to collect all spectral information. Therefore, there is not much advantage in using 2D photon detector such as high resolution CCD camera. The 1D grating is major bottleneck for spectral data collection and limit maximum data collection volume in single measurement. As a result, tedious and costly sequential spectroscopic measurement with varied resolution or spectral regions has to be done to capture both LRBR and HRNR information. As mentioned above, due to multiple factors which are difficult to control, the sequential measurement will lead to information lost, measurement artifacts and failure of the dynamics capturing. It can significantly reduce the impact of the spectroscopy measurement.

For instance, coherent EUV/X-ray radiation generated during high order harmonic generation process has very complex spectral structure as shown in figure 1. It has a broadband base with periodical spaced and harmonic comb. For many HHG applications such as HHG source optimization and HHG based molecular imaging, both low frequency (the broadband base) and high frequency (each single harmonics) structures are important for experimental diagnosis or data analysis. However, there is always a trade-

off between broad spectral bandwidth and high spectral resolution in traditional X-ray spectrometers. The former deploy a low groove density grating while the later utilizes a high groove density grating. Furthermore, with a fixed grating groove density, the spectral resolution will continuously reduce with the photon energy increasing. As a result, broadband spectrometer design cannot resolve the single harmonic information at high energy region, while the high resolution spectrometer has limit field of view and loses the information at low energy region as shown in figure 2. Specifically in figure 2, the first HHG spectral measurement 210 and the corresponding first spectral resolution diagram 215 show an ideal spectrometer with 2D VLS grating design, the second HHG spectral measurement 220 and the corresponding second spectral resolution diagram 225 show a broadband spectrometer with high groove density grating, and the third HHG spectral measurement 230 and the corresponding first spectral resolution diagram 235 show a high resolution spectrometer with low groove density grating.

Most diffraction spectrometers are realized using plane gratings, curved (spherical and toroidal) diffraction gratings and Fresnel zone plates. Designs based on diffraction gratings can provide very high spectral resolution at the expense of working bandwidth. Gratings with constant line spacing and groove density are the most widely used in various spectrometers due to its fabrication simplicity and low cost. For gratings with constant line spacing, the diffracted light after the grating actually can only be perfectly focused on a curved plane, which is called Rowland circle 310, rather flat plane as shown in figure 3. However, the detection panel of most photon detector like CCD is a flat plane. As a result, the diffraction pattern of different wavelength on the CCD is blurred and cannot be clearly resolved. This blur effect happens to all wavelength. For longer wavelength such as infrared and visible light, the Rowland circle 310 has very large radius and its effect on flat panel detector can be ignored for low or moderate resolution applications. For short wavelength such as EUV and X-ray light, the radius of Rowland circle 310 is small has significant effect on spectrometer performance. To solve this issue, 1D planar field grating 320 with curved surface is proposed. With this planar field grating 320, the focal plane is designed to be flat so that detectors such as a photodiode array, an X-ray streak camera, and a microchannel plate (MCP) can be easily applied.

The 2D grating design for broadband and high resolution spectrometer proposed is able to overcome the trade-off problems mentioned above between spectral bandwidth and spectral resolution in fix-line space grating and 1D grating design and shown in figure 3. Different from traditional planar field grating which is 1 dimensional, the 2D grating has

varied groove density and period function along the groove direction (z direction). In this way, the diffraction pattern on the CCD imaging plane becomes 2D other than 1D in the traditional spectrometer using 1D grating. The spectrum range and resolution varies along the z direction on the CCD. Therefore, their spectrum can be collected by one CCD

5 in a single shoot. This feature enables high speed broadband spectrum measurements without changing of grating or moving the detectors. Because spectra with different resolution as well as bandwidth range can be captured in same time, both high frequency and low frequency spectroscopic statistic and dynamic information can be captured simultaneously. By selecting the CCD pixel reading path, novel spectral measurement

10 function can be realized. For example, constant resolution spectrometer and constant central photon energy with varied spectral resolution are shown in figure 4 and table 1 below. Figure 4 shows the focus position on CCD imaging plane for (a) constant central frequency with multiple spectral resolving power (150 eV) 410 and (b) constant resolution (8 pixel/eV) 420. Table 1 shows a summary of the performance of the 2D VLS grating for

15 a constant incident wavelength and a constant resolution

	Spectrum range (eV)	Resolution (pixel/eV)
Constant Spectral Resolution	82 ~ 176	8
Constant Spectral Central Photon Energy with multiple spectral resolving power	150 eV	1.51~9.9

Table 1

Furthermore, the 2D grating can be designed to capture different spectral range using

20 different line of CCD pixel, ultra-broad band spectrum can be captured without switching the gratings or changing the mounting position of the camera. The time consumption of broadband spectral measurement can be greatly reduced. The detail of the 2D grating modelling and design will now be described as follows.

25 The schematic of 2D VSL 510 grating is shown in figure 5. Different from traditional VSL grating, the 2D VSL grating 510 has varied groove density and period function along the z direction (i.e. along the groove direction). In this way, the diffraction pattern on the CCD imaging plane becomes 2D rather than 1D in the traditional spectrometer using 1D VSL grating. The spectrum range and resolution at different z position on the CCD plane is

30 different. The groove density function $G(z)$ and period function $d(y, z)$ are designed to

focus the incident EUV/X-ray source on the CCD imaging plane. An algorithm is also developed to read out the 2D spectrum mapping on the CCD imaging plane.

Figure 6 shows the groove pattern of the proposed 2D VLS grating. The groove density G is linearly increased from 300 to 1500 along the positive z direction where $G(z)$ varied from 300 line/mm to about 1500 line/mm and b_2 vary from -19.5 to -19.59, where b_2 is the first order coefficient of the period function. This gratings design covers the spectral range from 10eV to 1500ev. With a CCD camera pixel size of 13.5um, the resolvable maximum HHG spectrum (415eV with minimum resolution of 1.33pxiel/eve with a grating length of 30mm (see table 2 below). The period function (based on equation (5) below) can be expressed as

$$d(y) = \frac{1}{G(z) \left(1 + \frac{2b_2(z)}{R} |y| \right)}$$

With $G(z) = G_{\min} + \frac{G_{\max} - G_{\min}}{L} z$ and $b_2(z) = b_{\min} + \frac{b_{\max} - b_{\min}}{L} z$; L is the length of the grating effective area; $G_{\max}$, $G_{\min}$, $b_{\max}$, $b_{\min}$ are determined by the designed spectral range and resolution range expected to be covered and can be found in table 3; and z is between 0 and 30mm with a 15mm offset to shift the line of $z=0$ to the center of the grating forming a symmetrical design. It should be noted that due to fabrication capability, the simulation and test results as provided in this disclosure are limited to groove density of 300 line/mm, 1200 line/mm and 2400 line/mm. While the simulation and test results for groove density of 1500 line/mm are not provided in this disclosure, one skilled in the art will recognise that the results for groove density 1500 line/mm can be easily derived from the simulation and test results in relation to groove density of 1200 line/mm and 2400 line/mm.

The CCD imaging plane is placed 235 mm away from the grating center along the y direction as shown in figures 7A and 7B. The EUV/X-ray incidence has different diffraction patterns on the CCD imaging plane along the z direction when diffracted from the 2D VLS grating 710. Figure 7A shows the imaging plane of the incident light at low resolution 740 position when $G(z) = 300$. The interception of the x and y axis show the grating position at $x=0, y=0$ projecting to the CCD imaging plane 730 at $y=235$. The lightly shaded part 740 shows the imaging position of high photon energy region (>123 eV), which has very low resolution due to the linear dispersion of and the out of focus at the CCD imaging plan. However, as shown in figure 7B, when the incident light is diffracted

from the high resolution position when $G(z) = 1500$, the resolution 750 for a particular wavelength, e.g. 150 eV, becomes higher. In short, the imaging plane with higher groove density as shown in figure 7B has better resolution compared to the imaging plane with lower groove density as shown in figure 7A. Based on 150 eV incidence, the imaging position shift from high photon energy region to low photon energy region with improved resolution when the groove density is increasing.

Table 2 below summarizes the performance of the 2D VSL grating, which can measure spectrum range from 10 eV to 415 eV light with minimum resolution (1.33 pixel/eV) capable to resolve the HHG pumped by 800 nm laser.

Performance	Spectrum range (nm)	Resolution@150ev (pixel/ev)	Max photon energy resolvable
Low resolution	2.5 to 50	2.56	123 ev
Medium resolution	1.4 to 16.5	7.82	293 ev
High resolution	0.8 to 9.5	9.90	415 ev

Table 2: The summary of the performance of the 2D VLS grating.

To avoid focus curvature in traditional grating with constant groove density and extend the spectral ranges to EUV/soft X-ray regions, the 2D grating are optimized using the VLS method to focus EUV/X-rays radiation from 10eV to 1500eV into a flat field. Then EUV/X-ray spectrum is spectrally resolved by single X-ray CCD camera at fixed position. The details of the 1D VLS grating design process will first be discussed below followed by the 2D VLS grating according to this disclosure.

Grating is one of the most commonly used optical components in spectrometers due to the designable light dispersion capabilities. Both gratings and prisms can be used as the dispersive optical components in visible and infrared spectrometers. However, in EUV/X-ray region, gratings become the most practical choice as the material absorptions become one of the major concerns in the spectrometer design. Furthermore, the absorption also leads to the limited choice of EUV/X-ray optics, which affects the EUV/X-ray spectrometers design in two aspects: 1) the incident light is focused or collimated using glazing incident mirrors before reaching the entrance slit. 2) The grating with imaging plane is designed to meet the requirement of the detectors, e.g. flat imaging plane for CCDs and MCPs, to avoid further absorption of collimation optics between grating and detector. Therefore, it is essential to understand the principle of diffraction gratings to choose or design the gratings the EUV/X-ray spectrometers.

Figure 8 shows a schematic of grating illuminated by monochromatic light. On the left of figure 8 indicated as reference (a), the plane wave expansion of the sphere wave emitted by a single point on the grating. On the right of figure 8 indicated as reference (b), the plane wave emitted from adjacent grating pitches.

When illuminated by incident monochromatic light with wave vector k_0 , each point on the grating surface emits a sphere wave with electric field $E(r) = E_0 \frac{e^{ik'r}}{r}$, which can be expanded by using plane waves as shown on the left of figure 8 indicated as reference (a) and expressed in the following expression

$$E(r) = \frac{1}{(2\pi)^{3/2}} \iiint f(k) e^{ikr} d^3 k \quad (2)$$

$$\text{where } f(k) = \frac{1}{(2\pi)^{3/2}} \iiint E_0 \frac{e^{ik'r}}{r} e^{-ikr} d^3 r = \sqrt{\frac{2}{\pi}} \frac{1}{k^2 - k'^2}$$

The wave vector k_i determine the reflection angle β_i of each plane wave component. For the points from adjacent grating pitches (e.g. A and D as shown on the right of figure 8 indicated as reference (b)), the emitted plane wave $E_i e^{ik_i r}$ with same reflection angle β_i has optical path difference OP as

$$OP = AB - CD = d \sin \alpha + d \sin \beta \quad (3)$$

These angles are measured from the grating normal, which is the dash-dot line perpendicular to the grating surface at its center (shown on the right of figure 8 indicated as reference (b)). The sign convention for these angles depends on whether the light is diffracted on the same side or the opposite side of the grating as the incident light. With reference to grating in figure 8 indicated as reference (b), the angles $\alpha > 0$ and $\beta_i < 0$ are measured counterclockwise and clockwise from the grating normal, respectively.

Therefore, the grating function can be written as

$$d(\sin \alpha + \sin \beta) = m \lambda \quad (4)$$

where m is the diffraction order of the grating and λ is the incident wavelength.

The flow chart of the spectrometer design is shown in figure 9. Firstly, a grating is selected based on the requirement for the proposed specifications. The choice of the grating determines the key specifications of the spectrometer, including the resolution R ,

throughput T and the spectrum range SR . There are always trade-offs between different specifications of the spectrometers. For example, a large groove density is preferred to increase the resolution at given incident wavelength, which will inevitably decrease the spectrum range. Therefore, the grating design is the key innovation of a spectrometer.

- 5 Once the grating design is finished, the mounting parameters of the grating, i.e. the incident angle α , the diffraction angle β , the incident distance r and the focal distance r' , will define the entrance slit and CCD position. Then further optimization is required to meet the spectrometer specifications, e.g. the choice of metal filter, the pre-focus optics and the slit opening.

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Figure 10 shows a schematic of spherical varied-line-space (VLS) grating. Most conventional EUV/X-ray spectrometers utilize grazing-incidence concave gratings as shown in figure 10 in which the dispersion and focusing functions of spectral images are combined in a single optical element for high throughput. The gratings are designed with
 15 varied line space to fit the imaging plane of the detectors (e.g. CCD, MCP). Therefore, those gratings can be defined as the concave curve radius R , groove density G and period function $d(w)$

$$d(w) = d_0 / (1 + \frac{2b_2}{R}w + \frac{3b_3}{R^2}w^2 + \dots) \quad (5)$$

- 20 Figure 10 shows the schematic of a spherical VLS grating when the incidence is from a point source A and focused at point B and the optical path of the incidence satisfy the following equation.

$$(AO + OB) - (AP + PB) = m\lambda \quad (6)$$

where $O(0,0)$ is the center of the grating and chosen as the origin of the Cartesian
 25 coordinates system and $P(u, w)$ is an arbitrary point on the grating surface.

Define

$$\begin{aligned} F(u, w) &= AP + PB + m\lambda \\ &= F(0,0) + wF_{01} + w^2F_{02} + uwF_{11} + u^2F_{20} + T(w^3) \end{aligned} \quad (7)$$

where

$$30 \quad F_{ij} = \sum_{i,j=0}^{\infty} \left\{ \frac{1}{(i+j)!} \sum_{i,j=0}^{i+j} \frac{(i+j)!}{i!j!} \frac{\partial^{(i+j)} F(u,w)}{\partial u^i \partial w^j} \Big|_{(0,0)} u^i w^j \right\} \quad (8)$$

$F(0,0) = AO + OB$ and $T(w^3)$ is a term with in w^3 or higher

$(u - R)^2 + w^2 = R^2$ since $P(u, w)$ is on the grating with curve radius R

Let $AO = r, OB = r'$

$$x = r \cos \alpha, y = r \sin \alpha \text{ and } x' = r' \cos \beta, y' = r' \sin \beta \quad (9)$$

Substitute Eq. (4) and Eq. (5) to Eq. (7)

$$F(u, w) = \sqrt{(r \cos \alpha - u)^2 + (r \sin \alpha - w)^2} + \sqrt{(r' \cos \beta - u)^2 + (r' \sin \beta - w)^2} + d(w)(\sin \alpha + \sin \beta) \quad (10)$$

Every F_{ij} term can be expressed as by substituting Eq. (10) and Eq. (5) to Eq. (8)

$$F_{ij} = C_{ij} + \frac{m\lambda}{d_0} M_{ij} \quad (11)$$

where

$$C_{01} = -\sin \alpha - \sin \beta \quad (12)$$

$$M_{01} = 1 \quad (13)$$

$$C_{02} = \frac{1}{2} \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} \right) + \frac{1}{2} \left(\frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{R} \right) \quad (14)$$

$$M_{02} = b_2/R \quad (15)$$

Substitute Eq. (6) to Eq. (7)

$$wF_{01} + w^2F_{02} + uwF_{11} + u^2F_{20} + T(w^3) \dots = 0 \quad (16)$$

Since $P(u, w)$ is an arbitrary point on the grating,

$$F_{ij} = 0 \quad (17)$$

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The selection of the grating parameters is the first and the most important step towards building up a EUV/X-ray spectrometer. The most important parameters of gratings are concave curve radius R , groove density G and period function (Eq. (5)), which, together with the incidence, define the imaging plane of the grating. Other parameters including the grating pitch profile, substrate and coating materials affect the efficiency of the grating. For glazing-incidence gratings, the radius R is very large (several meters). Therefore, $w \gg u$, when P is on the grating with curve radius R . Therefore, uwF_{11} , u^2F_{20} and $T(w^3)$ are much smaller when compared with wF_{01} and w^2F_{02} . The grating parameters are randomly given and evolved using certain functions f_i . Then the imaging plane $B(\lambda)$ is derived by

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$$F_{01} = C_{01} + \frac{m\lambda}{d_0} M_{01} = 0 \quad (18)$$

$$F_{02} = C_{02} + \frac{m\lambda}{d_0} M_{02} = 0 \quad (19)$$

Substitute Eq. (12) and Eq. (13) to Eq. (18)

$$\beta = \arcsin\left(\frac{m\lambda}{d_0} - \sin\alpha\right) \quad (20)$$

Substitute Eq. (14) and Eq. (15) to Eq. (19)

$$5 \quad r' = \frac{rR\cos^2\beta}{r[\cos\alpha + \cos\beta - 2(\sin\alpha + \sin\beta)b_2] - R\cos^2\alpha} \quad (21)$$

The x and y coordinates, i.e. B_x and B_y of the imaging point B are the functions of λ

$$B_x = r' \cos\beta \quad (22)$$

$$B_y = r' \sin\beta \quad (23)$$

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Figure 11 shows the flowchart of a process for selecting grating parameters using genetic algorithms. The y coordinates of the imaging point for each wavelength, i.e. $B_y(\lambda)$, is designed to be the same in order to meet the requirement of flat imaging plane of MCP or CCD. Therefore, grating parameters R, G and $d(w)$ are evaluated by targeting parameters, e.g. the standard deviation of $B_y(\lambda)$. The optimization process is repeated to form the next generation of grating parameters until the targeting criteria is reached.

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A grating of $G = 1200$ lines/mm is designed to have a plane imaging when the incident wavelength is from 5 nm to 20 nm (248 eV to 62 eV). The radius of the grating $R = 5650$ mm, the incident light is a point source with $r = 237$ mm and the incident angle $\alpha = 87^\circ$ are fixed to simplify the optimization process. The imaging plane can be derived by substituting G, R, α, r and λ into Eq. (16-19) as shown in figures 12A and 12B. Figure 12A and 12B show an evolution of the imaging plane by optimizing period function of the grating with groove density of 1200 lines/mm. Figure 12B shows different imaging plane when b_2 is from -30 (left) to -20 (right). Figure 12A shows the standard deviation of B_y in the interested wavelength range (62 eV to 248 eV) at different b_2 . Figure 12A shows how the imaging plane is changed by the optimization of the grating period function. The imaging plane of the interested wavelength range is highlighted with darker line. Here, the evolution function is chosen as $f_3(b_2) = b_2 + 1$. The initial value of the b_2 is chosen as -30. The targeting parameters is chosen as the standard deviation of $B_y(\lambda)$ and the optimization process is stopped until the standard deviation of $B_y(\lambda)$, is less than 0.5 mm as shown on figure 12B. In this way, a flat imaging plane along the y axis can be achieved by the optimization of $b_2 = -20$. It should be point out that the flatness of the

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imaging plane, i.e. the standard deviation of $B_y(\lambda)$, is affected by the incident wavelength range.

The flatness of the imaging plane is very poor at shorter and longer wavelength, i.e. from 1 nm to 5 nm and 20 nm to 80 nm, which is shown on figure 12A. Therefore, high groove density grating, e.g. $G = 2400$, should be used in shorter wavelength region while low groove density grating should be used at longer wavelength region for the sake of the spectrometer performance.

Figures 13A, 13B, 14A and 14B show the optimization of grating parameters for the incident wavelength range from 10 eV to 62 eV and 248 eV to 1500 eV respectively. Specifically, figures 13A and 13B are based on grating of $G = 300$ lines/mm while figures 14A and 14B are based on grating of $G = 2400$ lines/mm. The optimization process is the same as discussed with reference to figures 12A and 12B. It should be pointed out that the optimization of the grating radius is also important for the flat image plane when the groove density variation is very large. The proposed spectrometer can work from 10 eV to 1500 eV with flat imaging plane by using three different gratings with optimized parameters summarized in table 1, which shows that the grating radius is similar for $G=300$ and 1200 grating while the radius is tripled for $G=2400$ grating.

The details of the 1D VLS grating design for EUV/X-ray spectrometer is shown in the table 3 below. G is the groove density, b_2 is the first order coefficient of the period function and R is the radius of the concave grating.

<i>Frequency range (eV)</i>	<i>G (lines/mm)</i>	<i>b₂ (n.u.)</i>	<i>R (mm)</i>
10 ~ 60	300	-19.5	5650
60 ~ 250	1200	-20	5560
250 ~ 1500	2400	-54.8	15000

Table 3

We now return back to the 2D VSL grating as shown in figure 5. By optimizing the 2D grating pattern, all the diffraction beams are focused at the same one flat plane. Figure 5 shows the schematic of 2D VLS grating design where the variation of the groove density along z direction enables the broadband and high resolution spectrometer using 2D detectors array. Figure 6 shows the zoomed-in view of the groove pattern of proposed 2D VLS grating. The table 4 below shows the design parameters of the 2D VLS grating. It should be noted that in the design parameters, z is 30mm in height with a 15mm shift

such that the center of the grating is 300 lines/mm (when $z=0$) and the ends are about 1500 lines/mm (where $z=-15$, $z=15$). The 2D VLS grating is focused to 7mm on the CCD. The spectral range is from 10eV to 1500eV. With a CCD camera pixel size of 13.5 μm , the resolvable maximum HHG spectrum (1.33 pixel/eV, means about 5 pixels to cover the 3eV distance between neighbour HHG odd order) is 415eV.

Grating parameters		
Incident angle	Incident distance	Grating radius
87°	237mm	5567mm
$b_2 = -19.5 - 0.003z$	$G(z) = 300 + 40.1z$	
CCD position (mm)	$X = 17\sim 43, y = 235, z = -3\sim 3$	

Table 4

We now turn to the arrangement of the 2D VLS grating. It is important to know where to put the incident slit and the 2D detector, e.g. CCD. Grating mounting parameters are those parameters corresponding to the relative positions of grating to entrance slit and detectors, which include the distance between the entrance slit and grating central r , the focal length of the grating r'_1 and r'_2 , the incident angle α , the position of the CCD imaging plane (y_0 , x_1 and x_2) as shown in figure 15. Briefly, figure 15 shows a schematic of a 2D VLS grating with mounting parameters.

The grating mounting parameters can be calculated by using Eq. (20) and Eq. (21). By substituting the incident light parameters λ , r and α into Eq. (16) and Eq. (17), the mounting parameters of the CCD camera can be calculated using $x(\lambda) = r'(\lambda)\cos(\beta(\lambda))$ and y_0 is the mean value of the $y(\lambda)=r'(\lambda)\sin(\beta(\lambda))$ over the interested frequency range. Figure 16 shows the calculation results of the mounting parameters for a grating with groove density 300 lines/mm 1610, 1200 lines/mm 1620 and 2400 lines/mm 1630. The bottom right of figure 16 shows the deviation angle between the incident and reflected light with different photon energies. Specifically, the solid 1640, dash 1650 and grey 1660 lines represent gratings with groove density of 300, 1200 and 2400 lines/mm. The table 5 below summarizes the mounting parameters of each grating working at different frequency region.

Frequency range (eV)	G (lines/mm)	α (degree)	r (mm)	y_0 (mm)	$x_1 \sim x_2$ (mm)	Deviation angle (degree)
10 ~ 60	300	87	237	234.34	28.70~67.05	164.07~170.04
60 ~ 250	1200	87	237	235.38	28.88~54.09	161.04~170.03
250 ~ 1500	2400	88.65	237	234.97	9.11~30.37	169.66~174.80

Table 5: The mounting parameters of the CCD for different gratings

It should be noted that the parameters in table 4 are the optimized design parameters used in experiment and are selected from the parameters in table 5. Hence, the 2D VLS grating is not limited to the parameters in table 4. The parameters in table 5 are general calculation. Therefore, the parameters used in table 4 are within the parameters as shown in table 5. In other word, the parameters of the 2D VLS grating can be selected from the parameters in table 5. Hence, $y=235$ in table 4 is within the range of 234.34 and 235.38 in table 5; $X=17-43$ in table 4 is within the range of 9.11 and 67.05 in table 5.

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The table above shows the mounting parameters of CCD for different gratings that are close to each other: 1) the y_0 variation is approximately 1 mm which is less than 0.5%. 2) The total range of $x(\lambda)$ is 57.94 mm which can be easily covered by a standard DN100 port for vacuum chamber. 3) The total deviation angle variation range is within 15° . The merits of the mounting parameters are two folds. One is that the CCD can be mounted at one position which simplifies the chamber design. The other is that the flat imaging plane almost overlaps with each other which ensure a fast detection speed with CCD or dipoles array. Also, it only requires 1D translation when the detector plane of the CCD is not big enough to cover 57.94 mm. These mounting parameters are achieved by the optimization of grating parameters.

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The HHG source is very weak, typically 10^7 photons/s, and ultra-broadband from 10s eV to 3 Kev. Therefore, it is essential to collect as much incident light as possible to meet the sensitivity of the detectors. In other words, it is important for the design of optical component to increase the throughput of the entrance slit before the entrance slit. Another concern is that the entrance slit opening has to be as small as possible to maintain the resolution and block the stray light from the pump laser. The typical spot size of HHG source at the pump laser focal spot is tens of microns. However, neither the entrance slit nor the grating can be mounted so close to the pump laser focus without being damaged by the ultra-high intensity of the pump laser, which is approximately 10^{14} w/cm². Therefore, in the proposed spectrometer, HHG source is focused at slit position along the direction perpendicular to the slit edge (x-direction) using a spherical mirror as

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shown in figure 17A. A cylindrical mirror is used to focus the EUV/X-ray source at the imaging plane along z-direction for higher intensity at imaging plane. The incident angle of both spherical mirrors θ_1 and cylindrical mirrors θ_2 are 85° . Figure 17A shows the schematic of optical path for the EUV spectrometer. The distances between the HHG source, spherical mirror, cylindrical mirror and the entrance slit are defined as L , L_1 and L_2 , respectively. L , L_1 and L_2 satisfy the following equations

$$\frac{1}{L} + \frac{1}{L_1 + L_2} = \frac{2}{R_s \cos \theta_1} \quad (25)$$

$$\frac{1}{L + L_1} + \frac{1}{L_2 + 237 + 235.3} = \frac{2 \cos \theta_2}{R_c} \quad (26)$$

where $R_s = 6500$ mm and $R_c = 67.14$ mm are the radii of the spherical mirror and cylindrical mirror, respectively. The size of spherical lens is 30 mm in diameter while the cylindrical mirror is 30 mm $\times$ 60 mm. Here, for the uniformity of the simulation the HHG source spot size is chosen to be 60 μm unless specified.

In certain measurements, a concave mirror may be required to implement projection function in EUV range. This is assuming a flat 2D VLS grating 1710 is implemented. As shown in the top drawing of figure 17B, the flat 2D VLS grating 1710 is arranged very close to the concave mirror. The distance between the flat 2D VLS grating 1710 and the concave mirror is small, typically 10mm compared with r and y which are several hundred mm to 1m. This arrangement of concave mirror and flat 2D VLS grating 1710 can approximately play the same function as a curved 2D VLS grating 1720 as shown in bottom of figure 17B. Alternatively, we may simply use a curve 2D VLS grating 1720. Specifically, the curve 2D VLS grating has a curved surface. This will eliminate the requirement of a concave mirror to project the incidence to the 2D VLS grating. It should also be noted that in EUV range, it is very hard to implement collimation. Hence, only projection is required, which means imaging the small spots at slit to a small spots on CCD surface. It is also worth mentioning that the curved 2D VLS grating is more suitable for wavelengths other than EUV.

Figure 18A shows the simulation results of the mirror mounting position as the function of the distance between HHG source and spherical mirror L . Eq. (25) and Eq. (26) have two sets of solutions (1810 and 1820) when L is smaller than 1200 mm. The second set of solution 1820 has smaller L_1 1821 when compared to L_1 1811 of the first set of solution 1810 and larger L_2 1822 when compared to L_2 1812 of the first set of solution 1810. The

focal distance of the spherical mirror 1830 decreases when L is increasing as shown in figure 18B. Therefore, the spot size along x-direction decreases as L is decreasing as shown in figures 19A and 19B. However, the spot size reach the diffraction limit of 10 eV light source when L is larger than 617.5 mm, which means the spot size cannot be further reduced with current setup for HHG lower than 10 eV. Figure 19B shows the spot size of the cylindrical mirror has already reach the diffraction limit as the focal distance of the cylindrical mirror is much larger than the spherical mirror. Therefore, it is pointless to have L larger than 617.5 mm for broadband spectrometer design with spectrum range including 10 eV. Besides, larger L also induces large EUV absorption and difficulty to maintain the vacuum level.

Figures 18A and 18B show the mounting position between the X-ray optics and the corresponding focal distance. Specifically, figure 18A shows the distance between the spherical mirror 1812 and 1822 and cylindrical mirrors 1811 and 1821 and the distance between the entrance slit and the cylindrical mirrors 1811 and 1821 as the functions of L . Figure 18B shows the focal distance of the spherical mirror 1830 and cylindrical mirror 1840. Figures 19A and 19B show the spot size on the entrance slit and CCD imaging plane as the functions of the objective length of the X-ray source. Specifically, figure 19A shows the width of the spotsizes on the entrance slit (x-direction) 1910 and the diffraction limit of the spherical mirror at 10 ev 1920 and 15 ev 1930. Figure 19B shows the height of the spotsizes on the CCD screen (z-direction) 1940 and the diffraction limit of the cylindrical mirror at 10 ev 1950 and 15 ev 1960.

Figure 20 shows the transmission of the entrance slit as the function of L at different slit openings, namely, slit opening of 100 μm 2010, slit opening of 80 μm 2020, slit opening of 60 μm 2030, slit opening of 40 μm 2040, and slit opening of 20 μm 2050. The slit transmission increases as the L is increasing. The slit transmission is larger than 95% when the slit opening is larger than 80 μm and L is larger than 550 mm. Therefore, the slit opening in the spectrometer design is chosen to be 80 μm for high throughput without further sacrifice the resolution. L_1 and L_2 is chosen according to the physical constrain of the mirrors. The distance between spherical mirror and cylindrical mirror L_1 are limited by their widths and incident angles. L_2 is limited by the chamber separation, which is much larger than 200 mm. Therefore, the pre-focusing optics mounting parameters are chosen as $L = 570.1$ mm, $L_1 = 72.0$ mm and $L_2 = 490.9$ mm.

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Spectral Resolution

The spectral resolution of a spectrograph based spectrometer is a measure of its ability to resolve features in the electromagnetic spectrum. In EUV/X-ray frequency region, frequency spectra are often used, which is more directly corresponding to the photon energy other than the wavelength. The spectral resolution of the spectrometer is determined by several parameters including the entrance slit opening, the signal spot size on the grating, the spatial dispersion of the grating, the detector pixel size and the incident wavelength. Altogether, they define the resolution of the whole spectrometer. Therefore, it is very important to understand where the bottleneck of the spectral resolution comes from to ensure the selected gratings, detectors entrance slits are compatible with each other and avoid unnecessary cost for the EUV/X-ray spectrometer.

The spectral resolution of a planar grating is determined by

$$R = \frac{\lambda}{\Delta\lambda} = m \cdot N \quad (27)$$

where λ is the central wavelength, m is the diffraction order, N is the number of grooves illuminated by the beam. The full width half maximum (FWHM) of the central wavelength is defined by $\Delta\lambda$. Eq. (27) shows that the best resolution R is achieved when the maximum number of grooves is illuminated, which is determined by the signal spot size diameter on the grating ϕ_g and the groove density of the grating G where $N = \phi_g \times G$. Here the gratings are working at first diffraction order $m = 1$ for better diffraction efficiency.

The spot size on the grating is determined by the incident spot size on the entrance ϕ_s slit and the slit opening

$$\phi_g = \phi_s \sqrt{1 + \left(\frac{Z}{Z_r}\right)^2} \quad (28)$$

where $Z_r = \frac{\pi\phi_s^2}{\lambda}$ is the Rayleigh length of the Gaussian beam. Here, slit opening is chosen to be 80 μm , which is similar as the HHG spot size on the slit.

The linear dispersion of the grating D_g is defined by the spatial separation Δx on the imaging plane over the photon energy ΔE difference of the HHG source while $D_g(E) = \Delta x(E)/\Delta E$. The linear dispersion of gratings for different groove densities is shown in figure 21A. The linear dispersions of the gratings are decreasing as the incident photon energy increases, which indicate that high photon energy light is more difficult to be resolved. Figure 21B shows the spectral resolutions for different gratings when the slit opening is fixed at 80 μm .

Figures 22A and 22B show the spectral resolution determined by the CCD with pixel size of 13.5 micron and gratings at different slit openings. Here the resolution is derived by Eq. (27) and Eq. (28) for different slit openings. The CCD resolution is calculated by using $\frac{D_g}{\text{pixel size}}$. Figure 22A shows the limitation of system resolution is caused by low groove density when $G = 300$. Therefore, decreasing the slit opening will increase the system resolution since smaller slit opening results in large spot size on the grating and higher resolution power. However, the CCD pixel size becomes the bottleneck of the system resolution as the grating groove density is increased to $G=2400$ as shown in figure 22B. Therefore, the changes to the slit opening will not increase the spectral resolution of the spectrometer. Figure 23 shows the spectral resolution of the whole spectrometer system under grating groove density $G = 300$ 2310, $G = 1200$ 2320, $G = 2400$ 2330. The highlighted part is the spectral resolution of each grating under their incident spectrum range as shown in Table 1.

Throughput of the Imaging Spectrometer System

The HHG source is attenuated by many factors before it reach the detector, including the reflection of the spherical and cylindrical mirrors R_{sphere} and R_{cylinder} , the transmission of the entrance slit T_{slit} , the diffraction efficiency of grating η_{grating} and the filter transmission T_{filter} . Here the throughput of the imaging system can be expressed as

$$T_{\text{sys}} = R_{\text{sphere}} \times R_{\text{cylinder}} \times T_{\text{slit}} \times \eta_{\text{grating}} \times T_{\text{filter}} \quad (29)$$

The material reflection and filter transmission coefficient can be obtained in the online data base from Center for X-Ray Optics, Lawrence Berkeley National Laboratory. Figure 24A shows the reflection coefficient of gold mirror under different incident angle, namely 87 degree 2410, 85 degree 2420 and 83 degree 2430. Figure 24B shows the transmission coefficient of Al (Aluminium) filters with different thickness, namely 200nm 2440 and 500nm 2450. The reflection coefficient is highly depended on the incident angle, especially for the high photon energy region. The Al filter transmission coefficient decreases as the thickness increases, especially for low photon energy region. Figure 25A shows the measured diffraction coefficient of the first order for $G=1200$ grating 2510 and $G=2400$ grating 2520. The grating contributes to the major attenuation of the whole spectrometer system. The total throughput of the spectrometer is shown in figure 25B, which is below 2.5%. Although the Al filter does not dominate the attenuation of the

spectrometer system, the cut off frequency at 72 eV still can be clearly observed in figure 25B, which can be used for the calibration of the HHG spectra.

- Most materials are highly absorptive in EUV region and the atoms ionized by X-ray can affect the CCD detector which is barely protected for better sensitivity. Therefore, the spectrometer system is designed to work at vacuum environment. The major concern of the chamber design is the angle between incident and diffracted light, which is defined as deviation angle. Figure 26 shows the deviation angle as the function of incident photon energy calculated using the parameters of a grating with groove density 1200 lines/mm.
- The detectable photon energy ranges are also shown in table 6 below for different ports.

Input Ports	Angle range ($^{\circ}$)	Photon energy range
A1	(32.8, 123.2) U (152.8, 180)	17ev to 1500 ev
A2	(58.8, 123.2) U (130.8, 180)	10ev to 1500 ev
A3	(58.8, 145.2) U (152.8, 180)	17ev to 1500 ev
A4	(32.8, 83.2) U (94.8, 180)	10ev to 1500 ev

Table 6

Test results

- A prototype is fabricated using silicon lithography to demonstrate the working principle of 2D VLS grating as shown in figure 5. The groove density $G(z)$ ranges from 300 to 100 lines/mm. This is lower than that described above due to limitation of fabrication facilities available. To avoid edge effect at high groove density region, the grating is designed symmetry along the axis of $z=0$ ($G(z)=G(-z)$). The grating is characterized using a 632-nm laser and a 532-nm laser. Figure 27A shows the scattering pattern of 632-nm laser on a white board. Figure 27B shows the scattering pattern of 632-nm laser detected by CCD. Figure 27C shows the scattering pattern of 532-nm laser detected by CCD. The far field scattering pattern of 632-nm laser is shown in figure 27A. The laser is incident on the center of the grating with the beam size of 9.3 mm. The first order diffraction pattern is split into different spots due to the variation of groove density $G(z)$ along the z direction.
- The spot diffracted from high groove density region is far away from 0th order spot and has larger spot size along x direction, which indicates higher resolution with smaller spectrum range. The first order scattering pattern is focused onto a CCD (acA2500 BASLER) using a convex lens. The scattering pattern from two different lasers with same incident angle and incident position are detected by the CCD as shown in figure 27B and 27C. A pin hole is placed before the 2D VLS grating to control the spot size of both lasers. The spots diffracted from the same groove density of the 2D VLS grating of both

lasers are identified by changing the spot size of the lasers. They are given the same spot number (SN) for calibration purpose.

The reading from CCD is integrated along z direction and then converted to optical intensity using known quantum efficiency. The normalized intensity as the function of pixel number along x direction is shown in figures 27B and 27C. Here, the normalized intensities are read from different CCD area marked with SN, which have fixed area size of 100 pixels. The separations of 532-nm laser peak 2710 and 632-nm laser peak 2720 are increasing with SN, which indicates an increasing in resolution.

Figure 28 shows the normalized optical intensity as the function of pixel number along x direction. The gray and thick black lines represent the optical intensity of 532-nm laser 2810 and 632-nm laser 2820, respectively. The SN number represents the spots at different CCD positions as shown in figures 27B and 27C.

The 632-nm laser is used as the calibration light to obtain the spectrum of the green laser. First, the 632-nm laser is measured using a commercial spectrometer USB4000 from Ocean Optics, which shows the central wavelength of the laser is 632.8 nm. Then, the incident angle and the distance between the CCD plane and grating center is calibrated by using the peak positions of the 632-nm laser. Finally, the pixel number of figure 28 is converted to wavelength based on the calibration results. Therefore, the spectra of the 532-nm laser is obtained. For visible spectral measurement, the total spectral range with central 6 grating lines and 2000 CCD pixels (in box 2830) is 300nm to 1000nm with resolution varied from 3884.2 to 1553.6 and bandwidth varied from 341.5nm to 554.9nm. When same grating used EUV and X-ray spectral measurement, the central 6 grating lines with 500 CCD pixels is able to cover the spectral range from 9.4eV (110nm) to 1600eV (0.76nm) with resolution varied from 81 (0.5eV/pixel @100eV) to 49.85 (0.3eV/pixel @100eV) and bandwidth varied from 800ev to 1600eV.

Figure 29 shows the measured spectra of 532-nm laser using proposed 2D VLS grating. The top line shows the measurement results from commercial spectrometer (USB 4000 from Ocean Optics). The rest lines show the measurement results from 2D VLS grating derived from different areas of CCD marked as spot number (SN), which shows different detection range and resolution. On the right shows the spectrum range and resolution as functions of CCD reading area. Figure 29 shows the measured spectra results of 532-nm laser using 2D VLS grating, which agree with the measured results from commercial

spectrometer. It proves that by reading the scattering pattern from different CCD area, the spectrum range (23.2 nm to 13.1 nm) and resolution (2293.1 to 4061.0) can be varied more than 75%, which is limited by the smallest feature size of our fabrication process.

- 5 The possible application includes X-ray industry such as tabletop X-ray source calibration, X-ray based spectroscopy and imaging, defect inspection; biological and medical industry such as lensless imaging of biological samples, real-time inspection of medicine production, high speed optical coherent tomography; and material industry such as material characterization and inspection, molecular dynamics study.

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While the invention has been illustrated and described in detail in the drawings and foregoing description, such illustration and description are to be considered illustrative or exemplary, and not restrictive; the invention is not limited to the disclosed embodiments. Other variations to the disclosed embodiments can be understood and effected by those

- 15 skilled in the art in practising the claimed invention.

Claims

1. A spectrometer comprising:

5 a 2 dimensional detector that captures multiple spectra within a lower resolution broad range (LRBR) and a higher resolution narrow range (HRNR) simultaneously; and

a 2 dimensional grating having grooves with variable groove density and period function, the groove density $G(z)$ and period function $d(y, z)$ are adaptable to
10 focus incident EUV/X-ray source from a slit onto the 2 dimensional detector where z is a direction along the grooves and y is a direction across the grooves.

2. The spectrometer according to claim 1 wherein the groove density G is linearly increased from 300 to about 1500 along a positive z direction where the
15 period function can be expressed as

$$d(y) = \frac{1}{G(z) \left(1 + \frac{2b_2(z)}{R} |y| \right)}$$

where $G(z) = 300 + 40.1z$, $b_2 = -19.5 - 0.003z$, $R = 5567\text{mm}$ and z ranges between 0-30mm.

20 3. The spectrometer according to claim 1 wherein the 2 dimensional grating is arranged such that the incident angle from the slit is 87° and at an incident distance of 237mm.

4. The spectrometer according to claim 1 wherein the 2 dimensional detector is
25 apart from the 2 dimensional grating by a distance of 235mm from a center along the y direction of the 2 dimensional grating, between -3.5mm and 3.5mm of the z direction, and between 17 and 43mm in an x direction, the x direction being perpendicular to the y direction.

30 5. The spectrometer according to claim 1 further comprising a cylindrical mirror and a spherical mirror arranged such that the cylindrical mirror is between the spherical mirror and the slit.

6. The spectrometer according to claim 5 further comprising a concave mirror
35 arranged between the slit and the 2 dimensional grating.

7. The spectrometer according to claim 5 wherein the 2 dimensional grating has a curved surface.

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