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Ex situ metrology of x-ray diffraction gratings

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A R T I C L E I N F O

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A B S T R A C T

The idea of measurements of groove density distributions of diffraction gratings suggested and first realized in Proceedings of SPIE 5858, (2005) 58580A consists of determination of the spatial frequency of the first harmonic peak appearing in the power spectral density (PSD) distribution of the grating surface profile observed with a microscope. Using a MicroMap™-570 interferometric microscope, it was experimentally proven that this technique is capable of high precision measurements with x-ray gratings with groove densities of about 250 grooves/mm, varying along the grating by ±5%. In the present work, we provide analytical and experimental background for useful application of PSD characterization of groove densities of diffraction gratings. In particular, we analyze the shape of harmonic peaks and derive an analytical fitting function suitable for fitting the PSD peaks obtained with gratings with a variety of groove shapes. We demonstrate the capabilities of the method by application to the groove density distribution measurements with a 300-groove/mm grating suitable for soft x-ray applications.

1. Introduction

In the present work we consider metrology of x-ray gratings with interferometric microscopes. These gratings are the main elements of x-ray spectrometers and monochromators. There has been constant development of this instrumentation by improvement of grating fabrication and by simultaneous tightening of the requirements for the shape (groove distribution and profile) and fabrication tolerances of the gratings, associated with corresponding strengthening of requirements of the dedicated metrology.

A revolution in both concept and implementation of monochromators for soft x-ray wavelengths was begun with the seminal paper of Petersen [1]. The novel design separates the focusing and diffracting modalities allowing for better focusing performance over a wider x-ray energy range than spherical grating monochromators (SGM) where both functions are combined in a single optic. It also allows the monochromator to operate in the angular range where the efficiency of the grating is a significant fraction of the maximum attainable. The design [1] incorporates a unique patented mechanism that permits a single carefully selected rotation axis just behind the grating to maintain the focal properties when the grating and plane pre-mirror are rotated as a unit [2]. A systematic review of the new design compared to the classical SGM has been published in Ref. [3], 12 years after the original paper.

Concurrently with these revolutionary developments, Harada, Hettrick and their collaborators pioneered both the design and mechanical fabrication of new designs by the ruling and usage of varied line space (VLS) gratings [4,5]. It was only natural for the original idea and VLS to be combined and modified in various new ways [6–9]. For example, VLS gratings were made by interferometric methods [6], or the original concept of Ref. [1] was modified to use the grating in collimated light [10]. Recently, for undulator beams which naturally have quite small numerical apertures of emission, the use of this general approach has been further broadened by retaining the elegant single rotation of the pre-mirror/grating combination, but placing all of the focusing into the varied line space nature of the grating [11]. Even the shaping of the mirrors by heat loading from absorption of the beams may be taken into account [11]. A typical optical schematic of such a monochromator utilizing a VLS grating is shown in Fig. 1.

In this case, the VLS groove density function $g(w)$ is specified by a polynomial:

$$g(w) = g_0 + g_1 w + g_2 w^2 + \ldots \tag{1.1}$$

where w is the distance along the grating parallel to the optical path ($w=0$ is the grating center), g_0 is the groove frequency at the center of the grating, g_1 allows a linear variation of the groove frequency, and g_2 allows a quadratic variation of the groove frequency.

The grating equation in groove frequency units:

$$\mathrm{Sin}\,\alpha + \mathrm{Sin}\beta = m\lambda g_0 \tag{1.2}$$

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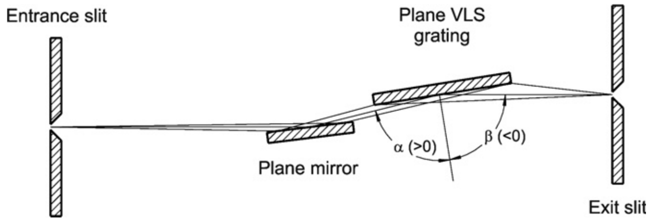

Fig. 1. Typical optical schematic of a monochromator utilizing a VLS grating.

when combined with the focusing equation for a VLS plane grating:

$$\frac{\mathrm{Cos}^2\,\alpha}{r}+\frac{\mathrm{Cos}^2\,\beta}{r'}=m\lambda g_1 \tag{1.3}$$

gives the defocusing function which must be minimized by the parameters of the design:

$$\mathrm{Sin}^2\,\beta\left(-\frac{1}{r}-\frac{1}{r'}\right)+\mathrm{Sin}\,\beta\left(\frac{2m\lambda g_0}{r}\right)+\left[\frac{1}{r}+\frac{1}{r'}-m\lambda g_1-\frac{(2m\lambda g_1)^2}{r}\right]=0. \tag{1.4}$$

The quadratic term in Eq. (1.1) is used to minimize the next order (spherical) aberration, and can also affect higher order terms.

Once these designs are optimized by ray trace and/or wavefront propagation methods, and the gratings are fabricated; it is the role of optical metrology to certify that the varying spacing of the grooves on the gratings are within specification so that the brightness of the beams may be preserved, and not destroyed by the monochromator system.

Let us estimate the required accuracy of groove density measurements with a typical x-ray VLS grating. Applying the results of work [12] to standard errors δg_0, δg_1, and δg_2 for the second order polynomial [Eq. (1.1)] coefficients g_0, g_1, and g_2, determined via linear regression analysis of a trace $g(w_i)$ of equidistant (with an increment Δw) points w_i ($i=0,1,\ldots,N$, $N\cdot\Delta w=L$ is the total length of the trace), one can write asymptotic ($N\gg 1$) expressions:

$$\begin{aligned}&\delta g_0=1.5\sigma/\sqrt{N},\\&\delta g_1=3.5\sigma/\left(\sqrt{N^3}\Delta w\right)=3.5\sigma/\left(\sqrt{N}\cdot L\right),\ \text{and}\\&\delta g_2=13.4\sigma/\left(\sqrt{N^5}\Delta w^2\right)=13.4\sigma/\left(\sqrt{N}L^2\right)\end{aligned} \tag{1.5}$$

where σ is the standard error of the groove density measurement of a single point. For a 150 mm long grating measured with 5 mm increments ($N=30$), expressions (1.5) give:

$$\begin{aligned}&\delta g_0=0.3\sigma\ \text{lines/mm},\\&\delta g_1=4\times10^{-3}\sigma\ \text{lines/mm}^2,\ \text{and}\\&\delta g_2=10^{-4}\sigma\ \text{lines/mm}^3.\end{aligned} \tag{1.6}$$

As an example of a typical specification, let us consider a VLS grating with the parameters $g_0=600$ lines/mm, $g_1=0.25$ lines/mm^2, and $g_2=4\times10^{-5}$ lines/mm^3 and requirements of fabrication accuracy on the level of:

$$\begin{aligned}&\delta g_0/g_0<0.2\%\ \text{or}\ \delta g_0<1.2\ \text{lines/mm},\\&\delta g_1/g_1<0.5\%,\ \text{or}\ \delta g_1<1.3\times10^{-3}\ \text{lines/mm}^2,\ \text{and}\\&\delta g_2/g_2<20\%,\ \text{or}\ \delta g_0<0.8\times10^{-5}\ \text{lines/mm}^3\end{aligned} \tag{1.7}$$

with an additional restriction applied to the appearance of higher order terms. Comparing (1.6) and (1.7), we conclude that the illustrated typical specification requires groove density distribution measurements with an accuracy of $\sigma\le 0.08$ lines/mm. This value corresponds to an absolute accuracy of about 100 nm/mm in linear displacement measurements with a grating. Note that the parameter of quadratic variation g_2 is the most difficult to measure in spite of the fact that only 20% accuracy is specified. Thus, extraction of the linear constant with the specified accuracy requires a measurement accuracy only $\sigma\le 0.3$ lines/mm.

The required and even significantly higher accuracy (30 nm/mm and better) is available with dedicated metrology instrumentation [13–16], such as, for example, the precision one-dimensional interferometrically controlled comparator designed and built at the German National Metrology Institute (PTB) for precise calibration of linear encoders and line scales [17]. However, such instrumentation is hardly available at any x-ray facility metrology laboratory. Instead, a method utilizing a more common x-ray optical metrology tool, namely the surface slope measuring long trace profiler (LTP), has been suggested and, to our knowledge, first realized at the ALS OML [18]; and now a number of modifications of the method are used worldwide [19–23].

A comprehensive analysis of LTP measurements with x-ray diffraction gratings is provided in Ref. [19]. It is shown that with an LTP error of 0.5 μrad rms the relative accuracy of groove density measurement in a particular grating position $\delta g(w)/g(w)\le10^{-5}$ is basically achievable. Indeed, LTP measurements are very sensitive to the relative change of the groove density distribution. Obtaining absolute values of the groove density requires significant additional effort to stabilize and calibrate the wavelength of the LTP light beam (especially in the case of a diode laser), to account for surface slope variation of the grating substrate, to precisely measure diffraction angle (e.g., corresponding to the Littrow configuration), as well as to compensate instrumental systematic (especially when measuring a VLS grating), mechanical, and drift errors. As a result, the practically achievable relative accuracy is on the level of $\delta g(w)/g(w)\le10^{-4}$ [20–23]. Moreover, special experimental arrangements are required for characterization of gratings with curved surface shape [22]. Additionally, the spatial resolution of LTP measurements is fixed by the cross-section of the light beam (1.5–2 mm), magnified in the Littrow configuration by the cosine of the diffraction angle.

In this work we report further developments of a novel method for ascertaining the VLS function of the grooves on the grating [24]. The method consists in characterization of x-ray diffraction gratings via a power spectral density (PSD) treatment of the grating surface topography, directly measured with an interferometric microscope. Possessing its own limiting factors, the method is generally free of the problems characteristic of diffraction angular measurements with a grating, discussed above. It has been successfully used at the Advanced Light Source (ALS) optical metrology laboratory (OML) for metrology of VLS gratings for the Linac Coherent Light Source (LCLS) AMO beamline and for the ALS MAESTRO project.

Here, we first systematically describe the mathematical foundation of the method and provide directions for increasing the accuracy of the method. We also suggest an application of interferometric microscope measurements with a reference grating as a possible method for performance testing of stitching procedures developed for the instrument.

We organize the paper as follows. In the next section (Section 2), we discuss a fitting procedure for determining the spatial frequency of harmonic peaks in the PSD distributions of the grating surface profile. An analytical fitting function is derived; and high correspondence of the predicted peak shape to the shape of the peaks measured with a 300-groove/mm VLS grating is demonstrated. In Section 3, we suggest and demonstrate improvement of the accuracy of the groove density measurements via averaging over spatial frequencies determined for the entire set of harmonic peaks observed in the PSD distribution of the grating. In the conclusion (Section 4) we analyze the complementarity of LTP and interferometric microscope based metrology