Diffraction efficiency of reflective metallic gratings operating in the THz range

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***Abstract*— Far IR spectrometers have a prominent role to play in future space IR missions devoted to unveiling the obscure universe. Diffraction gratings are the heart of these instruments that, when operating in the range of a few THz, shall cover a wide spectral range, provide the highest resolution and maximize the efficiency, generally for only a single polarization. Therefore, the diffraction grating design and optimization become a determinant exercise where the main grating parameters shall be univocally established and ensured for maximizing the diffraction efficiency for the complete spectral range. This paper describes the optimization of the reflective diffraction efficiency for order *m* = 1 by comparing two different methods. Since the grating period is of the same order of magnitude as the wavelength, it is necessary to solve Maxwell's equations rigorously to obtain the best diffraction efficiencies. Results obtained with the methods based on RCWA (Rigorous Coupled-Wave Analysis) and FEM (Finite Element Method) are compared. Manufacturing errors are a severe limiting factor for performance, so their identification, parameterization, and modeling must also be considered.**

Keywords— Terahertz, Far-IR optics, IR spectrometer, diffraction gratings, diffraction efficiency.

I. Introduction

This work presents the design process of a diffraction grating for a THz spectrometer for space applications operating in the spectral band from 70 to 114 microns. The design of gratings for a THz spectrometer uses the equations of the blazed diffraction grating. Blazed gratings are used to enhance the amount of radiation that is forwarded toward a selected diffraction order. The grating profile was optimized in this case to guide the light toward the $m = 1$ diffraction order. The relation between the angle of incidence, ε, the grating period, d, the diffraction angle θ, and the wavelength of the incident light, λ, is given by the grating equation:

$$d(\sin \varepsilon + \sin \theta) = m \lambda ,$$

where m is the diffraction order [1].

In this case, the efficiency obtained for the ideal geometry of a sawtooth profile for a plane wave TM (transverse magnetic mode) at a fixed incidence angle is included. Two modelization different methods were used, the RCWA and a FEM-based model, analyzing similarities and discrepancies in the diffraction efficiency response [2]. Additionally, the diffraction grating has been fabricated, and morphologically characterized, and its behavior modelized to determine the impact of the manufacturing errors on the diffraction grating performances.

II. Results

A. Diffraction grating design

In the design of a diffraction grating, three fundamental parameters must be considered: period, morphological profile, and spectral range. These parameters have been individually optimized to achieve a diffraction grating with a maximum diffraction efficiency for TM polarization and m=1 order, while the other orders are minimized. In this contribution, FEM is applied using COMSOL-Multiphysics®, and RCWA is realized using GSolver® (Grating Solver Development Company, UT, USA) and S^4 (Stanford Stratified Structure Solver, Stanford University) programs. These approaches solve the Maxwell-Equations for periodic structures quite efficiently. FEM requires an appropriate mesh of the calculation domains and customization of the boundary conditions. Even though RCWA is a mesh-free method, it also needs a fine-tuning of some internal parameters of the calculation (number of internal orders, number of slices, etc.). Fig. *1* shows that under the same conditions, similar efficiencies are observed. Those obtained with the FEM method are higher than those calculated with RCWA. The discrepancies can be attributed to the fact that RCWA generates an inter-order energy distribution that depends on the definition of the internal computational parameters, while FEM only depends on the meshing.

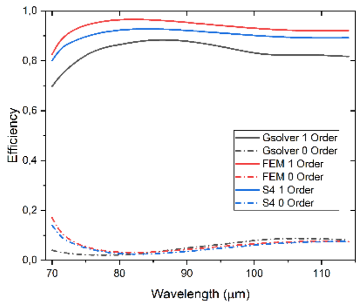

Fig. 1: Comparison of diffractive efficiency obtained by RCWA and FEM methods. m=1 and m=0 orders are shown.

Regarding the diffraction grating efficiency, efforts have been focused on optimizing the period and the blaze angle. As can be seen in Fig. *2*, a change in the thickness of the profile produces a variation in the blaze angle. The effects of modifying these variables have been studied by RCWA. The slant angle, the deviation from 90° of the sawtooth profile, was analyzed as an unavoidable manufacturing defect.

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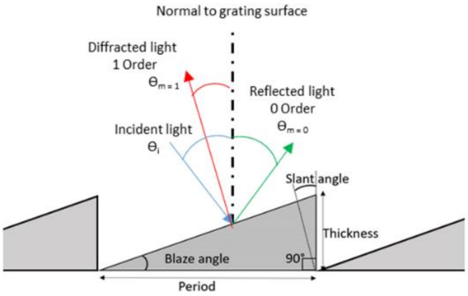

Fig. 2: Sawtooth profile of the blazed diffraction grating.

a) Period: The simulation starts from a period value centered in the wavelength range getting for that period multiple diffraction orders. Cut-off anomalies appear when energy redistributes due to the disappearance of diffraction orders. As can be seen in Fig. 3, this effect can be eliminated by reducing the value of the period. In this case, lowering the period to 76 µm gives a better response for efficiency.

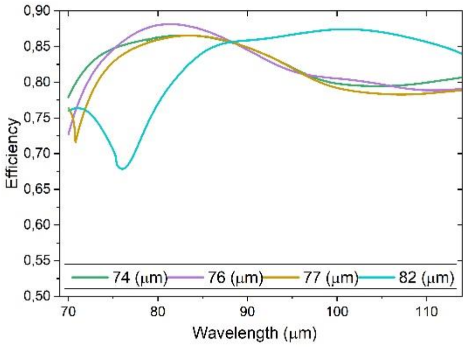

Fig. 3: Diffractive efficiency at different period values.

b) Blaze angle: An increase in this angle produces an increase in the efficiency at longer wavelengths and a decrease in the efficiency at shorter ones as can be observed in Fig. 4.

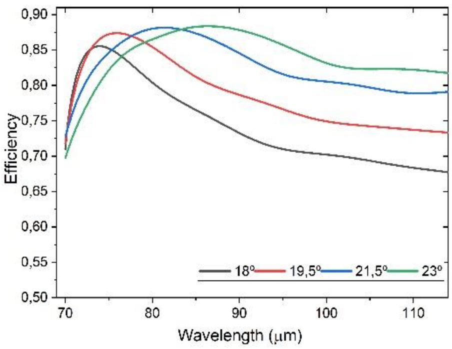

Fig. 4: Diffractive efficiency at different values of blaze angle.

c) Slant angle: When calculating the behavior of the grating as a function of the slant angle from 0 to 30°, for a fixed value of the blaze angle, 24°, and a period a 76µm, we find that the efficiency calculated by the FEM method remains above 90% in the whole spectral range. So, adding a slant angle at the sawtooth profile enhances the diffraction efficiency. The green curve labeled as "Nominal" in Fig. 6 shows the diffraction efficiency for a slant angle of 10°.

B. Diffraction efficiency analysis of manufactured gratings

The manufacturing process distorts the geometry of the theoretical design and generates unavoidable discrepancies between the ideal profile and the actual one. In our case, a blazed diffraction grating with sawtooth-shaped geometry and a total area of 54×40 mm^2 has been manufactured by micromachining on a metallic substrate, specifically aluminum 6061T651, which is the most suitable material for space applications due to its mechanical and thermal properties. Fig. 5 shows an image taken by confocal microscopy. It can be observed that the sawtooth profile is not like the ideal one that was modeled and contains fabrication defects.

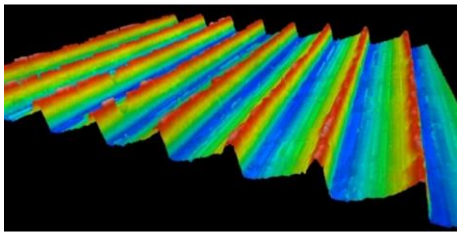

Fig. 5: Confocal image of the micromachined diffraction grating.

The results from the topographic measurements have been used to evaluate the response of the fabricated grating. Fig. 6 shows the diffractive efficiency for the real manufactured profile (red line), and the response to the nominal theoretical ideal profile (green plot). Even though the fabricated topography largely departs from the nominal, the calculated efficiency is above 65% for the whole spectral range.

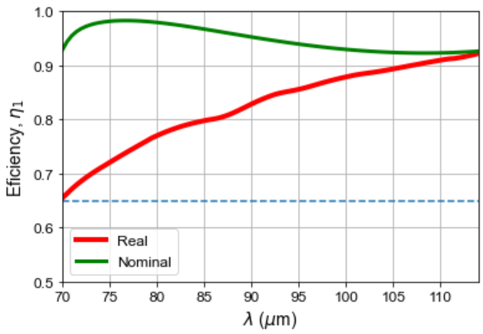

Fig. 6: Diffractive efficiency calculated for the fabricated grating (red) and the nominal profile (green)

III. CONCLUSIONS

A detailed numerical analysis has been made using two main computational electromagnetism methods: the RCWA and the FEM. Both of them produce similar values of efficiency and can be used to optimize the performance of the grating by changing the geometrical parameters. After considering all these issues in the design, we have fabricated an aluminum blazed grating with a period of 76 µm, a blazed angle of 24°, and a slant angle of around 10°. This grating has been fabricated by micromachining. The actual geometry has been also included in the simulations and the diffraction efficiency has been evaluated.

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