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Simulated versus measured efficiency comparison of a mechanically ruled, variable-line-spacing blazed diffraction grating manufactured for ALS MERLIN

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Abstract

Inprentus has developed proprietary software to predict diffraction efficiency of manufactured diffraction gratings for arbitrary groove shapes and scattering conditions. This software uses rigorous coupled-wave analysis (RCWA) and has been verified with both GSOLVER and Nevière's Gradif code. In this paper, we present the simulated efficiency of a variable-line-spacing (VLS) grating manufactured by Inprentus for the MERLIN beamline upgrade at the Advanced Light Source (ALS) in Lawrence Berkeley National Lab (LBNL). We compare the simulated efficiency of the manufactured grooves to that of perfectly triangular grooves. We also present measurements taken by Eric Gullikson at ALS Beamline 6.3.2 which show the grating's actual efficiency exceeds the simulation predictions.

1 Introduction

A blazed diffraction grating gives the highest efficiency for photon-starved applications. Master gratings are the preferred choice in applications requiring UHV compatibility and radiation hardness like the monochromators and spectrometers in soft x-ray and EUV beamlines. A direct way to assess grating performance is in-beam efficiency measurements, but this tends to be time consuming and unavailable during the manufacturing process. Lacking a tool to assess efficiency of manufactured groove shapes, beamline grating designers have had to resort to specifying geometric angles and facet roughness. This has led to some specifications and their importance being open to interpretation. To bridge the gap between groove shape assessment and performance efficiency, the industry needs a tool to simulate efficiency of arbitrary groove shapes at the desired energy range, diffraction order, and illumination conditions. This simulation software needs to be compatible with the manufacturer's preferred method of probing the groove shape, tolerant to imperfect groove shapes, and efficient in its use of computational resources. Such a tool tool would be immensely useful for expediting the grating manufacturing process and increasing manufacturing yield.

Mechanical ruling is done line-by-line by burnishing the substrate surface with a diamond scribe. This process often introduces random variations in the groove shape. Previous work done by Nevière et. Al. has produced a code to simulate the efficiency of a handful of predetermined, parametrized groove shapes, but a tool that can simulate arbitrary groove shapes has been unavailable. Inprentus has produced a proprietary software to solve this problem and its application are presented in this paper. We probe the groove shapes fabricated for the ALS MERLIN beamline grating using an atomic force microsope (AFM) and use the real groove shapes to predict grating efficiency. We show how this efficiency compares to a perfect sawtooth groove shape and how it compares to real beamline efficiency measurements.

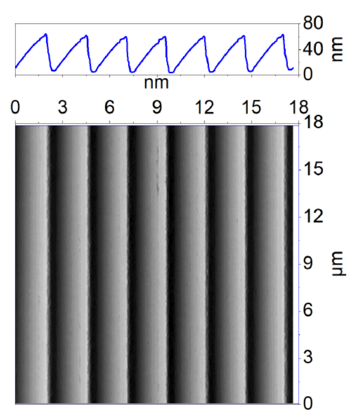

Figure 1: Surface profile of seven mechanically ruled grooves of the MERLIN beamline grating are probed with an AFM and column averaging provides shape profile (blue line).

2 MERLIN Beamline Grating Simulations

A 100 mm x 20 mm grating was ruled on a 160 mm x 40 mm x 40 mm single-crystal Si substrate of tangential cylinder geometry following the deposition of thin layer of gold on the optical surface. The VLS grating has a central line density of 400 lines/mm and a 1.6 deg blaze angle. The grating was probed with an AFM and Figure 1 shows a representative 2D height map scanned at the grating center. Figure 2 shows the Inprentus angle analysis software used to fit angles to the manufactured groove shape, obtaining statistical details on the shape variation. The ruled grating was overcoated with 50 nm of carbon with density $> 2.05\ g/cm^3$ using a third-party vendor.

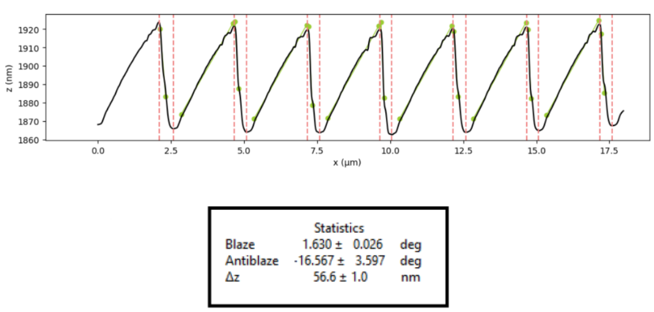

Figure 2: Inprentus' automated angle-fitting software gives statistical data on groove shape during both machine alignment and grating metrology.

The groove shape profiles are loaded into Inprentus' proprietary efficiency simulator to produce efficiency plots as shown in Figure 3. Inprentus software simulates a single material (carbon, in this instance) in transverse electric polarization. The simulator is extremely flexible with configurable design photon energies, diffraction orders, and incident-beam angles. In Figure 3, The orange curve represents the mean simulated efficiency from 13 scan locations along the grating length. This is compared with expected efficiency from a perfect sawtooth of specified angles (black curve).

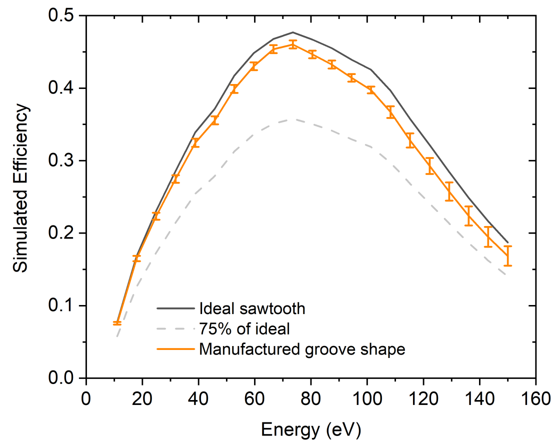

Figure 3: Simulated efficiency predictions for the MERLIN beamline grating. The black curve shows the expected efficiency from the perfect sawtooth-shaped groove, the orange curve shows the expected efficiency from the manufactured groove shape, and the dashed gray line shows 75% of ideal grating efficiency.

3 ALS Measurements

ALS measured the efficiency of the delivered MERLIN beamline grating in test beamline 6.3.2 and provided the following plot. The MERLIN grating efficiency exceeded Inprentus' simulations.

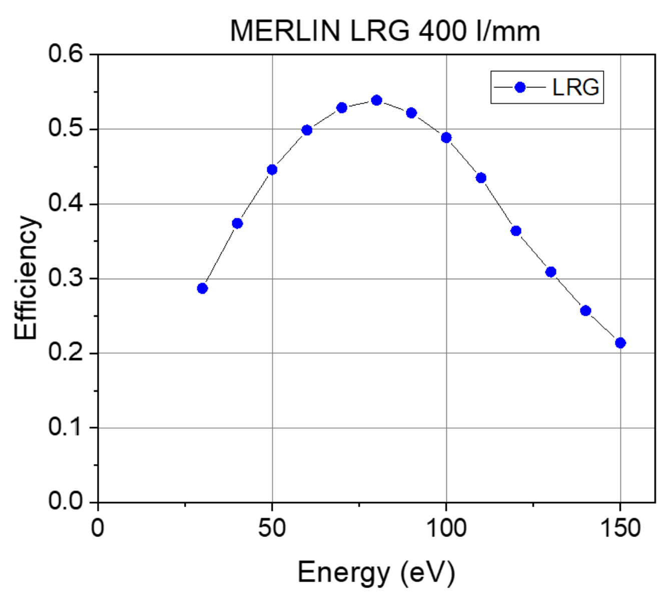

Figure 4: Efficiency of MERLIN grating measured at ALS Beamline 6.3.2 by Eric Gullikson and shared by Andrew Doran.