Design and Analysis of an Optical System (Optical Spectrometer)

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Laboratory Practice III

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Abstract

The aim of the laboratory work is to design and analyze a spectrometer. The spectrometer design consists of a collimating lens, a binary transmissive grating, an achromatic doublet and a Charge-Coupled device (CCD). The light source was taken to be red LED of wavelength range 610 − 760 nm. The laboratory work consists of three parts: geometrical design with analytical calculation and spectrometer design using OpTaliX as well as rigorous grating optimization. Geometrical analysis and analytical calculation were done to obtain parameters for a starting point for refining the system with OpTaliX. Also, analytically obtained grating period was used in grating optimization to achieve high transmission efficiency throughout the whole wavelength range.The optimization was done using Fourier Modal Method (FMM) with the help of Matlab.

Keywords: lens; grating; geometrical analysis

Contents

Chapter I

Introduction

Optical spectrometers are used as a very important tool in science and technology, i.e. Chemistry and astronomy. The basic principle of the spectrometer is the interaction of electromagnetic radiation with a sample and the resultant reflection, refraction or transmittance gives the characteristics of the material.The history of spectrometer dates to centuries. The first known study of spectrometer was done by Newton in 1666. His experiment was based on the dispersion of the sunlight by glass prism and the observation of spectrum by an additional lens. This process was improved by William Wollaston in 1802 with the introduction of a narrow slit instead of small aperture. However, significant advancement in the spectrometer design was achieved by Joseph von Fraunhofer in 1814 as he used convex lens between slit and the prism, and a telescope was added to view the spectrum for more improved measurement [1].

Modern spectrometer is way more complex. Instead of using prism for light splitting, diffraction grating is used for the dispersion of the spectrum. On the other hand, Charge-Coupled Device (CCD) is used as detector instead of photographic plate. Based on the characteristics of the spectral lines, i.e. position, height, depth, width and general shape, it is possible to characterize the observed body [2].

This work is based on the design and analysis of a spectrometer. In the 2nd chapter, theoretical background of diffraction grating as well as description of different components of spectrometer will be discussed briefly. The third chapter is on the development of geometrical design and related calculation for optimization. In the chapter four, optimization using OpTaliX as well as corresponding results will be presented while in the fifth chapter, optimization of grating parameters based on

FMM method will be discussed . The last chapter is on the summery of the whole work.

Theory

Optical spectrometer is a device that creates the image of the input slit at the detector. Basically, it consists of two types of lens systems: collimating and focusing lenses, as well as a diffraction grating that is used in between the lenses to disperse light according to their wavelength. In this chapter, theoretical background of diffraction phenomena as well as the diffraction grating, and Fourier Modal Method through which grating efficiency is calculated will be discussed.

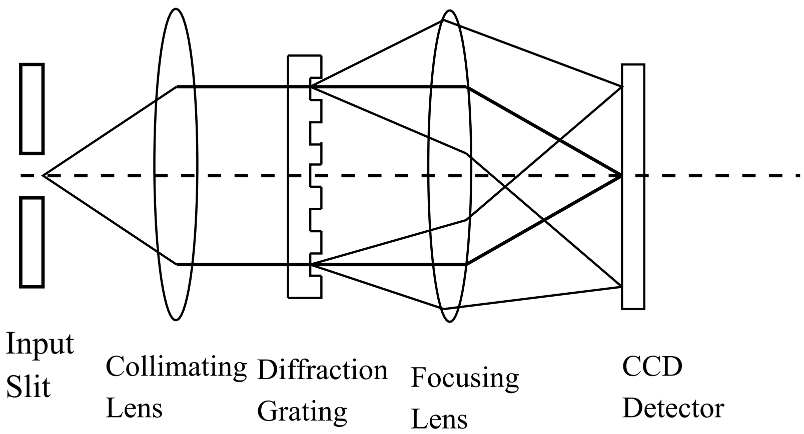

Figure 2.1: Scheme of an optical spectrometer [3].

2.1 Collimating and focusing lens

In this laboratory work, two types of lenses are used: a collimating lens which is normally a convex lens and an achromatic doublet as focusing lens. The light coming through the input slit is not collimated. Therefore, collimating lens is used to make rays parallel. Also, it helps to do the necessary modification for the filed of view, collection efficiency and spatial resolution in the spectrometer setup [4]. On the other hand, an achromatic lens is used to reduce the chromatic aberration of the system which is due to the inability of the system to focus the light of different wavelengths at the same focal spot. An achromatic doublet generally consists of two different lenses joined together. Generally, a positive low-index (crown) element and a negative high-index (flint) element are added together for the formation of achromatic doublet [5].

2.1.1 Spot size evaluation

The spot size determines the resolution of image and Rayleigh criteria is used to calculate the spot size of the focused beam. According to the Rayleigh criteria, any two images are resolvable when the center of the diffraction pattern of the first image overlaps the first minima of the other. The radius of the focused spot can be expressed as ,

$$x = 1.22\frac{\lambda f}{D}. \tag{2.1}$$

Here, f is the focus distance of the lens and D is the beam diameter at the lens [6].

2.2 Diffraction grating

A diffraction grating is a set of repeating elements which can be either transmitting or reflecting, separated by a specific distance. The distance must be comparable to the wavelength of the light used in the process. The basic property of a diffraction grating is the spatial modulation of refractive index. A series of transparent slits are used as transmitting elements in an opaque screen while reflecting grooves on a substrate are used as reflecting elements. The first diffraction grating was a half inch wide grating with fifty-three apertures which was developed by American astronomer, David Rittenhouse [7] in 1785. Diffraction grating can be different types: reflection grating, transmission grating, master grating and replica grating. Reflection grating formed on reflective surfaces while the transmission grating formed on transmission surfaces. Master grating is based on surface relief pattern which is created by holographic recording while the surface relief pattern of replica grating is formed by molding the relief pattern of another grating.

2.2.1 Grating equation

Fig. 2.2 shows the scheme of a diffraction grating. The grating period of the diffraction grating is d. A light wave of wavelength λ is incident on the diffraction grating at an angle θ_i with respect to the surface normal. After diffraction light exit the grating at an angle θ_m. Based on the geometry, grating equation can be expressed

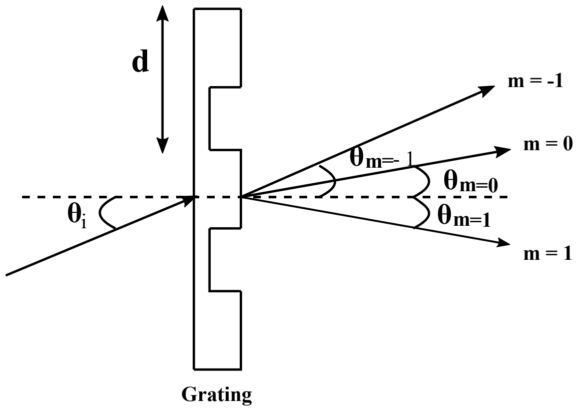

Figure 2.2: Scheme of a diffraction grating and propagation of light through the diffraction grating.

as,

$$d(Sin\theta_m + Sin\theta_i) = m\lambda. \tag{2.2}$$

Here, θ_i and θ_m are positive since they are opposite sides of the surface normal. m is the diffraction order and m $= \pm 1, 2, 3, ...$

2.2.2 Transmission grating

In this laboratory work, single layer transmission grating was used for spectrometer design which is illustrated in Fig. 2.3. The structure of the grating is defined by three factors: grating height h, grating period d and fill factor $ff = c/d$ (see Fig.2.3). Here, the input material (substrate) is silica and the output material is air.

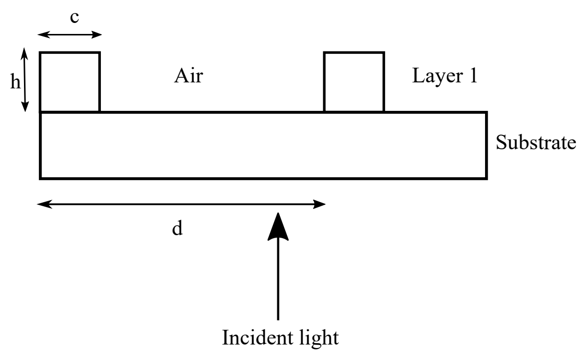

Figure 2.3: Single layer transmission grating and its parameters.

2.2.3 Grating efficiency calculation based on Fourier Modal Method

Grating efficiency can be explained in terms of energy distribution of a given wavelength diffracted by a grating. The diffracted light of different spectral order is governed by specific parameters: polarization of incident light, incidence and diffraction angle, refractive index of the grating surface and grating structure [8]. The grating efficiency is defined by the ratio of diffracted light intensity to the incident light intensity. In this work, Fourier Modal Method (FMM) was used to design the diffraction grating and optimization of grating efficiency. In this method, field outside the permittivity-modulated region is represented as the Rayleigh plane-wave expansions formula while the field inside the modulated region is considered as the superposition of guided modes. By using the Fourier series method, eigenvalue equations are solved and applying the electromagnetic boundary condition, system of linear equations are found. This method is widely used for its clarity and versatility [9].

2.3 Detector

In this laboratory work, Charge-Coupled Device (CCD) detector was used. The CCD in question is a line camera which works in the wavelength range of 350 nm to 1100 nm while the detector length is 29.184 mm. The detector has a 3648-pixel array while the pixel size is 8 $\mu m \times$ 200 μm.

Calculations based on geometrical design

In this chapter, geometrical approach of a spectrometer design will be developed to obtain different parameters that can be used in the actual spectrometer design. During the analytical calculation, the wavelengths were considered in red LED region. Also, incident light was assumed to be collimated.

3.1 Basic geometrical design

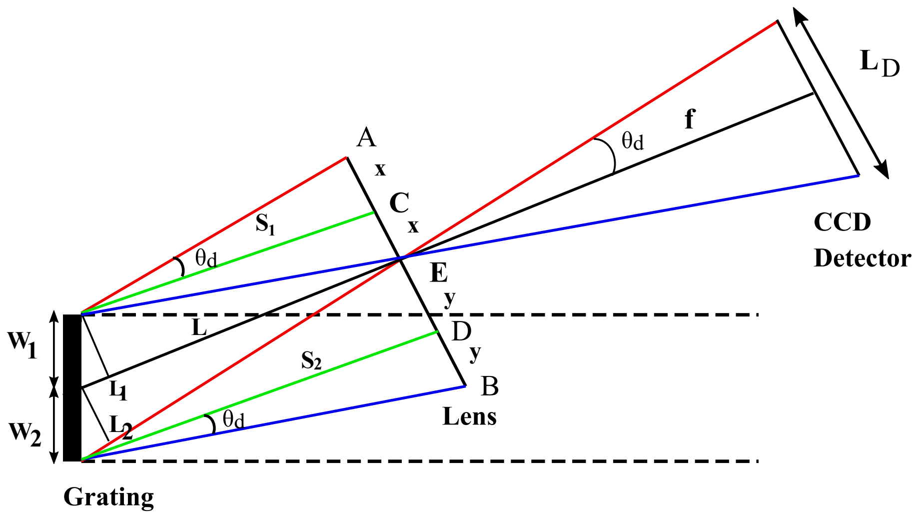

Figure 3.1: Geometry of the spectrometer.

The spectrometer design for the geometrical analysis is shown in Fig. 3.1. According to the geometry, as the incoming light strikes the grating, different wavelengths diffract at different angles. The diffracted light rays are focused by an achromatic lens at the CCD detector. Here, full length of the detector was used. For this reason, the distance between the lens and the detector will be varied while the distance between the grating and the lens will be kept fixed.

From the figure, it is seen that the width of the diffraction grating is W = $W_1 + W_2$ = 10 mm. The distance between grating and lens is L while the distance between lens and detector is denoted by f. Lens diameter AB = 22 mm, which is smaller than actual one inch diameter, is considered to avoid edge aberration. Also, AC = CE = x and ED = DB = y. After diffraction, the light beam is divided into components with wavelengths λ_{max}, λ_{avg}, and λ_{min} and the corresponding diffraction angles are given by θ_{max}, θ_{avg}, and θ_{min}. The diffraction order is $m = 1$.

Using the Pythagorean theorem, following parameters are obtained from the figure:

$$W_1 = \sqrt{x^2 + L_1^2}, \tag{3.1}$$

and

$$W_2 = \sqrt{y^2 + L_2^2}. \tag{3.2}$$

From the trigonometry,

$$x = S_1 \tan\theta_{\mathrm{d}}, \tag{3.3}$$

$$y = S_2 \tan\theta_{\mathrm{d}}, \tag{3.4}$$

Here, $\theta_{\mathrm{d}} = \theta_{\mathrm{max}} - \theta_{\mathrm{avg}} = \theta_{\mathrm{avg}} - \theta_{\mathrm{min}}$, and S_1, S_2 and L are related by

$$S_1 = L - L_1, \tag{3.5}$$

and

$$S_2 = L - L_2. \tag{3.6}$$

Using Eqs. (3.3)-(3.6) in Eq. (3.1) and Eq. (3.2) we get ,

$$W_1 = \sqrt{(L - L_1)^2(\tan\theta_{\mathrm{d}})^2 + {L_1}^2}, \tag{3.7}$$

$$W_2 = \sqrt{(L + L_2)^2(\tan\theta_{\mathrm{d}})^2 + {L_2}^2}. \tag{3.8}$$

So the grating width becomes,

$$W = W_1 + W_2 = \sqrt{(L - L_1)^2(\tan\theta_{\mathrm{d}})^2 + {L_1}^2} + \sqrt{(L + L_2)^2(\tan\theta_{\mathrm{d}})^2 + {L_2}^2}. \tag{3.9}$$

Also, focal length can be expressed as

$$f = \frac{L_D}{2\tan\theta_\mathrm{d}}. \tag{3.10}$$

Here, L_D is the detector length. Finally, the beam width at the lens is given by,

$$D = \frac{W\cos\theta}{\cos\theta_\mathrm{d}}. \tag{3.11}$$

3.2 Calculated parameters based on the geometrical design

The wavelengths of the red LED are $\lambda_{max} = 610$ nm, $\lambda_{min} = 760$ nm, and $\lambda_{avg} = 685$ nm. Also, grating period is selected as 1036 nm while the grating width is 10 nm. These design parameters are used to calculate the diffraction angles θ_{max}, θ_{min} and θ_{avg} by using Eq. 2.2. Also, focal length and spot size was calculated from Eq. 3.10 and Eq. 2.1. Calculated values of different parameters obtained from the geometry is presented in Table 3.1.

Table 3.1: Calculated parameters for the spectrometer design.

Grating period [nm]	Focal length [mm]	θ_{max}	θ_{avg}	θ_{min}	spot size [mm]
1036	149.9504	47.1883	41.6302	36.0721	0.0169

CHAPTER IV

Spectrometer design with OpTaliX

In this chapter, the design of spectrometer based on the analytical data will be implemented for achromatic doublet and singlet lens with OpTaliX design software. OpTaliX is a software for designing optical systems, thin film multilayer coatings and illumination systems. First, the spectrometer will be constructed for achromatic doublet to get the optimized spot size and then will be compared with the spot size obtained for the singlet lens.

4.1 Spectrometer with achromatic doublet lens

A focal length of 150 mm, close to the calculated focal length of 149.9504 mm is selected from the Thorlabs achromatic doublet catalogue [10]. The tilt angle of the lens is -41.60 degree while the distance from the grating to lens was set to 130 mm for the system requirement.The main design parameters are presented in the Appendix A.2. Fig. 4.1 shows the spot diagram of achromatic doublet before the optimization while Fig. 4.2 shows the spot diagram after the optimization. It is observed from the both figures that spot size changes significantly after the optimization. This is probably because the lens-detector distance was not optimized. The optimization was done by making lens to detector distance as variable.The lens to detector distance was 146 nm before optimization. Making the lens-detector distance variable makes the distance 145.86 mm after optimization. The analytically calculated, diffraction limited spot size was 16.9 μm which is calculated from Eq. 2.1. The r.m.s spot size in OpTaliX after optimization was 39.01 μm. The change in the spot size is probably due to chromatic aberrations although it is reduced in achromatic doublet lens compared to the other lenses. Appendix A.3 shows the values of optimized spot sizes for the achromatic doublet.

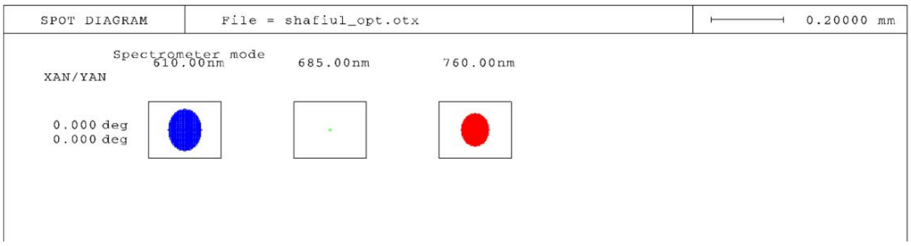

Figure 4.1: Spot diagram of achromatic doublet before optimization for $\lambda_{max} = 760$ nm, $\lambda_{avg} = 685$ nm, and $\lambda_{min} = 610$ nm.

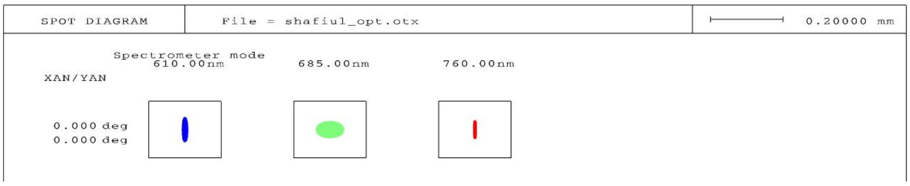

Figure 4.2: Spot diagram of achromatic doublet after optimization for $\lambda_{max} = 760$ nm, $\lambda_{avg} = 685$ nm, and $\lambda_{min} = 610$ nm.

4.2 Spectrometer with singlet lens

The achromatic doublet is replaced with a singlet lens from the Thorlabs catalog to compare it with the doublet lens. A N-BK7 Bi-Convex Lenses (Uncoated) of focal length 150 mm was chosen from the catalogue [11]. All the specifications of the lens are obtained from the catalogue. The design parameters are presented in the Appendix A.5. Fig. 4.3 and Fig. 4.4 shows the spot diagrams of singlet lens for red LED before and after the optimization. Like the achromatic doublet similar kind of change was observed for singlet lens. The size of the spot diagram changed after the optimization as the lens to detector distance is optimized. Like the achromatic doublet, the optimization was done by making the lens to detector distance as variable. The optimized lens to detector distance was 148.6754 mm while

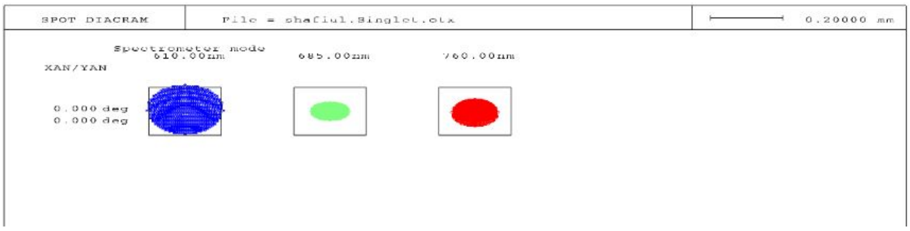

Figure 4.3: Spot diagram of singlet before optimization for $\lambda_{max} = 760$ nm, $\lambda_{avg} = 685$ nm, and $\lambda_{min} = 610$ nm.

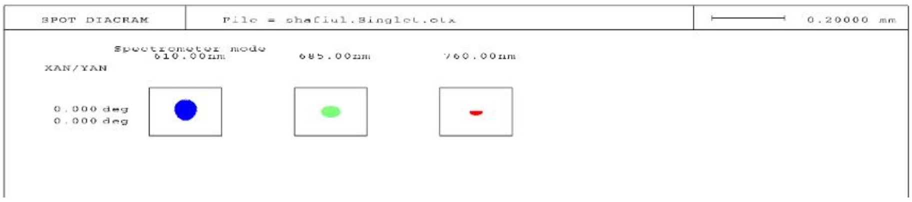

Figure 4.4: Spot diagram of singlet after optimization for $\lambda_{max} = 760$ nm, $\lambda_{avg} = 685$ nm, and $\lambda_{min} = 610$ nm.

the distance was set 149 mm before optimization. The analytically calculated spot size was 16.9 μm while the r.m.s. spot size was 32.71 μm. Appendix A.5 shows the values of optimized spot sizes for the singlet lens.

The optimized spot size is larger in achromatic doublet than in the singlet lens. But, both of them are still larger than the analytically calculated diffraction limited spot size. So, better performance is obtained if the spectrometer is designed with the singlet lens.

CHAPTER V

Analytical optimization for grating parameters

In this chapter, for obtaining maximum transmission efficiency, grating height and fill factor of the grating, grating structure is optimized by using FMM with the help of MATLAB.

5.1 Colormap, selection of grating height and fill factor

In the design of binary grating, grating materials, i.e. substrate, layer 1 were considered silica. The incoming light is assumed to be unpolarized. Therefore, TE and

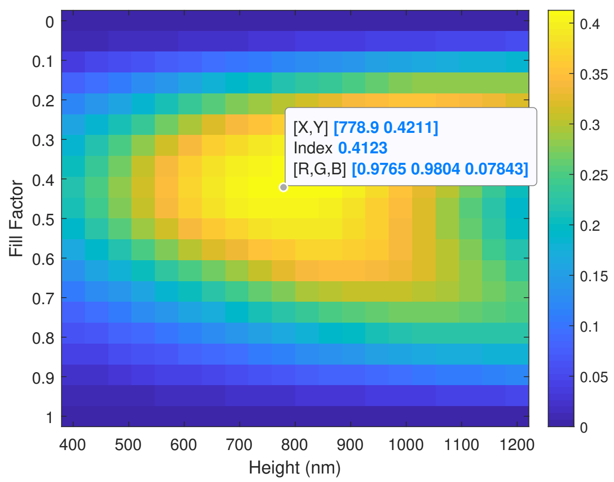

Figure 5.1: Color map of binary grating with red LED source for grating period 1036 nm.

TM mode of the light, i.e. light parallel and perpendicular to the grating grooves are considered. For obtaining the best result, propagating orders of diffracted light was considered 10. Fig. 5.1 represents the color map of binary grating with red LED source for 1036 nm grating period. The colormap gives average grating efficiency over a wavelength range for different height and fill factors pairs. At the center of the color map, i.e. deep yellow region gives the maximum value of average efficiency and the optimum values of grating height and fill factor is obtained from it. Table 5.1 represents the optimal parameters are obtained from the colormap plot for red LED source. Fig. 5.2 shows the efficiency curve obtained for the values obtained

Table 5.1: Calculated parameters obtained from color map.

Grating period (nm)	Grating height (nm)	fill factor	average efficiency(%)
1036	778.9	0.4211	41.23

from Table 5.1. From the average efficiency plot, it is clearly observed that 41.23 % average efficiency obtained for red LED light with the grating period of 1036 nm.

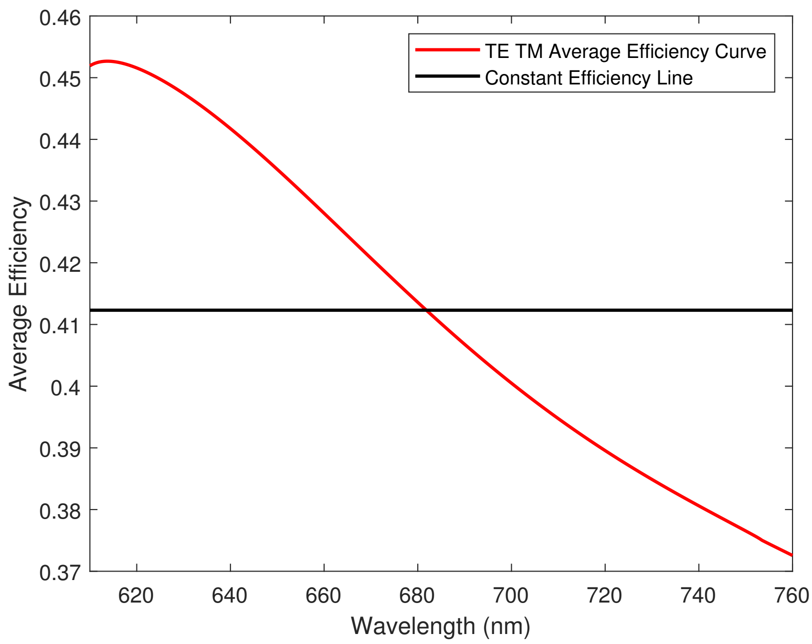

Figure 5.2: Efficiency curve for optimized value for red LED source.

Chapter VI
Conclusions

In this laboratory work, a spectrometer was designed for red LED wavelength range of 610-760 nm. The work was divided into three steps. First, the spectrometer was designed analytically and geometrically. The analytically obtained parameters, i.e. focal length, grating period are used to select the the actual lens from the Thorlabs catalogue. Finally, to optimize the grating structure for optimal efficiency FMM method was used. Best efficiency, i.e. 41.23 % is obtained for 1036 nm of grating period which was confirmed by average efficiency curve. The grating height and fill factors are 778.9 nm and 0.4211 respectively.

Two types of lenses, i.e. achromatic doublet and singlet lens were used to refine the geometrically designed spectrometer with OpTaliX design software. The spot size obtained from the analytical calculation were compared with the r.m.s. spot size obtained from OpTaliX design. Design with singlet lens gave the smaller spot size and therefore, better performance was obtained with it.

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Appendix A

OpTaliX layout and different parameters

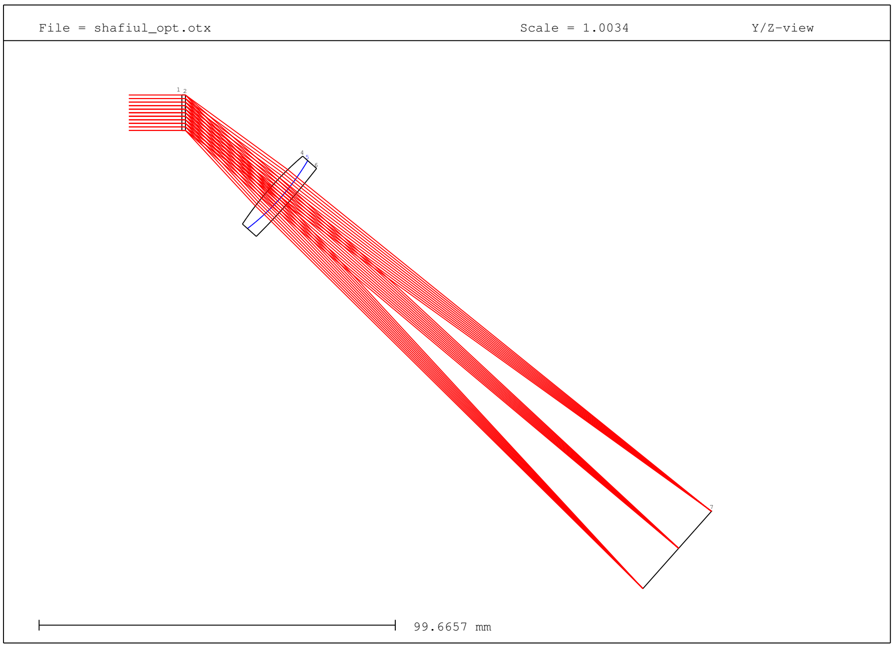

Figure A.1: OpTaliX design with achromatic doublet.

Surface Editor: C:\Users\shafiual\Downloads\shafiul_opt.otx

Standard Data | Decenter, Tilts | Asphere | GRIN | Solves | Special Apertures | Hologram | Misc. | Array

	TYPE	Radius	.	Distance	.	GLASS	.	APE-Y	*	Shape	Glb	THR	.	Comment	Coating	Coat_orientation
OBJ	S	0.00000000		0.1000000E+21				0.000	0	circular	0	0.00000				automatic
STO	S	0.00000000		1.000000		B270		5.000	0	circular	0	0.00000				automatic
2	SH	0.00000000		0.000000				5.000	0	circular	0	0.00000				automatic
3	SXD	0.00000000		31.70000				0.000	0	circular	0	0.00000				automatic
4	S	91.6000000		4.000000		N-BK7		12.700	0	circular	0	0.00000				automatic
5	S	-66.7000000		2.500000		SF5		12.700	0	circular	0	0.00000				automatic
6	S	-197.700000		145.8640	v			12.700	0	circular	0	0.00000				automatic
IMG	S	0.00000000		-1.121615				14.592	0	circular	0	0.00000				automatic

Figure A.2: Optimized lens data for achromatic doublet.

```
                                  <---- RMS Spot Diameter ----> <--- ChiefRay ----> <---- Absolute --->
Field  Wavel.  Rel.Wgt                RMS      RMSx      RMSy    X_grav    Y_grav    X_grav    Y_grav
    1       1    1.000            0.04123   0.00561   0.04084   0.00000  -0.00005   0.00000   0.54335
    1       2    1.000            0.04621   0.03696   0.02774  -0.00000  -0.00000  -0.00000   0.54340
    1       3    1.000            0.02959   0.00220   0.02950   0.00000   0.00007   0.00000   0.54348
    Weighted RMS Spot :           0.03901   0.01492   0.03270                      -0.00000   0.54341

RMS Spot (all fields) :           0.03901   0.01492   0.03270
```

Figure A.3: Optimized spot sizes for achromatic doublet.

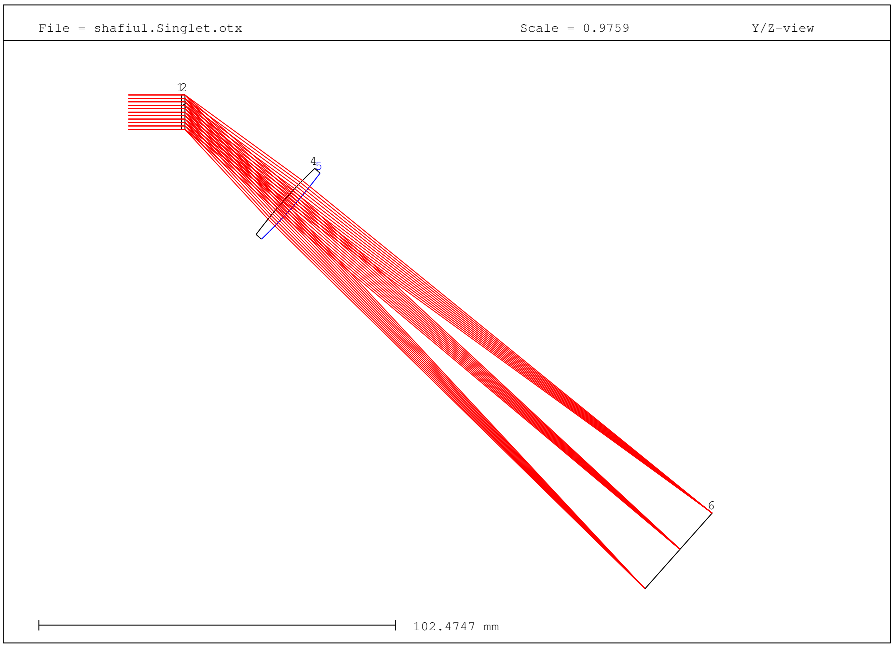

Figure A.4: OpTaliX design with singlet lens.

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Standard Data | Decenter, Tilts | Asphere | GRIN | Solves | Special Apertures | Hologram | Misc. | Array

	TYPE	Radius	.	Distance	.	GLASS	.	APE-Y	*	Shape	Glb	THR	.	Comment	Coating	Coat_orientation
OBJ	S	0.00000000		0.1000000E+21				0.000	0	circular	0	0.00000				automatic
STO	S	0.00000000		1.000000		B270		5.000	0	circular	0	0.00000				automatic
2	SH	0.00000000		0.000000				5.000	0	circular	0	0.00000				automatic
3	SXD	0.00000000		38.11700				0.000	0	circular	0	0.00000				automatic
4	S	154.200000		3.100000		N-BK7		12.700	0	circular	0	0.00000				automatic
5	S	-154.200000		148.6754	v			12.700	0	circular	0	0.00000				automatic
IMG	S	0.00000000		-0.9646334				14.592	0	circular	0	0.00000				automatic

Figure A.5: Optimized lens data for singlet lens.

			<---- RMS Spot Diameter	---->		<--- ChiefRay	---->	<---- Absolute	--->
Field	Wavel.	Rel.Wgt	RMS	RMSx	RMSy	X_grav	Y_grav	X_grav	Y_grav
1	1	1.000	0.04614	0.02464	0.03901	0.00000	0.00279	0.00000	0.57551
1	2	1.000	0.03403	0.02678	0.02100	0.00000	0.00010	0.00000	0.57282
1	3	1.000	0.01794	0.01722	0.00505	-0.00000	-0.00224	-0.00000	0.57048
Weighted RMS Spot :			0.03271	0.02288	0.02169			-0.00000	0.57294
RMS Spot (all fields) :			0.03271	0.02288	0.02169				

Figure A.6: Optimized spot sizes for singlet lens.

Appendix B

MATLAB Codes

MATLAB code for color map, fill factor and grating height

```
n3=1;   %refractive index of air
the=0; % incident angle
d=1036; % grating period
do=-10:10; %Diffraction Orders%
h_grat=linspace (400,1200,20); % varying height of the grating for
obtaining the optimized height.
ff_grat=linspace (0,1,20); % varying fill factor of the grating for
obtaining the optimized fill factor.
wl=linspace (610,760,20); % wavelength range for red source.
for p=1: length(h_grat)
    zl= [0 h_grat(p)];
    for m=1: length(ff_grat)
        tpl=[ff_grat(m) 1];
        for u=1: length(wl)
            n1=silica_n(wl(u));
            nl= [n1 1];
   [rm, tm, rma, tma] =eigml_tm (n1, n3, nl, the, wl(u), d, zl, do, tpl);
            y=tm (10);
   [re, te, rea, tea] =eigml_te (n1, n3, nl, the, wl(u), d, zl, do, tpl);
      y1=te (10);
            average(u)=((y)+(y1))/2;
        end
        avg (m, p) = sum(average)/ length(wl);
    end
end
imagesc (h_grat, ff_grat, avg)
```

```
 xlabel ('Height (nm)')
 ylabel ('Fill Factor')
 colorbar
```

MATLAB code for average efficiency curve for red LED

```
n3=1; %refractive index of air
the=0; % incident angle on the grating
d=1036; %Diffraction Grating period
do=-10:10; %Diffraction Orders%
output= [ ]; % efficiency calculated results  from TE to be stored  in this.
output_1= [ ], % efficiency calculated results  from TM to be stored  in this.
zl= [0 778.9]; % height ranges up to the corresponding grating period of the
desired grating period
tpl= [.4211 1]; % fill factor up to the corresponding grating period of the
desired grating period
wave=610:0.5:760;% for red source
for wl=610:0.5:760;
 n1=silica_n(wl);
 nl= [n1 1];
  [rm, tm, rma, tma] =eigml_tm (n1, n3, nl, the, wl, d, zl, do, tpl);
  tm; %Calculation of TM Efficiency%
 y=tm (10);
output= [output y];
 [re, te, rea, tea] =eigml_te (n1, n3, nl, the, wl, d, zl, do, tpl);
   te; %Calculation of TE Efficiency%
y1=te (10);
output_1= [output_1 y1];
end
avg=(output+output_1)/2; %Average Efficiency Calculation%
figure (99)
clf
plot (wave, avg,'r','LineWidth',1.5) %Plotting the Average Efficiency%
  hold on
  line_avg= sum(avg)/ length(avg)
plot_line= line_avg*ones ([1,301]) %Calculation of Constant Average of
Average Curve%

 plot (wave, plot_line,'k','LineWidth',1.5)
 set(gca,'xlim',[610,760])
  xlabel ('Wavelength (nm)')
```

```
 ylabel ('Average Efficiency')
legend ( 'TE TM Average Efficiency Curve', 'Constant Efficiency Line')
```