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Theoretical and measured performance of diffraction gratings

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Abstract

At the SRS at Daresbury Laboratory, we are undertaking a programme comparing the results from efficiency calculations of diffraction gratings, mainly using the GRADIF code of Neviere, with measured efficiencies. The deviations from the predicted performance are larger for higher orders than for first order. Higher order contamination is important in determining the usability of the beamline for certain types of experiments, particularly at energies below 100 eV. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

There can be significant differences between the theoretical and measured performances of diffraction gratings. In this paper, comparisons are made between calculated efficiencies and diffractometer measurements for four gratings, which have recently been acquired for two new XUV beamlines on the SRS at Daresbury Laboratory.

2. The calculations

Most of the calculations have been carried out using GRADIF, which is an update of the LUMNAB code of Neviere [1]. This code solves the differential equations from electromagnetic (EM) theory by integrating the equations through the grating. Upgrades to the code of relevance to these calculations include the ability to study trapezoidal profile gratings, to include more Fourier coefficients and use of the S-matrix propagation algorithm (Neviere and Monteil [2]) which increases the numerical stability of the integration.

For one grating, calculations were run by Li [3] using his own code which is based on the Chandezon method [4], an eigenvalue technique for solving the EM equations. The agreement with the results from GRADIF was in general 1%–2%, at worst 5% at a few energies in second order, over the energy range studied.

3. The measurements

Diffractometer measurements were taken, using existing SRS beamlines as the light source. Two types of measurements were carried out for the

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higher orders; type (a) when the efficiency of the second order at the same included angle as the first order but at twice the energy was measured; type (b) when the detector was rotated to measure the second order at the same incident angle and energy as the first order, but different included angle.

The most significant potential source of error in the measurements is higher order contamination in the beamline output. The two beamlines used for the measurements presented here have naturally low higher order content in the energy ranges used. Further, for the 300 and 600 lines/mm gratings, an undulator beamline (5U1) was used and the undulator was tuned to maximise the ratio of first to second order flux. A range of filters (0.15 and 0.3 μm Al, 0.13 and 0.26 μm B, 0.45 μm Si, 2 and 4 μm polypropylene) was also used. The high flux available on the beamlines allowed the filters to be used in various combinations to give good suppression.

The filters were chosen primarily to reduce second order content, but also gave sufficient reduction of the inherently much lower levels of third order light. Orders higher than third were not present in sufficient quantity to be a problem.

The effectiveness of the higher order reduction was checked by scanning the gratings under test over the first order diffraction peaks of the second and third order energies from the beamline. In almost all cases, these contamination peaks were absent or $\leqslant 0.1\%$ of the main peak. The diffraction efficiency for these peaks was checked to ensure that the absence of a peak was due to good suppression of the higher orders.

4. The gratings

The calculations were carried out using the profiles given in Table 1, which are from the manufacturer's, measurements taken at the grating centre. 'Lamellar' gratings in fact have trapezoidal profiles, the angles of which have been measured for the 300 and 390 lines/mm gratings. Ideal rectangular profiles have been used for the other lamellar grating. All the gratings are gold coated.

Table 1
Grating parameters used in the calculations

Profile	Line density (l/mm)	Depth (Å)/ blaze angle	Valley width (Å)/ apex angle
Trapezoidal 57°	300	493	24 600
Trapezoidal 50°	390	540	13 900
Lamellar	600	222	11 200
Blazed	1440	2.2°	165°

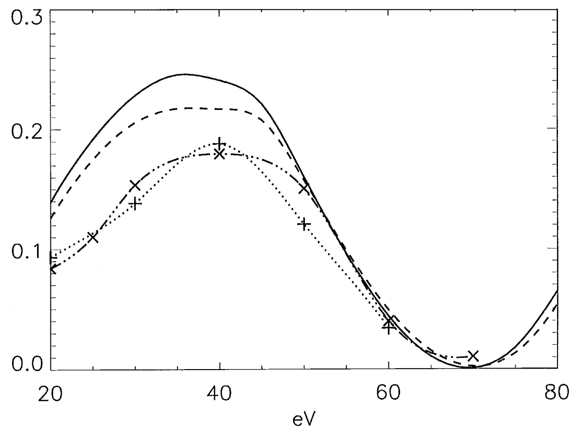

Fig. 1. First order efficiency of the 390 lines/mm lamellar grating as a function of photon energy; —— theory, trapezoidal profile; – – – – – – theory, lamellar profile; – · · · · – · · · · – · · · and .... diffractometer measurements. The + and × mark the measured points.

5. Results

The effect of using a trapezoidal (rather than lamellar) profile on the first order efficiency of the 390 lines/mm grating is seen in Fig. 1. For the same grating, the maxima in the second order efficiency were increased by about 20% when a trapezoidal profile was used. This is consistent with the results for grazing incidence found by Reichardt and Schafers [5].

For first order, the calculated efficiency versus energy curves have in general the same shape as the diffractometer results, although the peak value is lower. Examples are given in Figs. 1 and 2 for the 390 and 600 lines/mm lamellar gratings and in Fig. 3 for the blazed grating. The exception is for the 300 lines/mm grating (Fig. 4) where the

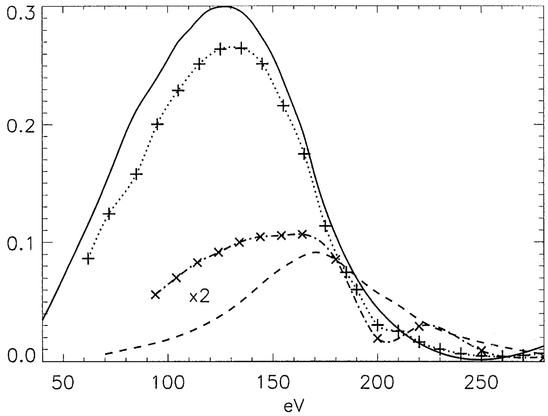

Fig. 2. Comparison of calculated and measured efficiencies for the 600 lines/mm lamellar grating: ———— first order theory; .... first order diffractometer measurements; – – – – – – – second order theory; – · · · · · · · · – · · · second order diffractometer (type a) measurements. The + and × mark the measured points. Note that the second order efficiencies have been multiplied by 2.

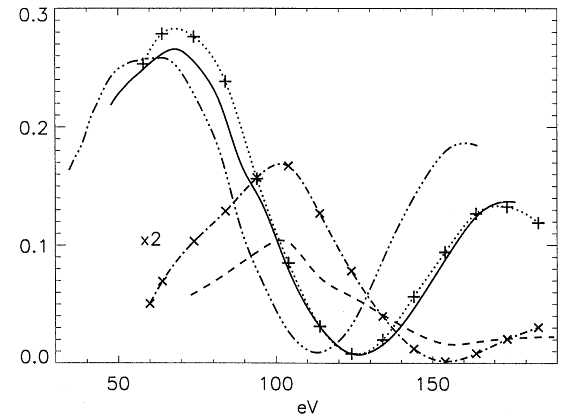

Fig. 4. Comparison of calculated and measured efficiencies for the 300 lines/mm lamellar grating: – · · · · · – · · · · · · first order theory (measured profile); ———— first order theory, valley depth 440 Å; .... first order diffractometer measurements; – – – – – – – second order theory, valley depth 440 Å; – · – · – · second order diffractometer (type a) measurements. The + and × mark the measured points. Note that the second order efficiencies have been multiplied by 2.

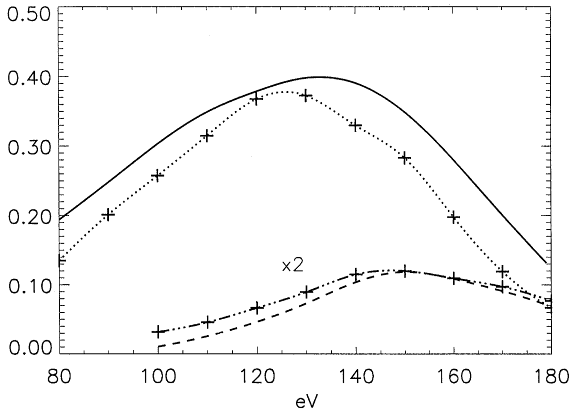

Fig. 3. Comparison of calculated and measured efficiencies for the blazed grating. ———— first order theory; .... first order diffractometer measurements; – – – – – – – second order theory; – · · · – · · · – · · · second order diffractometer (type b) measurements. The + marks the measured points. Note that the second order efficiencies have been multiplied by 2.

solid curve in Fig. 4. The spread in measured groove depth is from 483 to 495 Å. Calculations, using a different computer programme, subsequently carried out by the manufacturer have confirmed the theoretical results in this paper.

The situation is not so clear for higher orders, where there are fewer direct measurements. The best comparison is between theory and diffractometer type (b) results for the blazed grating, shown in Fig. 3. Figs. 2 and 4 give a comparison with the diffractometer type (a) results for the 600 lines/mm grating and the 300 lines/mm lamellar grating discussed above. For the latter, a depth of 440 Å was used in the calculations. It is seen that the measured efficiency can be about a factor 2 higher than predicted, even round the peak of the efficiency curves.

position of the minimum near 120 eV, which depends mainly on the groove depth, could not be reproduced using the depth value measured by an AFM. Close agreement with the measurements was found using a depth of 440 Å as shown by the

6. Conclusions

Work is still needed to understand the differences between calculated and measured efficiencies, particularly for second order, where the measured efficiency can be significantly larger than predicted.

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