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# Metallic Blazed Grating TE Mode Resonance Conditions and Diffraction Efficiency Optical Transfer Function

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Abstract-We introduce a general approach to study diffraction harmonics or resonances and resonance conditions for blazed reflecting gratings providing knowledge of fundamental diffraction pattern and qualitative understanding of predicting parameters for the most efficient diffraction.

### I. INTRODUCTION

In the existing work, there is a gap between theoretical models that can only be applied numerically, in practice, and simulations that are exclusively applied for a specific design with previously determined parameters. This work studies in-plane diffraction phenomena from 45° blazed (ruled) reflecting gratings. We present an approach to quantify diffraction efficiency (*DE*) for metallic gratings with transverse electric (TE) polarized light (Fig. 1a). *DE* is defined as the ratio between the power of light diffracted in a certain order and the power of incident light  $-DE = P(m,\lambda,\alpha)/P_0$ . Simulation result analysis are based on the classical diffraction grating equation in free space:

$$d\left(\sin\beta - \sin\alpha\right) = m\lambda,\tag{1}$$

where d – grating period;  $\alpha$  – incidence angle (polar);  $\beta$  – diffraction angle; m – diffraction order (DO);  $\lambda$  – wavelength. However, the diffraction equation does not include information about *DE* that is the primary criteria for the design and material. To simplify the description of the problem, the following transformation is being used:  $x \leftarrow |m|\lambda/d$  and  $y \leftarrow \sin \alpha$ . It is

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straightforward to show that diffraction can only occur if the following condition is met:

$$y(x) \cdot \operatorname{sgn} m \le 1 - x, \tag{2}$$

with sgn *m* being the sign function of DO. Note that  $y \in [-1;1]$  and  $x \in (0;2]$ , meaning, every DO can be analyzed separately in the same axis and values (Fig. 1c), where the primary physics meaning of *y* is the incidence angle, and of *x* it is the wavelength (or frequency) which is normalized with respect to *d* and *m*.

## II. RESONANCE CONDITIONS

In diffraction, harmonics are generated by grating resonances, i.e., when multiple orders interfere constructively, and thus harmonics are not a trivial solution of frequency multiples of the fundamental frequency (Fig. 1b). For reflection DE, we reveal that these harmonics concur with the so-called guidedmode resonance (GMR) regions describing grating couplers [1-2]. Here, we show the relevance of GMRs to reflecting gratings. In Fig. 1c, the lines originating from  $(x, y) = (0, \pm 1)$  correspond to a boundary of subsequent higher DO. Interference of multiple orders forms the aforementioned harmonics, i.e., the effective DO at which DE peaks will be observed. Intersections of these lines determine the resonance conditions and it is found that the effective order is equal to the sum of conterminous order numbers, e.g., in the case of m = -1 (Fig. 1c), two interfering orders would take the following form of mathematical description:  $m_n + m_{-n-1} \equiv -1$ ; *n* indicates the number of the DO.



Fig. 1. (a) Blazed grating geometry and definition of sign convention. TE angular OTF in terms of DE; (b) superimposed spectra in semi-log scale of all individual orders except the 0<sup>th</sup> order (the sum of all orders at any given point is equal to unity), dashed lines represent Littrow lines for the corresponding DO; (c) DE(x, y) spectrum of the -1<sup>st</sup> order diffraction, the red dots indicates resonance positions on Littrow line.

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Fig. 2. TE diffraction efficiency (*DE*) spectrum of the -1<sup>st</sup> order on Littrow curve for: (a) PEC; (b) aluminum (Al); (c) Al normalized against total reflection (approximately equal to (a)); (d) absolute difference in percent between (c) and (a). (e) PEC with axis transformed to the number of harmonics vs. grating period. For the reference – (a-d) shows all diffraction orders (DO) in a sequence 0,-1,-2,... from right to left; the blue line corresponds to the -1<sup>st</sup> order.

#### **III. SIMULATIONS AND RESULTS**

To generalize the problem and obtain optical transfer function (OTF), we reduce main simulations to perfect electric conductor (PEC) material gratings and show the relation to metallic materials in case of TE polarized light (Fig. 2a-d). It is known fact that *DE* of TE light is scaled accordingly to the reflection coefficient (if azimuth angle is zero). But transverse magnetic (TM) light involves the interaction of surface plasmons (SPs) and thus is not simply scaled by the reflection coefficient [3-4]. Rather extinction coefficient  $\kappa$  determines the interaction strength and coupling of SPs, thus the interference.

Simulations are performed using rigorous coupled-wave analysis (RCWA) method (total number of spatial harmonics – 50). PEC is mimicked by setting the refractive index n equal to zero and the extinction coefficient  $\kappa$  equal to 10, rendering a material similar to real metals in UV-VIS-NIR range for TE case. In such a way, it is ensured that the reflection coefficient always will be  $R \equiv 1$ . By TE simulations, it is confirmed that the value of n and  $\kappa$  does not affect DE peak positions (see Fig. 2a-c), as long as there is only one reflecting surface, i.e., all the transmitted light is being absorbed or not reflected back. Interference of back-reflected light requires separate analysis on case-by-case basis, like for those cases with leaky modes. Convergence was extensively studied to verify solution stability and conclusions. The main studied factors for the convergence were the spatial resolution of the grating profile and the total number of spatial harmonics used in RCWA method. Fig. 2e verifies the independence of OTF on the grating period if  $\lambda/d$  normalization is properly taken into account, and it also verifies a successful description of harmonics - resonance conditions.

The following important conclusions are drawn from the results:

- No efficient diffraction/resonance at 45° incidence is observed for the first-order as often assumed for the Littrow configuration; it is true for higher orders at shorter wavelengths;
- 2. Only certain wavelengths/frequencies (harmonics) are diffracted with the highest *DE*;
- 3. Large gratings are more efficient typically with small variation of *DE* in Littrow configuration, but requires larger illumination area to illuminate the same number of grooves;
- 4. *DE* dataset from the findings applies to any size of 45° blazed metallic diffraction gratings, thus can be used as an OTF of reflection gratings.

To interpret general diffraction patterns and resonance conditions, the work is being studied further for other types of grating profiles, including nonsymmetrical gratings in higherorder diffraction, and TM polarized light with SPs.

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