Diffraction grating based monochromators
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1. Reflection Gratings

The grating equation can be written for a reflection grating:

$$d(\sin\theta_{inc} \pm \sin\theta_{diff}) = m\lambda \qquad (1)$$

where d is the grating constant, defined as $d \equiv 1/N$, and
$N \equiv$ number of rulings per mm. The + holds when the diffracted beam is on the same side with the incident beam with respect to the normal to the grating's surface. The – sign is when incident and diffracted beams are on opposite sides with respect to the normal. For simplicity, we are assuming that the incident beam is a plane wave, that is its angular spread is near zero.

Differentiating, we obtain , with θ_{inc} constant:

$$d(\pm \cos\theta_{diff})d\theta_{diff} = m\, d\lambda$$

This equation gives us the angular resolution $d\theta_{diff} / d\lambda$ of the optical grating.

Now, we are ready to study the grating based monochromators.

Except of the case where intense laser beam is used, we have typically small optical signal directed to each angular direction due to the spectral analysis caused by the grating. Therefore, we are forced to use some concentrator (lens or mirror having a focal length f) in order to increase the signal to noise ratio. We need then to understand the effect of the chosen value of f on the spectrometer (monochromator) performance.

To simplify the above issue, we consider the quite simple case occurs when we have the so called Littrow arrangement, where we assume that

$$\theta_{inc} = \theta_{diff}$$

It is left as an exercise to show that the linear resolution , $d\lambda/dx$ is:

$$d(2\cos\theta_{diff})\, f\, d\theta_{diff} = m\, d\lambda\, f \quad \text{or:}$$

$$d\lambda/dx = d(2\cos\theta_{diff}) /(m\, f) \quad \text{and} \quad \delta x/\delta\lambda = m\, f / (d\, 2\cos\theta_{diff}) =$$

$$m\, f\, N / (2\cos\theta_{diff}) \equiv R_d \qquad (1)$$

where: R_d is reciprocal linear dispersion

Thus, for Δx=1mm, we have $\Delta\lambda$= 1 1000 mm 3600 grooves/mm

/(2 x .20) if $\cos\theta_{diff}$ = 0.2, N=3600 grooves/mm, and f=1000mm, and m=1.

Thus, $\delta\lambda/\delta x$=.4 mm / (1000 mm x 3600) $\approx$ 10^{-7} 10^{6} nm/ mm = 0.1 Angstroms/mm

Now, if the linear resolution is about 25 μm (dictated by the segmentation of a linear CCD array), we expect a resolution of the order :

$\Delta\lambda_{limii} \approx$ 0.1 Angstrom * 25 μm / 1000 μm $\approx 2.5 \times 10^{-3}$ nm. (2)

This could be one approach to the limiting resolution, but there may be another limit coming from the resolution of optical grating:

$\lambda/\Delta\lambda_{limit} \approx$ number of grooves= 3600 x 25 = 90000 for a typical grating .

Thus, for λ = 450 nm, we get $\Delta\lambda_{limit} \approx 0.6 \times 10^{-3}$ nm.

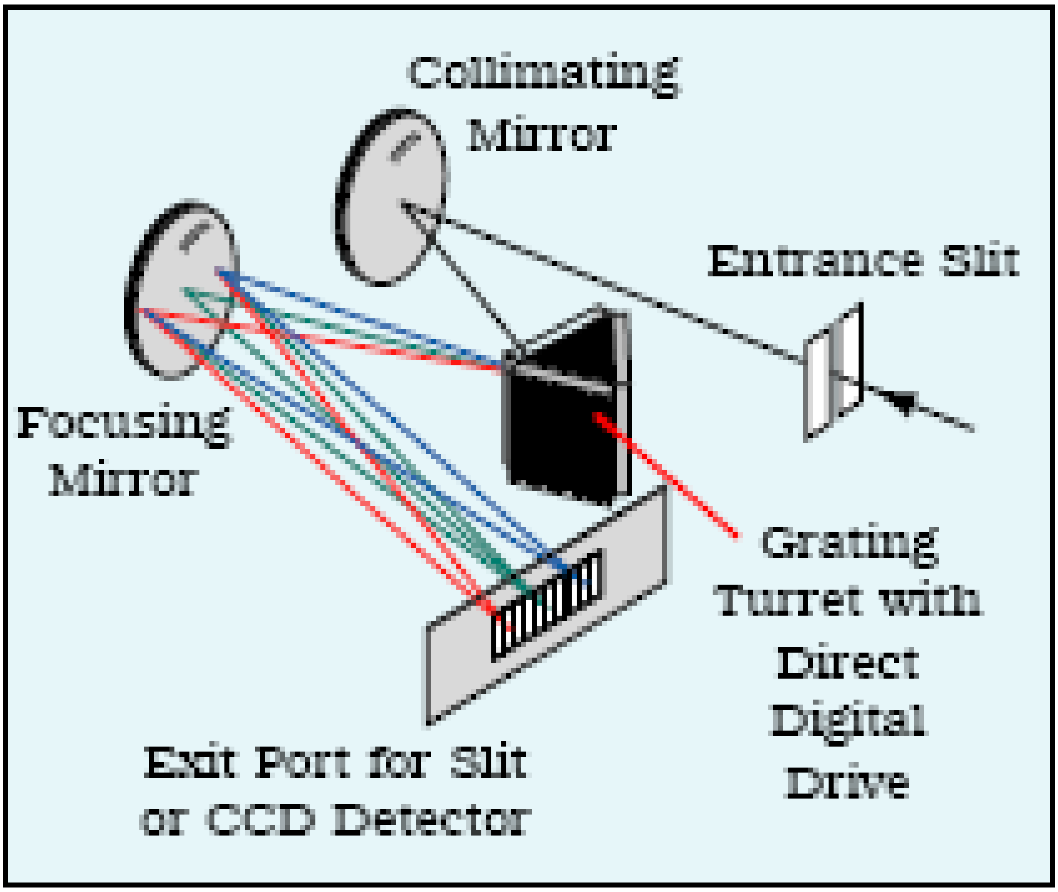
Thus, we see that this limiting resolution arising from Rayleigh's criterion is not inconsistent to the relationship (2) which gives the expected accuracy of the spectroscopic system considered. However, there may be other factors which will cause worsening of the resolution predicted from (2), such as small signal to noise ratio due to the weakness of the spectral line, optical aberrations of the mirrors or lenses used, finite size of the slit used in the entrance of the monochromators etc.

The actual resolution may be obtained experimentally by measuring many times an almost ideal monochromatic line and then obtaining the statistical error.

Another point of view on the accuracy of a grating Monochromator

We go now to see the effect of various aspects which limit the accuracy of wavelength determination. These are enumerated as follows:

a) Natural linewidth, b) Imaging error due to the lenses or mirrors which are part of the monochromators system, c) slit size effects (in either input or output of the spectrometer)



The effect of finite size of spherical mirrors may be estimated by forming the ratio f/d, where f the focal length and d the effective diameter of the mirror. This ratio is frequently called in optics "the f/number or f/# or f/No ". The larger the f/No , the smaller the contribution to the overall wavelength error. An optical instrument with large f/No has more accurate imaging capabilities than a small f/No instrument. That is why we frequently have long telescopes.

The resolution of a spectroscopic instrument is limited by the FWHM of Instrumental Profile:
More specifically,

$$FWHM = (d\lambda^2_{(slits)} + d\lambda^2_{(resolution)} + d\lambda^2_{(line)})^{1/2}$$

Where
$d\lambda^2_{(slits)}$ → *bandpass determined by finite spectrometer slit widths and the* ***linear dispersion of the grating.***

$d\lambda^2_{(resolution)}$ → *the limiting resolution of the spectrometer which incorporates system aberrations, diffraction effect of our system and the* ***laser line width*** *of our system**.

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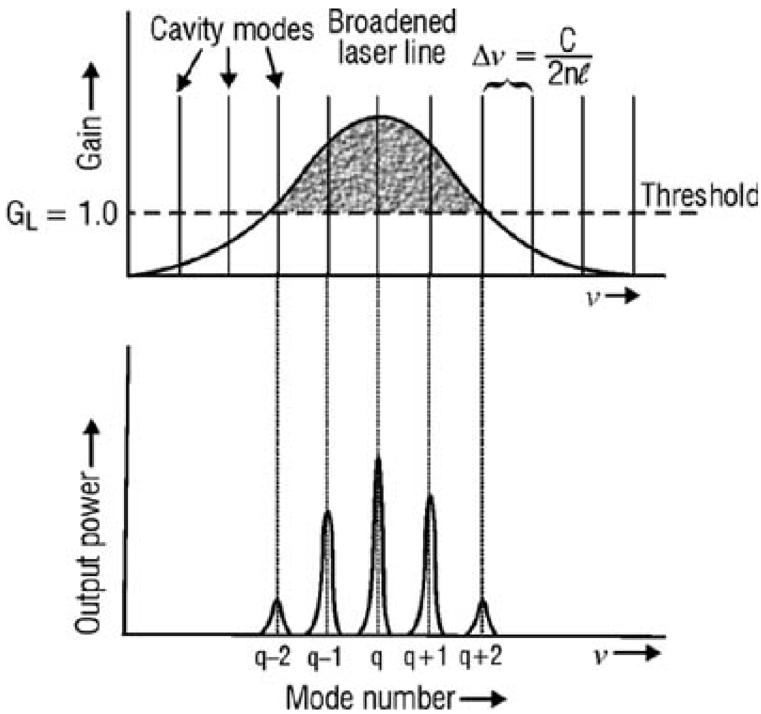
and,
$d\lambda^2_{(line)} \rightarrow$ natural line width of the spectral line being probed.
This FWHM is our limit of resolution for the spectrometer.

** In case the spectrometric system studies some laser line*

How do you calculate the FWHM of the Instrumental Profile?

- The instrumental profile FWHM is something you can measure experimentally.
- $d\lambda^2_{(line)}$: By only observing a laser line with the spectrometer we can eliminate the broadening of the FWHM due to the natural line width of a spectral line **.
- $d\lambda^2_{(slits)}$: The bandpass due to the slit width and the grating of the spectrometer can be calculated.
- $d\lambda^2_{(resolution)}$: The limiting resolution of the spectrometer is something that you solve for knowing the other variables of the FWHM equation.

** see the following graph to understand the thermal broadening of a line and at the same time the peaks corresponding to , longitudinal, laser modes within this line width:



How to Calculate Bandpass (BP)

We can apply , for this purpose, equation (1), above.

Then,

$BP = W \times R_d$

Where W is the slit width of the entrance or exit slit (which ever is larger)

Therefore, due to Equation (1),

$$BP = W\ m\ f\ N / (\ 2\ \cos\theta_{diff}) \qquad (2)$$

Thus, if we wish to achieve a specific band pass (BP), we can select the appropriate value of entrance slit , W, given the other values of m, f, N, and $\cos\theta_{diff}$.

Further discussion about the slit size W:

We may stress that we have two slits, the entrance slit and the exit slit of a monochromators. Normally, the two slits should be conjugate, that is the exit slit should be the image of the entrance slit. However, this need not be always the case. Thus, we propose that the value W inserted in formula (2) above, is the smallest of the two slits in the case that they are conjugage. If they are not conjugate, the W value should be the part of the smaller slit width imaged on the larger slit.

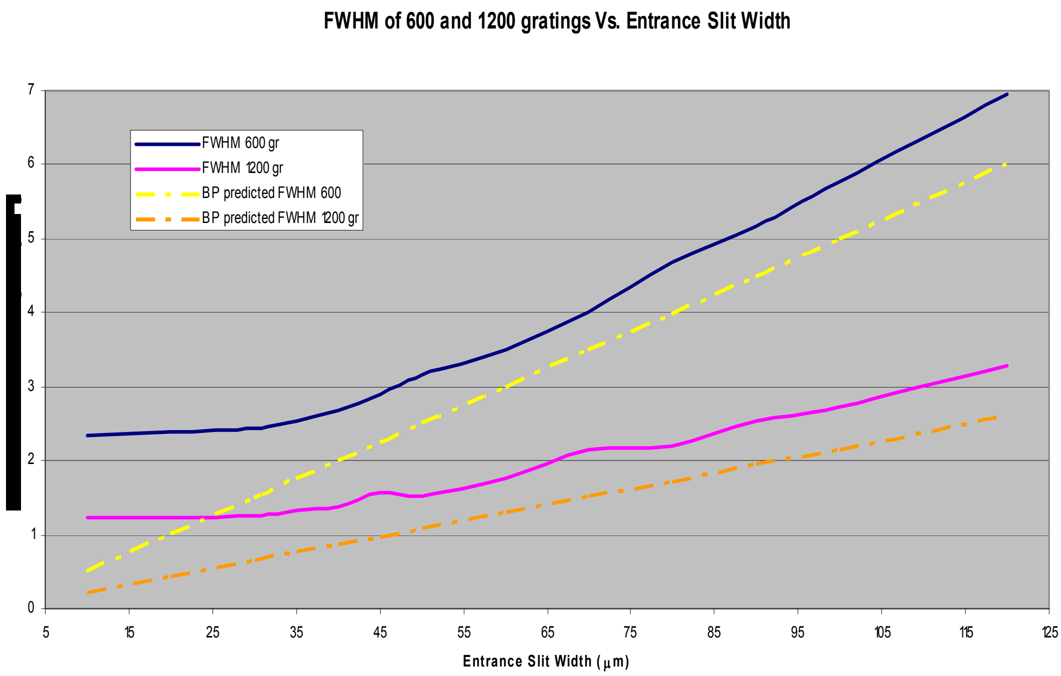


Figure 3.

We present in figure 3, a bibliographical case in which the bandwidth is computed with respect to the entrance slitwidth.

In the case we study in our lab exercise, where the number of groves per millimeter is 3600, we estimate that we may expect up to 3 times better bandpass than the one corresponding to the case 1200 groves per mm, all the other factors being equal.
To achieve this better result could be achieved, with a CCD based monochromators we must be careful that each CCD pixel is equivalent to an effective output slit size. We, therefore, must always take into account the pixel size.

Signal to Noise Ratio

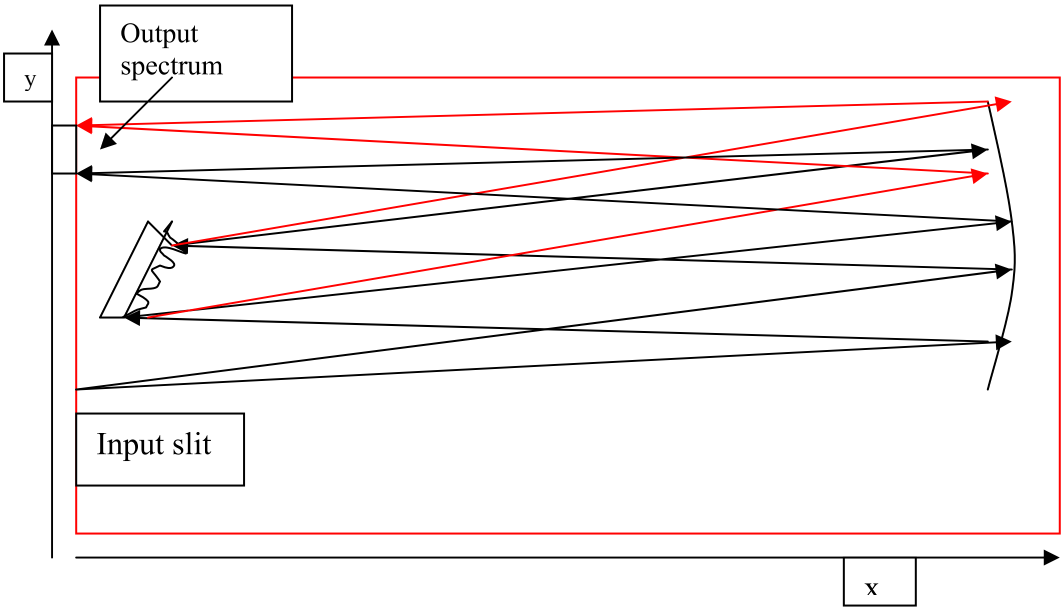
We must be aware, and worry!!, that frequently the CCD area is very small as typically, the CCD has a 20 μm x 100 μm area or even smaller. This means that the overall signal must be compared to the optical noise, which is independed from the optical signal to be measured. This is described by the so called "signal to noise ratio, or simply S/N". This can add another uncertainty in the wavelength to be measured, and therefore we have the expression:

$$FWHM = (d\lambda^2_{(slits)} + d\lambda^2_{(resolution)} + d\lambda^2_{(line)} + d\lambda^2_{(S/N)})^{1/2}$$

The latter expression is appropriate when we deal with weak line sources or line sources in the presence of appreciable optical background.

Application of Monochromator Theory in design of 1 meter spectrograph

Having discussed in some detail the monochromators design, we focus now in specific implementation to achieve a reasonable approach to the theoretical limit.
We have available one concave aluminum mirror of reflectivity near 93%, focal length 914 mm, and diameter 152 mm. The situation is seen in Figure 2.



In the plane xz, the view can be described as seen in Figure:

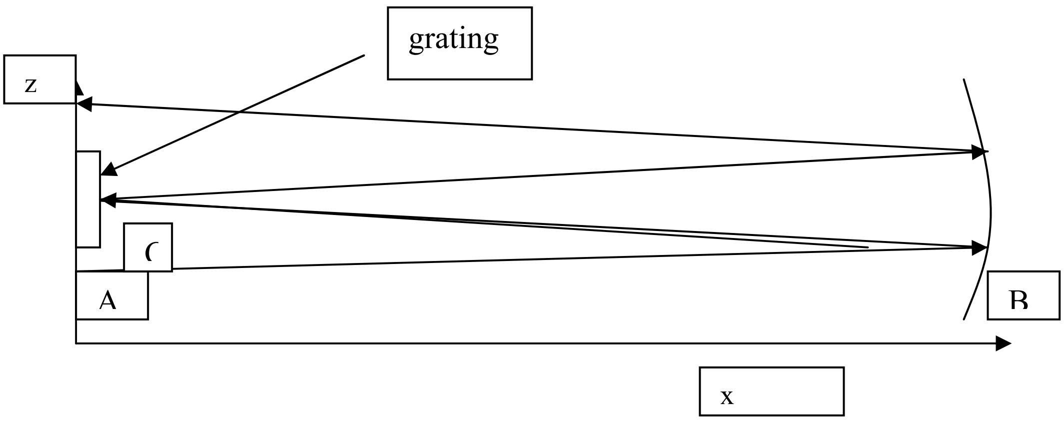
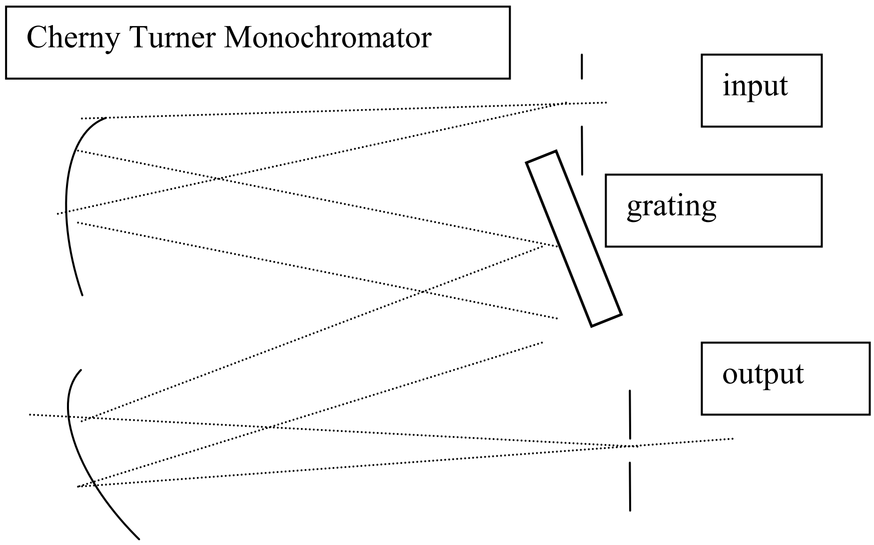


Figure. A: input slit, B: Mirror, C : Spectrum image



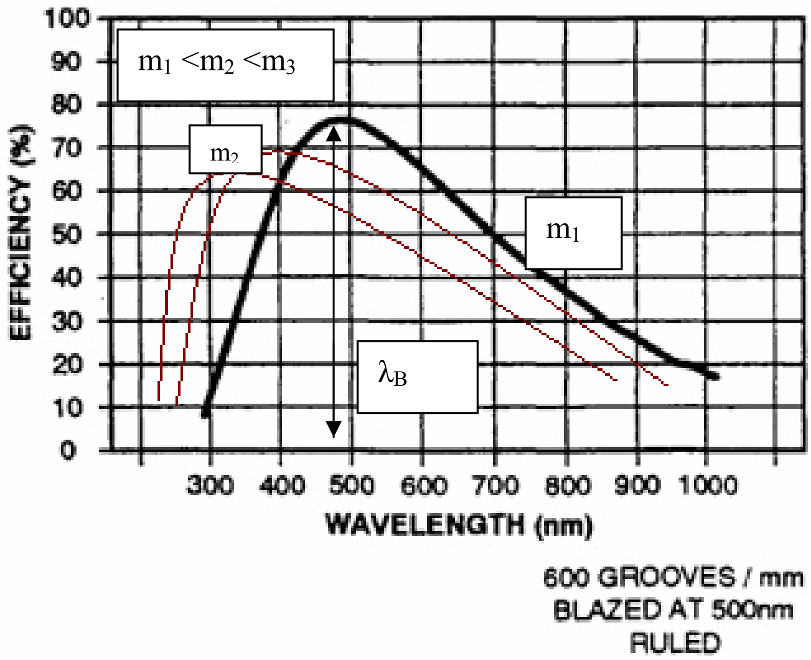
Factors influencing grating efficiency

The efficiency depends on:

- m (diffraction order)
- angles of incidence and diffraction
- λ/d
- polarization

P- Plane => no anomalies
S- Plane => anomalies

P-plane is TE polarized light
S-plane is TM polarized light



The above graph shows that the efficiency, that is , the percentage of intensity dispersed at a certain angle, depends on the wavelength.

Exercise:
Consider the grating with the following parameters:

Focal length(mm)	no. grooves/mm	blaze λ	blaze angle	ruled dimensions (Hx W)
998.8	2400	580 nm	44.2°	30mm x 80mm

(α)Determine the resolution of this grating,(β) A monochromators is constructed using this grating, with input and output slit of 50μm. Determine at the exit of the monochromators the plate factor, that is, the $\delta\lambda/\delta x$, where δx is the width of slit. (γ) Determine the wavelength resolution of the monochromators for the above slit sizes. Examine, the case with slit sizes 20 μm, and 10 μm

Solution:

(α)It is $\lambda/\Delta\lambda$ = No. Grooves x m = 192 000. Thus, for λ=580 nm, we have $\Delta\lambda = 3 \times 10^{-3}$ nm

(β)

Plate factor:

$d\lambda/dx = d(\ 2\cos\theta_{diff})/(m\ f) = (\ 2\cos\theta_{diff})/(N\ m\ f) \approx 2\ /(2400\text{mm}^{-1} \times 1000\text{mm}) = 2\text{ nm}/(2400 \times 1000 \times 10^{-6}\text{ mm}) = 0.83\text{ nm/ mm}$

(γ) The best we can expect , for the accuracy, is $\Delta\lambda_{slit}$ = (0.83 nm/ mm)x 50 μm=

=0.04 nm. For the case of 10 μm, we obtain, $\Delta\lambda \approx 0.008$ nm. Be careful, however, for the diffraction effects in the slits, as we have that the slit size is 20 times less than the wavelength.

2. **Transmission gratings**

In this case, we have the simplified expression,

$$d \sin \theta_{m,i} = m \lambda_i$$

where i is the index of the wavelength under consideration, assuming that the light beam is perpendicular to the grating surface. In reality, we have a deviation from the fully perpendicular case, and therefore , the exact expression is:

$$\pm d \sin\theta_{in} + d \sin \theta_{m,i} = m \lambda_i$$

with θ_{in} very near zero, and thus $\sin\theta_{in} \approx \theta_{in}$. For symmetrical orders, we have :

$$d \theta_{in} - (-d \theta_{in}) \;+\; d \sin \theta_{m,i} \;- d \sin \theta_{-m,i} = 2 m \lambda_i$$

or

$$\theta_{in} + \quad \sin \theta_{m,i} \;=\; m \lambda_i/d \qquad (1)$$

etc.

and

$$\theta_{in} = \; m \lambda_i/d \;\; - |\sin \theta_{m,i}|$$

This gives us an estimate of θ_{in}. By changing in very small steps the orientation of the grating, we may reduce very much the absolute value of θ_{in} until it is zero within errors. In this case, the angles $\theta_{m,i}$ and $\theta_{-m,I}$ should be equal, and in this way, we may get rid of one important systematic error. This systematic error may lead to wavelength errors of the order of 5-20 nm!! If we donnot pay enough attention to assure a perpendicular to the grating beam.

On the other hand, by using a calibrated spectral line λ_{calib} , we may use equation (1) to determine the value of θ_{in} , which we may use to determine unknown spectral lines with respect to the line λ_{calib}. Thus, we may use as calibration line the one at 586 nm of the Hg spectrum, and therefore determine the value of wavelength of the line at 588 nm with respect the calibration line. If we work with the 4^{th} order, then the experimental deviation from the expected 2 nm difference is normally around 1 nm, which indicates the expected statistical error in determining the peak corresponding to the 588 nm yellow line. Remember, that this error does not include the systematic error discussed above, which is due to the non perpendicular beam and perhaps to other reasons.

Vibrational spectroscopy. Atom spectroscopy:
http://www.tau.ac.il/~phchlab/Spect2005/Spectroscopy2005-6.pdf

Grating theory files:

1. GratingTheory-joa4_5_026
2. http://www.stsci.edu/stsci/meetings/nhst/talks/ErikWilkinson.pdf
3. **http://www.physics.arizona.edu/~haar/ADV_LAB/ROWLAND.pdf**

ROWLAND.pdf

4. **Optical grating fabrication:**

4.1 http://snl.mit.edu/papers/papers/2002/cc_SPIE2002.pdf

αρχείο:NanometerAccurateGrating….

4.2 GratingFabricationInterferenceLaserBeams

5. NIST:

http://physics.ship.edu/~mrc/pfs/308/atomic_spectroscopy/Pubs/AtSpec/index.html

5. http://www.astro.su.se/utbildning/kurser/astro_obs/spectroscopy2006.pdf

Αρχείο: AstrophysicsSweden-spectroscopy2006.pdf

6. http://www.chem.utoronto.ca/coursenotes/CHM249/StructureA.pdf
7. http://www.chem.utoronto.ca/coursenotes/CHM249/StructureB1.pdf

Αρχείο:SpectroscopyNotesStructureB1

8. http://www.chem.utoronto.ca/coursenotes/CHM249/StructureB2.pdf

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9. http://www.astro.su.se/utbildning/kurser/astro_obs/spectroscopy2006.pdf

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