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Optical Design and Performance Evaluation of a Mini Spectrometer for Space Applications

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Abstract

The mini spectrometer design is discussed, and two models using finite elements approach are presented. The simplest optical design is used to reduce the optical signal losses. The two models considered are based on the use of transmission and reflection gratings respectively. The two designs are compared based on the obtained wavelength resolution. Our results showed that the spectrometer based on the transmission diffraction grating performed better and showed good wavelength resolution with a small footprint making it suitable for space deployment.

1. Introduction

The traditional design of a Raman spectrometer is intended for general laboratory use with the focus on the resolving power and the flexibility in the spectral range coverage.

These spectrometers are generally heavy and bulky tabletop instruments. For mini spectrometer design the size of the instrument is also very critical due to many parameters such as heating effect, dimensions, weight, and resolution. Some compromises must be made between these parameters to have the best design for space applications [1,2].

In this paper, we investigate the optical design parameters of a Mini-Raman spectrometer optimized for best performance in harsh space environment. A Czerny-Turner spectrometer [3] was successfully modeled using finite elements method with COMSOL Multiphysics [4]. The performance characteristics of the design were investigated under ambient atmospheric environment.

The two models considered in this study showed that the spectrometer based on the transmission grating has higher resolution than the spectrometer based on the reflection grating. This is a good and promising result that further supports the high stability and mechanical structure of the transmission-based grating used in this configuration.

2. Spectrometer Operation Principle

The spectrometer is used to disperse and analyze the input light by providing the amount of light intensity as a function of the position on the Charge Coupled Device (CCD) detector.

The two designs considered in this study are described as follows: (1) A mini spectrometer with a transmission-based diffraction grating, and (2) A mini spectrometer with a reflection grating as shown in Figures 1 (a) and (b) respectively.

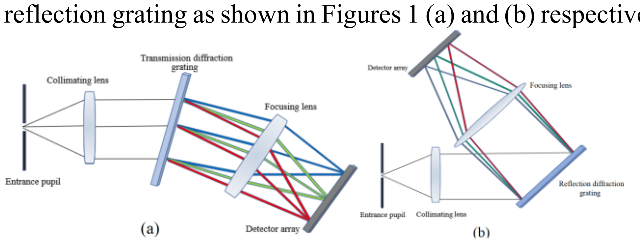

Figure 1. Schematic of a simplified spectrometer with a transmission-based diffraction grating (a) and a reflection-based diffraction grating (b).

In our case, the light from the sample under investigation enters the entrance slit on the spectrometer. The size of the slit determines the amount of light that can be measured by the instrument and hence affects the optical resolution as well as the efficiency and sensitivity of the spectrometer. The smaller the slit size, the higher is the resolution but at the expense of a lower signal intensity. The beam coming out of the slit is diverging and requires collimation to be a parallel beam. This is accomplished by using a collimating lens as shown in Figure 1. The collimated rays are then directed towards a diffraction grating. The grating acts as a dispersive element and splits the light into its constituent wavelengths [1].

In more details, the diffraction grating is an optical element that imposes a "periodic" variation in the amplitude and/or phase of an incident electromagnetic wave. It thus produces, through constructive interference, several discrete diffracted orders (or waves) which exhibit dispersion upon propagation. Diffraction gratings are thus widely used as dispersive elements in spectrographic instruments, although they can also be used as beam splitters or beam combiners in various laser devices or interferometers [2].

After interacting with the diffraction grating (transmission or reflection), the diffracted electromagnetic waves with different wavelengths are spatially dispersed and resolved then captured by a photodetector or CCD. The later captures the light spectra and measures the intensity of light as a function of wavelength (or position on the detector). After calibration of the CCD, the data is plotted as a spectrum of the normalized light intensity as a function of wavelength. A CCD is an integrated circuit etched onto a silicon surface forming light sensitive elements called pixels. Photons striking this surface generate charges that can be measured by specialized circuits [5].

After this brief description of the main working principle of spectrometers in general, we now proceed to the comparison of two optical configurations and designs for a mini-Raman spectrometer as the focus of this study.

To design a mini spectrometer that is more compact and have enough resolution to be used for Raman spectroscopy, we have selected the optical configurations shown in Figure 1. This choice is also driven by the fact that we wanted a simple design with less optical components to reduce the losses of the expected weak light signal and reduce the probability of instrument failure. In our study, we developed a finite element model for each of the optical configurations shown in Figure 1. The results of the two models are compared based on the characteristics of the output signal at the detector surface. We compared the spectrometer resolution at the detector surface. From our results, we found that the spectrometer design using the transmission grating gives the best results as shown and discussed in the next sections.

3. Theoretical Background

The key parameters needed for the design and characterization of a spectrometer are summarized in Table 1. Some of these parameters and the geometry used for the diffraction grating are also shown in Figure 2.

Table 1: Key parameters used in the spectrometer design

Parameter	Symbol	Value
Minimum wavelength	λ_1	220 nm
Maximum wavelength	λ_2	980 nm
Wavelength range	$\lambda_2 - \lambda_1$	760 nm
Resolution	$\Delta\lambda$	2.63 nm
Center wavelength	$\frac{\lambda_1 + \lambda_2}{2}$	600 nm
Grating groove density	G	500 gr/mm
Collimator focal length	L_c	100 mm
Focusing lens focal length	L_F	100 mm
Detector width	L_D	29.18 mm
Input slit size	w_{slit}	100 µm
Numerical aperture	*NA*	0.25

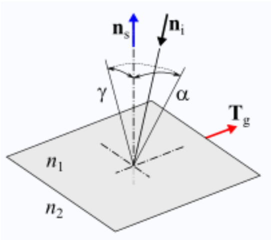

Figure 2. Schematic of the diffraction grating orientation and angles [4].

Using these parameters, we can derive the required governing equations along with the physical limitations of a specific spectrometer design and size. These design parameters are considered in the following consecutive steps:

1. Define the wavelength range $\Delta\lambda$, with appropriate groove density G, and geometry given by
$$\Phi = \alpha + \beta \quad (1)$$
2. Calculate the grating angles α and β from the grating equation [6]:
$$\alpha = sin^{-1}\left(\frac{\lambda_c G}{2\cos\left(\frac{\Phi}{2}\right)}\right) - \frac{\Phi}{2} \quad (2)$$
3. Choose the detector length: L_D
4. Calculate the focal length of the focusing lens and/or mirror from [6]:
$$L_F = \frac{L_D \cos(\beta)}{G(\lambda_2 - \lambda_1)} \quad (3)$$
5. Calculate the magnification from the following [6]:
$$M = \frac{L_F \cos(\alpha)}{L_C \cos(\beta)} \quad (4)$$
6. Calculate input slit width from [6]:
$$w_{slit} = \frac{G L_C \Delta\lambda}{\cos(\alpha)} \quad (5)$$

After steps 1-6 have been completed iteratively, the next step is to consider the physical limitations constraining the extent to which one can make the spectrometer more compact. These limitations are governed by the optical diffraction limit and the grating diffraction limit [7]. It is worth noting that the specific parameters L_C, L_D, and L_F from Table 1 are set based on the design requirements. For example, the lenses and the detector are chosen in accordance with the required size of the mini spectrometer and how compact it can be. For space applications, the size and weight are very important factors as the instrument deployment cost is very high.

It is important to note that steps 1-6 above, only allow us to achieve the best compact spectrometer design in terms of physical dimensions. However, an effective spectrometer should also exhibit optimal resolution, and the diameters of the focusing/collimating lenses should also transfer all the incoming light coming through the aperture. This is described by the numerical aperture (*NA)*. In the far field approximation, the numerical aperture is given by [8]:
$$NA \approx n\frac{D}{2f} \quad (6)$$
where *D* is the lens diameter, *n* is the refractive index (≈ 1 for air), and *f* is the focal length of the lens.

Spectral resolution is defined as a spectrometer's ability to resolve features in the electromagnetic spectrum. The resolution of a spectrometer is denoted by Δλ which is the smallest wavelength change that it can detect (resolve). The resolving power of a spectrometer is defined as follows [9]:
$$R = \frac{\lambda}{\Delta\lambda} \quad (7)$$
On the other hand, the diffraction grating is characterized by its grooves' density *G*, which is the number of lines per mm. Theoretically, the higher *G* is the better the dispersive resolution. However, this is still limited by the grating diffraction limit given by the following equation [9]:

$$\Delta\lambda_{diffraction1} = \frac{0.84\lambda_c \cos(\alpha)}{2GL_c \tan(\theta_{NA})} \quad (8)$$

Similarly, the spectral resolution is strongly tied to the optical diffraction limit as follows [9]:

$$\Delta\lambda_{diffraction2} = \frac{1.028\lambda_C M(\lambda_2 - \lambda_1)}{2L_D \tan(\theta_{NA})} \quad (9)$$

Hence, it is the optical part that must be chosen to make $\Delta\lambda_{diffraction2}$ as close as possible to the required $\Delta\lambda$.

The main motivation behind considering the two types of spectrometer designs in Figure 1, is their simplified design with less optical components. The spectrometer with the transmission-based grating is comparatively less sensitive to misalignments due to vibrations, which is important for portable /mini spectrometers. However, transmission-based gratings become less effective in the near infrared (NIR) wavelength region when the groove density exceeds 1000 lines/mm. In this case the distance becomes comparable to the wavelength of the electromagnetic wave making it less transmitting. The reflective diffraction grating, however, can have higher groove densities and work well in NIR.

4. Spectrometer Design

4.1 Design Parameters

As mentioned, all spectrometers are based on three main components: an entrance pupil, a diffraction grating, and a detector which have been described above. Proceeding to further details regarding spectrometer design, we now briefly describe the key parameters, governing equations, physical constraints and/or limitations, and optimization.

The design parameters used for both our models are kept the same except for the diffraction grating and the geometry associated with it. All the path lengths of the central optical beam are kept the same. The parameter values used for the models are listed in Table 1.

4.2 Transmission-based Grating Model

We investigated the performance of a Czerny-Turner spectrometer using two different models. The spectrometer design is shown in Figure 4.

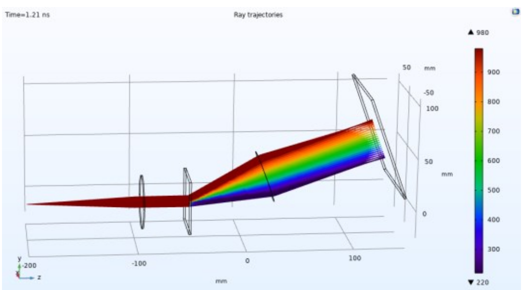

Figure 4. Transmission-based grating model of the spectrometer.

This is chosen as the simplest spectrometer design with the minimum number of optical components to reduce the light losses and interactions with the different surfaces. The first design is based on the transmission diffraction grating. The model was developed using finite elements approach with COMSOL Multiphysics. The geometry and the results of this model are shown in Figure 4. From Figure 4 we can see that the focal plane of the light spectrum does not fall exactly on the detector plane. This is due to the wavelength dependence of the focal distance and the diffraction angle. This affects the spot size and shape of the light deposited on the detector plane differently at different wavelengths. In Figure 5 we show the spot diagram of the light deposited on the target plane which is at the detector surface that is normal to the light beam for optimum sensing. In general, the spectrometer is designed to focus the central wavelength to achieve the best resolution. This is done by placing the target plane at the location where the central spot has the smallest diameter to optimize the resolution of the spectrometer. At this point we move the detector plane to the position of the target plane which is the best position for optimum spectrometer resolution.

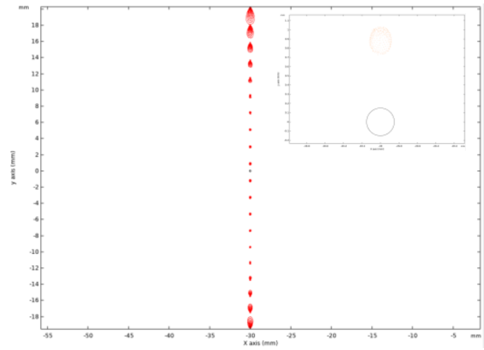

Figure 5. Spot diagram at the target plane of the detector (CCD). A closer view of the beam spot at the target plane is shown in the inset. The black circle with 300 µm diameter is shown in both figures for reference.

4.3 Reflection-based Grating Model

Similarly, we have developed a finite element model using COMSOL Multiphysics for a reflection-based grating spectrometer. The model diagram and results are shown in Figure 6. The diffraction grating is placed at 45° with respect to the incident beam. The light beam is deposited on the detector plane at normal incidence.

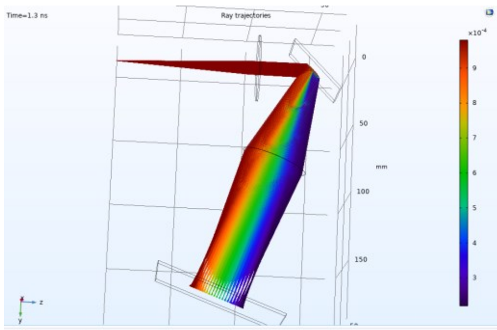

Figure 6. Reflection-based grating model of the spectrometer.

In Figure 7 we show the spot diagram of the light deposited at the target plane on the detector. This is the optimized position for the best spectrometer resolution. The inset shows a closer view of the spot diagram at the detector plane. The small circle in the inset is for reference and has a diameter of 300 µm.

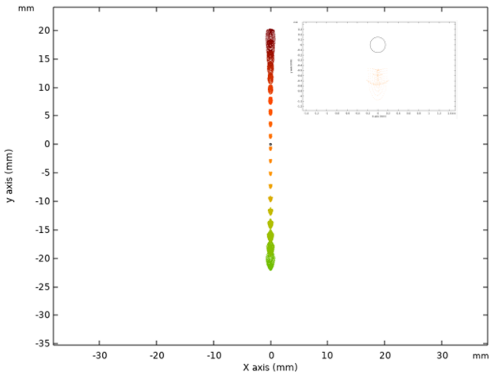

Figure 7. The spot diagram of the reflection-based grating model on the detectr plane. The inset shows a circle with 300 µm diameter for reference.

5. Results and Discussion

To compare the results of the two models we consider the following parameter N:

$$N = \frac{Spot\ diameter}{pixel\ width} \tag{10}$$

The parameter N gives the number of pixels needed to cover the spot diameter on the CCD. The results are in Table 3.

Table 3: Spot size comparison between the two models

Model	Spot size (µm)	CCD Pixel width (µm)	N (Pixels)
Transmission Grating	290	8	36
Reflection Grating	540	8	68
Comparison			1.9

From the result above we can see that the number of pixels needed to cover the light spot at the detector in the reflection grating configuration is almost double that needed for the transmission grating configuration. This is an indication of the higher resolution achieved by the transmission-based spectrometer. To illustrate this further we can consider two adjacent light spots at the detector with a width of 36 pixels each. In this case the two spots will be resolved in the transmission-based grating spectrometer while in the case of the reflection-based grating spectrometer they will overlap and cannot be resolved. This is clearly shown previously in Figure 3. We also notice the beam spot distortions away from the central wavelength in both cases. These distortions are observed to be more pronounced in the case of the reflection-based grating.

Based on our models we can also calculate the resolving power of each spectrometer using Equation 7. The results found are $R_1 = 109$ and $R_2 = 62$ for the transmission-based and the reflection-based spectrometer designs respectively. This shows almost double the resolving power for the transmission-based grading spectrometer design. We believe this is due to the larger amount of stay light and sensitivity of the reflection process to small changes in the surface orientation. The reflection on the grating surface will behave like a mirror and hence the reflected light (as well as the diffraction) will rotate by twice the angle change of the mirror surface. These secondary rays in addition to the phase change associated with reflection could play an important role in this observed broadening of the spot size.

6. Conclusions

We have designed two mini spectrometers for potential applications in space. At this initial stage, we focused on the choice of the proper geometry and best components for harsh space environment. We have developed two mini spectrometer models using transmission-based and reflection-based gratings to investigate their performance. From our results, we confirmed that the spectrometer design based on the transmission diffraction grating has double the resolution of the reflection-based grating spectrometer design. Additional work is in progress to evaluate the thermal and mechanical stabilities of both designs under space environment with wide temperature variations and intense vibrations.

7. Acknowledgment

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