

Freeform Design of Blazed Diffraction Gratings for THz Frequencies

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ABSTRACT

Achieving high diffraction efficiency over broad spectral bandwidths has become a key requirement for next-generation terahertz (THz) spectroscopic systems. In THz spectrometers, system complexity can be reduced if the diffraction grating operates efficiently across the entire wavelength range of interest. In this work, we address this challenge through optimized stepped-profile gratings that account for realistic fabrication constraints while enabling complex profile geometries. The angular overlap of diffraction orders across broad spectral ranges is mitigated through order-selection strategies implemented at the detector plane. The designs are evaluated through computational electromagnetic simulations based on realistic instrument specifications. Experimental realization is enabled by laser ablation techniques applied to aluminum, allowing the fabrication of complex stepped profiles. Results show that the optimized geometry achieves diffraction efficiency values above the 65% for the $m = 1$ diffraction order over the 40 μm to 139 μm wavelength range, demonstrating strong potential for compact broadband THz spectrometers.

Keywords: Terahertz, Far-IR Optics, Computational Electromagnetism, IR Spectrometer, Diffraction Gratings, Diffraction Efficiency,

1. INTRODUCTION

The development of far-infrared instrumentation is crucial for future space missions¹, particularly in the context of next-generation observatories that envision large telescopes² equipped with spectrometers operating in the terahertz (THz) range: 1–10 THz. Achieving compact instrument architectures, which are essential for meeting strict mass and volume budgets in space applications, often requires dividing the spectral range into narrower sub-bands³, each addressed through a dedicated optical design. Within the broader objective of developing cryogenic infrared spectrometers, particular attention is devoted to the development of high-efficiency reflective metallic gratings with extended spectral response. The design of these diffraction gratings must simultaneously satisfy the spectrometer requirements – such as spectral resolution, diffraction efficiency, and operational bandwidth – and the constraints imposed by fabrication technologies capable of accurately reproducing complex surface topographies.

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In multispectral THz spectrometers, the complexity of the optical system can be significantly reduced if the diffraction grating at its core operates efficiently over a broad spectral interval. Achieving such broadband performance requires working in two directions: On one side, we study the blazed geometry with advanced grating design strategies that consider fabrication techniques capable of accurately reproducing complex surface profiles. On the other hand, extending the operating spectral range typically requires the use of higher diffraction orders, which inevitably leads to angular overlap between adjacent orders. Therefore, efficient spectral-selective solutions at the detector plane are needed to isolate the desired diffraction order.

This contribution addresses both challenges. The analysis is based on the specifications of previously proposed THz instruments and investigates strategies for designing broadband diffraction gratings while enabling optimized diffraction-order selection at the detection plane.

2. FUNDAMENTALS

Diffraction gratings are periodic optical elements that modulate the phase of incident radiation in order to separate it into its constituent wavelengths. Their performance is commonly quantified by the diffraction efficiency, defined as the ratio between the diffracted and the incident optical energy. Conventional blazed diffraction gratings, typically based on linear sawtooth profiles, can achieve high efficiency for a given diffraction order and polarization over a limited wavelength range. In the simplest configuration, blazed diffraction gratings are optimized to operate in only one diffraction order, $m = 1$, in TM polarization. The design, optimization, fabrication, and experimental validation of blazed diffraction gratings in the THz range have been previously reported by the authors. In those works, the target diffraction efficiency threshold of $\eta_1 = 0.65$ was significantly exceeded in numerical simulations.⁴ Experimental characterization of the fabricated gratings, performed using monochromatic THz sources,⁵ revealed that deviations from the predicted performance were primarily associated with discrepancies between the designed and manufactured surface profiles. Furthermore, accurate validation required accounting for Gaussian beam propagation in order to properly estimate the angular spread of the incident radiation.

In these designs, the grating period is on the same order as the incident wavelength, making scalar diffraction theory insufficient for reliable efficiency predictions. Consequently, the design process relies on computational electromagnetic techniques that rigorously solve Maxwell's equations. This approach enables a precise evaluation of the grating performance for both Transverse Electric (TE) and Transverse Magnetic (TM) polarizations. The selection of the specific computational method is guided by the availability of commercial tools and the expertise developed in their application. In this contribution, we utilized the Rigorous Coupled-Wave Analysis (RCWA) method to simulate the performance of a grating with a stepped profile.

The principal geometrical parameters considered in the design analysis of the compound-blazed grating, along with the constraints imposed by the system mechanical envelope, are summarized in Table 1. The geometry of a blazed grating (Fig. 1) is primarily characterized by the grating period d , the angle of the blazed surface, γ , and the slant angle, β . The slant angle accounts for manufacturing limitations that prevent the realization of perfectly sharp edge transitions. The relationship between the angle of incidence of the radiation, θ_{inc} , on the surface of the reflective grating and the diffraction angle, θ_m , follows the grating equation:

$$d(\sin \theta_{\text{inc}} + \sin \theta_m) = m\lambda, \quad (1)$$

where λ is the wavelength and m is the diffraction order which determines the angular location of the diffracted light.

In previous work by the authors⁴, the Rigorous Coupled-Wave Analysis and Finite Element Method (FEM) were investigated as numerical approaches for evaluating the diffraction efficiency of blazed gratings. The study showed that, for an aluminum blazed grating with a period of $d = 76\mu\text{m}$ and a blaze angle of $\gamma = 23.5^\circ$, the diffraction efficiencies of orders $m = 0$ and $m = 1$ exceeded 65% over the wavelength range from 70 to 139 μm . The FEM predictions yielded slightly higher values of the first-order diffraction efficiency, η_1 , than those obtained with RCWA; however, this discrepancy progressively decreased as the number of slices and Fourier-expansion terms used in the RCWA model increased, indicating convergence between both methods. Building on these results, the objective of the present work is to develop a grating capable of maintaining diffraction efficiencies

Table 1. Initial Operational Requirements

Variable	Values
Spectral range, λ	$[40, 140] \mu\text{m}$
Angle of incidence, θ_{inc}	57°
Period, d	$76 \mu\text{m}$
Diffraction order, m	1
Polarization	TM
Efficiency threshold, η_{thres}	0.65
Resolving power, R	200

above 65% over an extended wavelength range spanning from 40 to 139 μm , thereby enabling efficient operation at shorter wavelengths while preserving the high performance achieved in the previous design.

In the literature, we found a variety of approaches that have been proposed by other authors to broaden the operating range of diffraction gratings. These include the use of gratings with two concentric regions⁶, each characterized by a different blaze angle; mosaic-like structures⁷ in which each individual section has its own blaze angle; multi-blaze profiles that continuously combine sawtooth shapes⁸ with differing blaze angles; and profiles featuring two distinct^{9,10} slopes.

3. RESULTS AND DISCUSSION

In this work, a freeform profile incorporating two facets with different inclination angles, together with flat regions positioned at different height levels, was designed to extend the wavelength range over which high diffraction efficiency can be achieved. The simulations were carried out using software based on the RCWA method¹¹ (GSolver, Grating Solver Development Company, UT, USA), which was selected due to its lower computational requirements compared with FEM. The initial specifications required are listed at Table 1: In all simulations, the grating period (76 μm), the material (aluminum), the polarization (TM), the number of layers (100) and the number of diffraction orders considered (20) were kept constant. The following figures illustrate the influence of the different design parameters on the first-order diffraction efficiency over the wavelength range from 30 to 140 microns. The plots present color maps showing the efficiency variation as a function of wavelength and the parameter under study. The black contour line delimits the region where the diffraction efficiency exceeds 65%. Our design proposal for a single grating with an extended spectral range departs from a geometry with two blazed portions that are arranged within the period of the grating. These blazed parts do not cover the entire period, d , which also contains two flat portions that generate smooth transitions between the lower grating angle and the large grating angle. At the same time, these two flat portions produce a sharp transition that strongly affects the diffraction efficiency.

Because broadening the wavelength range of high diffraction efficiency leads to the emergence of additional diffraction orders, this effect was investigated in detail, and potential solutions for its implementation in a practical experimental system were identified and evaluated.

3.1 Compound Grating Profiles for Extended Range Operation

3.1.1 Effect of a double-blaze profile on diffraction efficiency

Fig.1 (left) shows that increasing the blaze angle enhances the diffraction efficiency at longer wavelengths while decreasing it at shorter wavelengths. In contrast, a larger slant angle leads to a reduction in diffraction efficiency, as illustrated in Fig.1 (right). The inclusion of the slant angle in the analysis is motivated by fabrication constraints, which inevitably introduce a certain degree of sidewall inclination.⁴

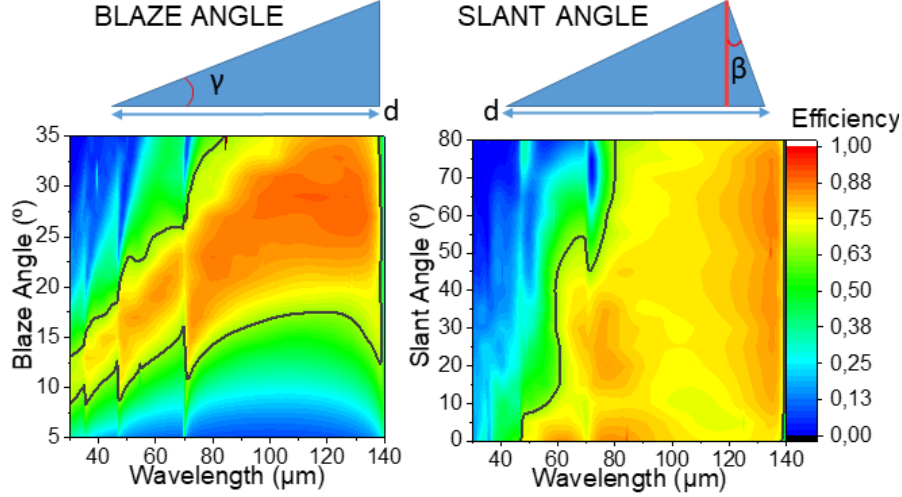


Figure 1. Diffraction efficiency *vs.* wavelength as function of blaze angle (left image) and slant angle (right image)

3.1.2 Influence of planar sections on the diffraction efficiency

The fabrication process based on laser ablation generates flat regions at the bottom of the grating profile. Figure 2 illustrates the effect of increasing the fraction of the period occupied by this bottom flat section while keeping both the blaze angle and the period constant. As the width of the flat region increases, the diffraction efficiency decreases, with the effect being particularly pronounced at shorter wavelengths. Conversely, introducing a flat region at the apex of the profile, as shown in Fig. 2 can enhance the efficiency at short wavelengths. However, when the top flat region exceeds approximately 35% of the profile base, the diffraction efficiency deteriorates at longer wavelengths.

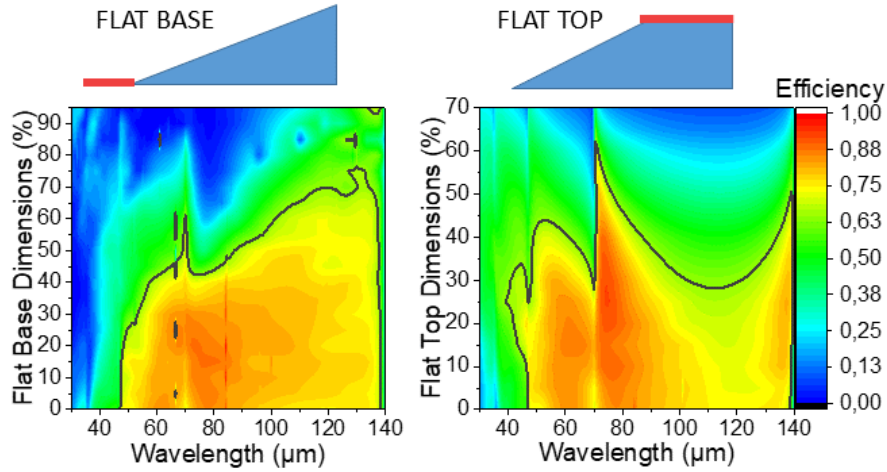


Figure 2. Diffraction efficiency as a function of wavelength, with a section of the profile flattened: on the bottom (left image) or on the apex (right image)

3.1.3 Influence of having a double blaze profile

In this case, we consider a profile with a double blaze; the structure of the sawtooth profile, instead of being a continuous slope, is divided into two distinct sections with different slopes (γ_1 and γ_2). We aim to improve the efficiency value at low wavelengths without reducing its value at high wavelengths. The proportion of periods corresponding to each section is varied, and the total height of the profile remains constant. Figure 3 (left)

corresponds to a first section with a blaze angle of $\gamma_1 = 10^\circ$ (according to previous simulations that gave good performance at short wavelengths) and a second section with a blaze angle of $\gamma_2 = 27^\circ$ (good performance at long wavelengths). It starts with a first simulation in which the first section occupies $7,6 \mu\text{m}$ and the second $68,4$ microns of the $76 \mu\text{m}$ period, until the last simulation in which the first section occupies 90% of the period. In Fig. 3 (right), the ratio of the periods occupied by each section remains constant ($38 \mu\text{m}$), while γ_2 is constant at 27° , and γ_1 varies from 5° to 23° . When the proportion of the period corresponding to the first section exceeds 50%, the efficiency drops, especially at medium and large wavelengths while the efficiency at short wavelengths increases slightly but does not reach the 65% efficiency requirement. When the proportion of the period covered by each section remains constant, an increase in the angle of the first blaze slightly improves the efficiency of the grating.

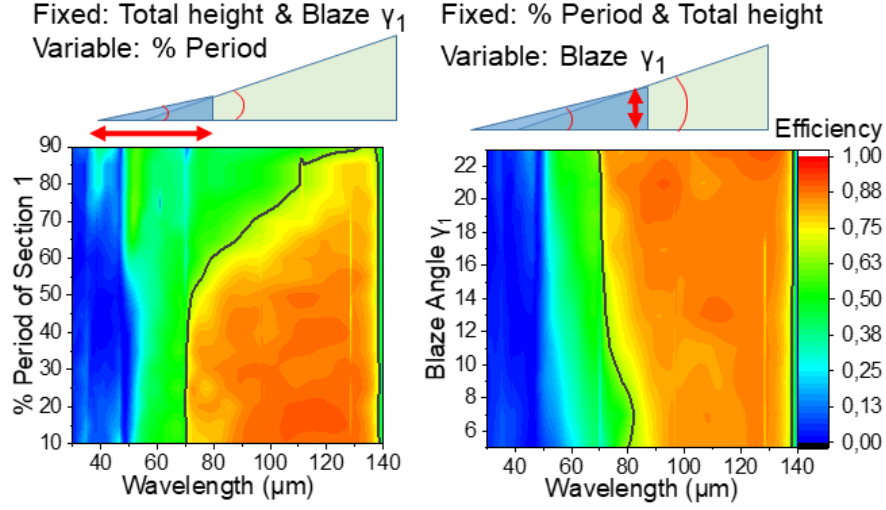


Figure 3. Diffraction efficiency *vs.* wavelength when introducing a double slope in the profile. At the left, the blaze angles of each slope remain constant but the percentage of period corresponding to the first section varies. At the right, the proportion of the period occupied by each slope is retained at 50% but the first blaze angle, γ_1 , is varied while keeping γ_2 constant

3.1.4 Combined effect of all parameters

The diffractive behavior of the grating when several parameters are combined differs from that expected when each element is considered separately. For example, by adding a flat surface at the top of the profile while maintaining the blaze angle, the overall height is reduced. Alternatively, incorporating a flat surface at the bottom of the profile alters the proportion of periods spent on each slope, which impacts efficiency. The grating has been optimized to consider all possible configurations using software based on the RCWA method.

To achieve a grating that operates in the whole range of interest with efficiencies above 65%, after the optimization process, the profile shown in Fig. 4 has been proposed. The description of which is summarized in Table 2. The profile consists of:

1. (a) A double blazed profile optimized to have good efficiencies at short wavelengths ($\gamma_1 = 10^\circ$, section A) without losing much efficiency at long wavelengths ($\gamma_2 = 33,5^\circ$, section B).
2. (b) A flat part at the apex of the profile that improves efficiency at short wavelengths (section C corresponding to 35% of the total period).
3. (c) A flat part at the base of the profile that occupies 5% of the total period (section D).

In Fig. 5 we have plotted the simulated efficiency for the 0th and 1st diffractive orders. It illustrates the simulated efficiency of a diffraction grating with the compound blazed profile described in Table 2 (black line),

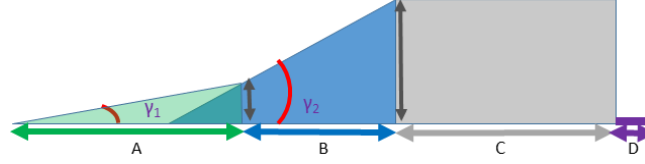


Figure 4. Profile diagram of compound blazed profile grating.

Table 2. Compound blazed diffraction grating parameters

Parameter	Dimension
Section A	27,66 μm
Section B	18,24 μm
Section C	26,45 μm
Section D	3,65 μm
Blaze angle (Section A), γ_1	10°
Blaze angle (Section B), γ_2	33,5°

and is compared to the baseline sawtooth profile (red line, period 76 μm and 23,5° blaze). The graph illustrates significant drops in the diffraction efficiency when specific diffraction orders disappear, as in the case of 47 μm , where the third order disappears, 69 μm , where the second order disappears, and 140 μm , where the first order is no longer present. Table 3 shows the average efficiency of the compound blazed profile grating and it is compared with the value of efficiency of the sawtooth profile grating. The average has been calculated for two different wavelength ranges. The compound blazed profile exhibits greater uniformity in efficiency throughout the wavelength range, as evidenced by the lower standard deviation; however, its efficiency is 4% lower than that of the sawtooth grating. The minimum efficiency of both profiles varies significantly. The minimum efficiency of the compound blaze profile is 66% at 70 μm , while the minimum efficiency of the sawtooth profile is 12% at 46.5 μm . The optimization of the proposed blazed profile grating aimed to enhance performance in the short wavelength areas while minimizing any decrease in the long wavelengths. This type of compound blazed profile grating maintains efficiencies greater than 65% throughout the wavelength range. In particular, it achieves an improvement 12% in the range of 40 to 70 μm , with a deviation less than that of the sawtooth grating.

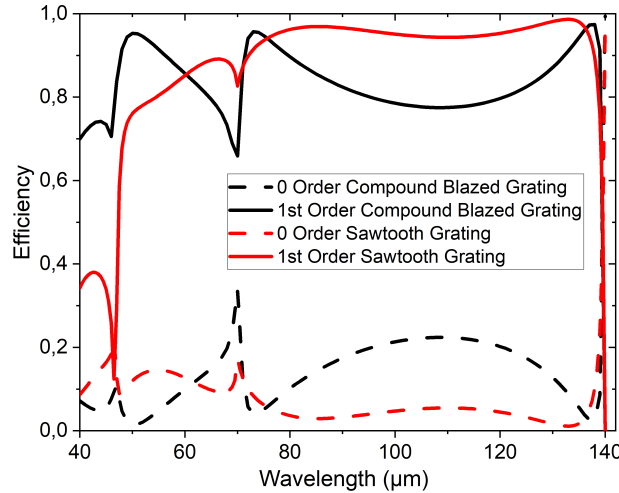


Figure 5. Diffraction efficiencies of both profiles for 0th and 1st orders for grating described in 3 (black) and comparison to the baseline sawtooth profile (red).

3.2 Emergence of Multiple Diffraction Orders

When the operational bandwidth of a diffraction grating is extended, wavelengths shorter than the grating period give rise to multiple diffraction orders. As a consequence, these higher orders lead to different wavelengths being

Table 3. Comparison of average efficiency between compound blazed profiles and sawtooth diffraction gratings in different λ ranges

Range (μm)	Compound blazed	Sawtooth
40-140	$0,83\pm0,07$	$0,87\pm0,17$
40- 70	$0,82\pm0,09$	$0,70\pm0,22$

diffracted at identical angles, producing spectral overlap. According to the grating equation (Eq. 1), spectral order overlap occurs when radiation of different wavelengths, diffracted in different diffraction orders, emerges at the same diffraction angle. This condition is fulfilled when

$$\lambda_2 = \frac{m_1}{m_2} \lambda_1, \quad (2)$$

where $m = 1$ and $m = 2$ denote the corresponding diffraction orders. As a particular case, radiation with wavelength (λ) diffracted in the first order m_1 propagates in the same direction as radiation with wavelength ($\lambda/2$) diffracted in the second order m_2 , since

$$\lambda_2 = 2\lambda_1. \quad (3)$$

Consequently, higher diffraction orders may overlap with shorter wavelengths, producing spectral ambiguities in the measured signal unless the unwanted diffraction orders are effectively suppressed or separated. Fig. 6 depicts the angular distribution associated with the various diffraction orders and clearly identifies the regions where such overlap takes place. The representation corresponds to the grating parameters listed in Table 1, where the radial coordinate denotes the wavelength and the angular coordinate represents the diffraction angle.

In this diagram, the red dashed curve marks the emergence of the second diffraction order ($m = 2$) at an angle of 12.5° . Likewise, the blue dashed curve indicates the third order ($m = 3$), showing that radiation with a wavelength of $40 \mu\text{m}$ is diffracted at an angle of $\theta = 47.8^\circ$. The brown dashed curve defines a critical wavelength of $\lambda = 76 \mu\text{m}$, which acts as a boundary beyond which only the fundamental order ($m = 1$) is present. For diffraction angles exceeding 12.5° , overlap between orders occurs for wavelengths shorter than $76 \mu\text{m}$, leading to potential ambiguity in the detected signal.

To mitigate this issue and avoid contamination from higher diffraction orders in the long-wavelength regime, it is necessary to employ long-pass optical filters with a cutoff wavelength above $76 \mu\text{m}$. By positioning these filters in front of detectors located within the affected angular regions, only the first-order diffraction component is allowed to reach the measurement system. When applied to diffraction-based spectrometers, particularly in space-borne instrumentation, metal mesh filters constitute an efficient means of mitigating harmonic contamination. Metal mesh filters specifically designed for operation in the terahertz (THz) spectral range have been widely reported¹² in the literature. These structures function as frequency-selective surfaces (FSS), where the electromagnetic response is determined by the precise geometry and periodicity of metallic patterns deposited on dielectric substrates. By carefully tailoring their unit-cell design, these filters can exhibit low-pass, high-pass, or band-pass behavior, typically characterized by steep roll-off regions and strong rejection outside the desired frequency band. Furthermore, these filters are especially well-suited for aerospace environments due to their mechanical robustness, high manufacturing reproducibility, and stable electromagnetic performance under cryogenic conditions. Consequently, they have become a standard solution in ground-based, balloon-borne, and space-based THz instrumentation platforms¹³.

4. CONCLUSIONS

A free form grating based on a double-ramp profile with different blaze angles and planar sections was investigated as a practical approach to achieve high diffraction efficiency over a broad spectral range. The grating geometry was optimized using rigorous electromagnetic simulations, which showed that efficiencies above 0.65 could be maintained across the target spectral range. The proposed methodology enables the design of high-performance free form gratings adapted to fabrication constraints while extending the operational spectral range. To mitigate crosstalk arising from the presence of multiple diffraction orders, the use of selective filters in the detection system

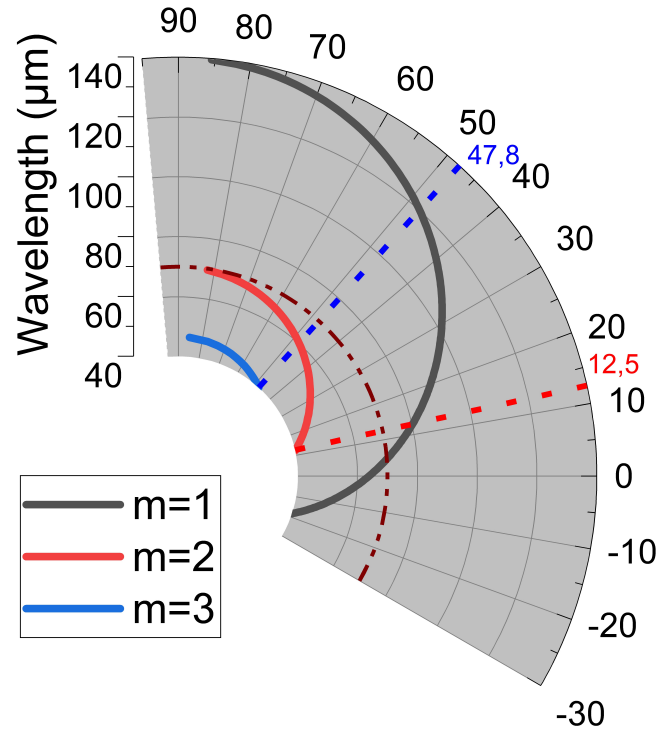


Figure 6. Angular and spectral mapping of diffraction orders is presented. It can be observed that the second-order contribution ($m = 2$) begins to overlap with the first-order component ($m = 1$) for angles $\theta > 12.5^\circ$. Furthermore, for angular values exceeding $\theta > 47.8^\circ$, an additional overlap involving the third order ($m = 3$) becomes evident.

is recommended. Overall, the results demonstrate the feasibility of efficiently operating a free form grating over a wide spectral range in the THz domain.

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