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Polarization Sensitivity Testing of Off-Plane Reflection Gratings

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ABSTRACT

Off-Plane reflection gratings were previously predicted to have different efficiencies when the incident light is polarized in the transverse-magnetic (TM) versus transverse-electric (TE) orientations with respect to the grating grooves. However, more recent theoretical calculations which rigorously account for finitely conducting, rather than perfectly conducting, grating materials no longer predict significant polarization sensitivity. We present the first empirical results for radially ruled, laminar groove profile gratings in the off-plane mount which demonstrate no difference in TM versus TE efficiency across our entire 300–1500 eV bandpass. These measurements together with the recent theoretical results confirm that grazing incidence off-plane reflection gratings using real, not perfectly conducting, materials are not polarization sensitive.

Keywords: Diffraction, gratings, grazing incidence, X-rays, polarimetry

1. INTRODUCTION

Off-plane reflection gratings offer a promising method to reach the high resolution and throughput required by the next generation of soft X-ray observatories.[1,2] The conical diffraction pattern of the off-plane (or 'conical') mount lends itself to favorable packing geometries compared to gratings in the in-plane mount, and gratings may also be blazed to preferentially disperse light to a single side of zero order, thereby increasing signal to noise in those orders and reducing the required detecting area.

There have been significant discrepancies in recent literature as to whether X-ray reflection gratings in the off-plane mount exhibit strong polarization sensitivity. Off-plane gratings were previously predicted to exhibit significant differences in efficiencies when linearly polarized light is incident in the transverse-magnetic (TM) orientation compared to transverse-electric (TE).[3] And indeed a difference in efficiency between the two polarization orientations was later reported for a 14° blazed off-plane reflection grating by Seely et al. 2006,[4] though the measured efficiency difference did not follow the theoretical predictions. However, more recent theoretical calculations by Goray & Schmidt 2010[5] show that the predicted polarization dependence largely disappears when calculations are carried out with rigorous treatment for the finite conductivity of the grating surface as opposed to the simplifying assumption of perfect conductivity applied in the previous studies.

Any variation in efficiency between linear polarization orientations must be well understood in order to employ off-plane gratings on future missions. Additionally, polarization sensitivity of off-plane gratings could offer a way to extend the polarimetry capabilities of future X-ray missions in the soft X-ray regime. Therefore to reexamine the potential polarization sensitivity of X-ray reflection gratings in the extreme off-plane mount, we performed efficiency measurements of laminar profile gratings at the Physikalisch-Technische Bundesanstalt (PTB) beamline at the BESSY II synchrotron facility between 300–1500 eV. We compare these findings to theoretical results and find good agreement with predictions for real, finitely conducting gratings. The experimental setup for this study is described in §2, results and modeling in §3, and discussion is given in §4.

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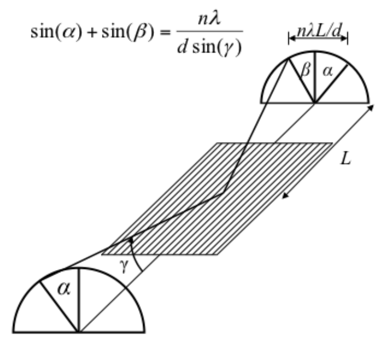

Figure 1: Geometry of the off-plane grating mount.[2]

2. TEST METHODOLOGY

2.1 Off-plane Geometry

A diagram of the off-plane grating geometry is shown in Figure 1. In the off-plane mount, light that is incident onto the gratings at a grazing angle and quasi-parallel to the groove direction is diffracted into an arc. The diffraction equation for the off-plane mount is

$$\sin\alpha + \sin\beta = \frac{n\lambda}{d\sin\gamma}, \tag{1}$$

where γ is the polar angle of the incident X-rays defined from the groove axis at the point of intersection, d is the line spacing of the grooves, α represents the azimuthal angle along a cone with half-angle γ, and β is the azimuthal angle of the diffracted light. The grooves are radially ruled such that the spacing between adjacent grooves decreases toward the focus to match the convergence of a telescope for a spectrometer instrument.

For gratings in the off-plane mount, we refer to linearly polarized light whose electric field vector lies in the plane defined by the grating normal and groove axis as TE polarization (p polarization), and define TM polarization as when the electric field vector lies parallel to the plane of the grating (s polarization). This is in contrast to the more familiar example of in-plane mounting, where s polarization corresponds to the TE case, and p polarization to TM. The switch is due to the altered groove orientation with respect to the field vectors.

2.2 Beamline Measurements

We tested an off-plane reflection grating for efficiency versus energy at two polarization orientations at the PTB soft X-ray beamline at the BESSY II electron storage ring.[6,7] The PTB soft X-ray radiometry beamline utilizes an SX-700 plane grating monochromator and covers a spectral range between 35–1700 eV. The synchrotron is linearly polarized in the axis of the storage ring. The samples are mounted in vacuum via the ellipsometer shown in Figure 2 which allows the samples to be measured at arbitrary polarization orientations.

The grating tested at the PTB beamline has a laminar (rectangular) groove profile and an average groove spacing of 6033 grooves/mm. The grating substrate is a 100 mm $\times$ 100 mm $\times$0.7 mm Si wafer coated with 80 nm of Au with a central grooved area of 25 mm $\times$ 32 mm. The mounting orientation is illustrated in Figure 3. Because the grating is not blazed and is thus not biased toward either side of zero order, it was mounted with the plane of incidence parallel to the grating groove direction (no yaw applied). The beam was incident at a graze angle of 1.5°. The grating was first mounted with the electric field vector perpendicular to the plane of incidence (TM polarization) and measurements taken between 300 − 1500 eV in steps of 50 eV at 0, $\pm1^{st}$, $\pm2^{nd}$, $\pm3^{rd}$, and $\pm4^{th}$ orders. The grating was then rotated 90° about the incident beam axis, and the same energy measurements were carried out in the TE configuration.

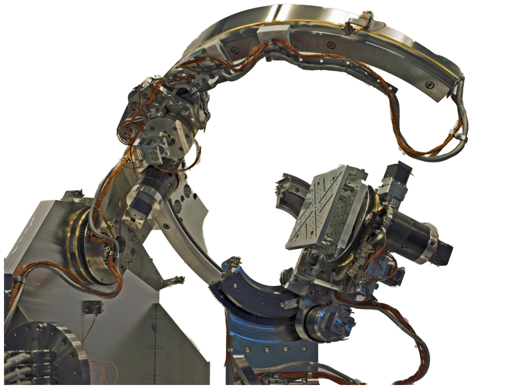

Figure 2: Ellipsometer operated at the BESSY beamline designed to carry out scattering and reflectivity measurements at specified polarization orientation.

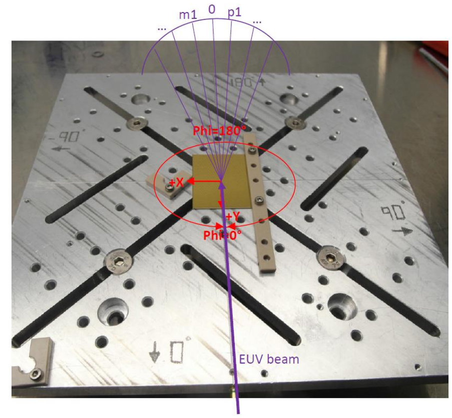

Figure 3: Diagram of the grating mount orientation to the PTB beam. Light is incident from the bottom of the image at a graze angle of 1.5° with respect to the grating plane and parallel with the groove direction. The diffracted orders are observed along an arc at the detector plane, where positive orders are diffracted to the right of zeroth order in the image.

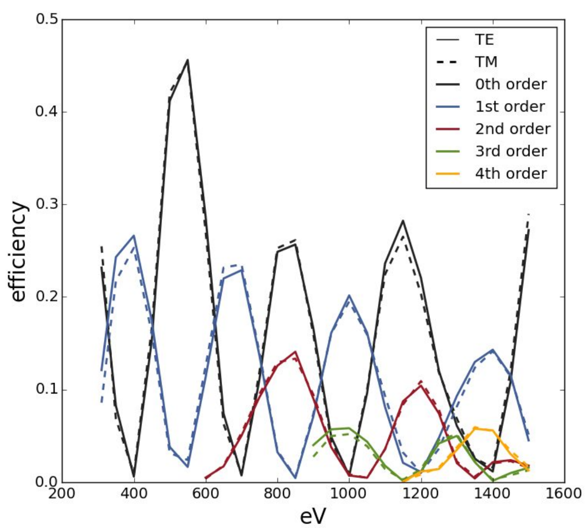

Figure 4: Measured efficiency versus energy for 0^{th} through 4^{th} orders where TE (TM) is plotted using solid (dashed) lines.

3. RESULTS AND MODELING

The efficiencies for 0^{th} through 4^{th} order TM and TE orientations measured at the PTB beamline are plotted in Figure 4. The measured TE efficiency is plotted using solid lines and TM using dashed lines. We observe no significant difference in the measured efficiencies at either orientation and thus find no polarization sensitivity for this grating.

To compare our empirical results to theoretical predictions, efficiency calculations for the grating were carried out using PCGrate-SX v.6.1. PCGrate-SX is a software suite which models the efficiency of diffraction gratings

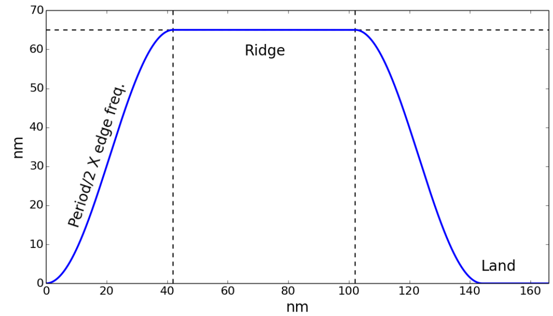

Figure 5: Example of the sine trapezoidal groove profile used to model the laminar grating response with PCGrate-SX.

for arbitrary groove profile and orientation, including in-plane and off-plane geometries. We model the laminar grating grooves as a sine trapezoidal profile (shown in Figure 5) which allows for realistic rounding of the groove corners apparent in Scanning Electron Microscopy (SEM) measurements of the grating.[2]

PCGrate-SX was also used in the previous study which predicted significant polarization sensitivity for gratings in the off-plane mount.[3] It is important to note that the efficiency calculations in PCGrate-SX v.6.1 are made through application of the theory of invariance.[8,9] This theorem is used to express the off-plane efficiencies of a perfectly conducting grating in the form of a linear combination of efficiencies in the simplified in-plane geometry. However, the resulting efficiencies are limited to the idealized case of a grating with infinite conductivity.

Goray & Schmidt 2010[5] carried out more rigorous integral method calculations including finite conductivity for blazed, off-plane reflection gratings in the X-ray regime, which demonstrate that the effect of real conductivity is non-negligible. The authors compare their results to those obtained under the assumption of perfect conductivity and find that the more rigorous treatment has little impact on the predicted TE efficiency. However, including finite conductivity strongly alters the predicted TM response. The resulting TM and TE efficiencies differ by no more than a few tenths of a percent. Thus, accounting for finite conductivity largely removes any polarization dependence on the predicted efficiency in the extreme off-plane mount at shallow graze angles.

It is the present authors' understanding that the PCGrate-SX v.6.6 allows for rigorous calculation of efficiencies, including finite conductivity for off-plane gratings. However, this method is slower to converge, and the calculation method precludes straight-forward treatment of rms surface roughness. Since the previously predicted polarization dependence disappears with rigorous finite conductivity treatment, it appears preferable to utilize the unaffected TE predictions from the simplified calculations. Use of the v.6.1 solver calculations is also favorable because it does not necessitate the procurement of a new software package.

Because the grating orientation does not impose a polarization sensitivity, the dominant polarization effect should in this case be due only to the reflection coefficients derived from Fresnel equations for a given surface material, incidence angle, and energy range. Thus, a small correction to produce TM efficiencies may be manually calculated from the TE predictions via these well known coefficients. For a grazing incidence angle, γ, the fraction of incident that will be reflected, R, is given as

$$R_{\mathrm{TE}} = \left| \frac{n^2 \sin\gamma - \sqrt{n^2 - (1 - \cos^2\gamma)}}{n^2 \sin\gamma + \sqrt{n^2 - (1 - \cos^2\gamma)}} \right|^2 \tag{2}$$

$$R_{\mathrm{TM}} = \left| \frac{\sin\gamma - \sqrt{n^2 - (1 - \cos^2\gamma)}}{\sin\gamma + \sqrt{n^2 - (1 - \cos^2\gamma)}} \right|^2, \tag{3}$$

for the TE and TM orientations, respectively. Here n is the energy-dependent complex index of refraction of the grating surface material. As the graze angle, γ, becomes very shallow, the ratio of these coefficients becomes

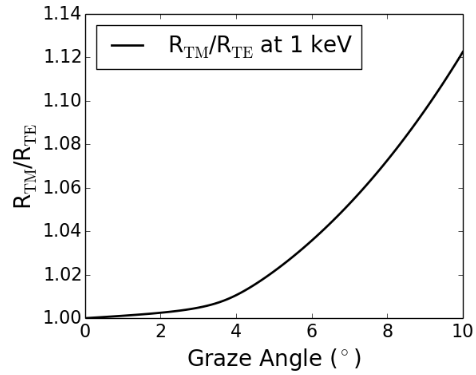

Figure 6: Ratio of the reflectivity coefficients for 80 nm Au-coated Si at 1 keV versus graze angle.

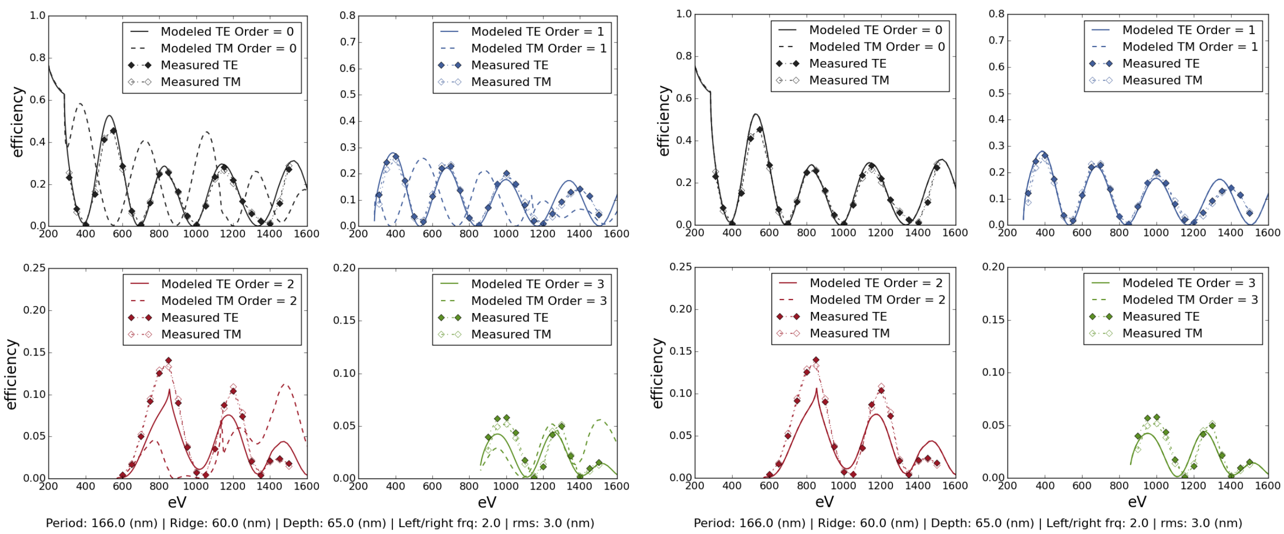

Figure 7: **Left:** Efficiency versus energy predicted by PCGrate-SX utilizing the invariance theorem (perfect conductivity). TE (TM) efficiency is plotted a solid (dashed) line. Each plot corresponds to a single order, with 0^{th} order plotted top-left, 1^{st} order top-right, 2^{nd} order bottom-left, and 3^{rd} order bottom-right. PTB measurements are plotted with filled (hollow) diamonds for the TE (TM) orientation. The sine trapezoidal profile parameters are listed at the bottom of the figure. **Right:** PTB measurements over-plotted onto modeled efficiencies where the TM response has been manually calculated from the TE PCGrate-SX predictions corrected by reflectivity coefficients, in agreement with calculations assuming finite conductivity.

very close to unity. Figure 6 is a plot of the ratio $R_{\mathrm{TM}}/R_{\mathrm{TE}}$ at 1 keV for a range of grazing incidence angles. At our graze angle of 1.5° this value differs from unity by a few tenths of a percent.

We performed a correction of the PCGrate-SX predicted TE efficiencies using the reflectivity coefficients to manually predict the expected TM response. In Figure 7 we present the PCGrate-SX modeled efficiencies assuming perfect conductivity (left) and compare to the corrected efficiency predictions (right). In both plots the measured TE and TM efficiencies are over-plotted as filled and hollow diamonds, respectively. In agreement with the calculations including finite conductivity presented by Goray & Schmidt 2010, we find good agreement with the perfect conductivity model predictions for the case of TE polarization, but poor agreement for the case of TM polarization. After applying the reflectivity correction to predict TM response, the TE and TM predictions lines are now indistinguishable in the right-hand plots, consistent with our measurements.

4. DISCUSSION

We carried out experimental measurements of an off-plane grating at the two fundamental linear polarization orientations in order to characterize any polarization sensitivity. We observe no polarization sensitivity with 6033 groove/mm, laminar reflection gratings at a graze incidence of 1.5° and 0° yaw. Our measurements support more recent theoretical results by Goray & Schmidt 2010[5] who demonstrate that the predicted strong polarization sensitivity of reflection gratings in the extreme off-plane mount disappears when real conductivity of the grating surface is taken into account. The authors show that calculations which make use of the invariance theorem, and thus assume perfect conductivity, strongly differ from the predicted response for finite conductivity gratings when light is incident in the TM orientation (E-field parallel to grating surface). However, the orthogonal TE orientation predictions are not strongly affected by the assumption of perfect conductivity.

In agreement with the recent theoretical results, we find that the TE model calculations utilizing the assumption of perfect conductivity are able to reproduce the measured efficiencies of our real gratings. Rigorous efficiency calculations including finite conductivity predict no significant polarization response. Therefore, we are able to produce predictions for TM polarization state by correcting the results of the perfect conductivity model TE efficiencies by the ratio of the reflectivity coefficients for a given grating material, incidence and angle and energy. Doing so yields predictions that match our empirical results.

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