Spectroscopy

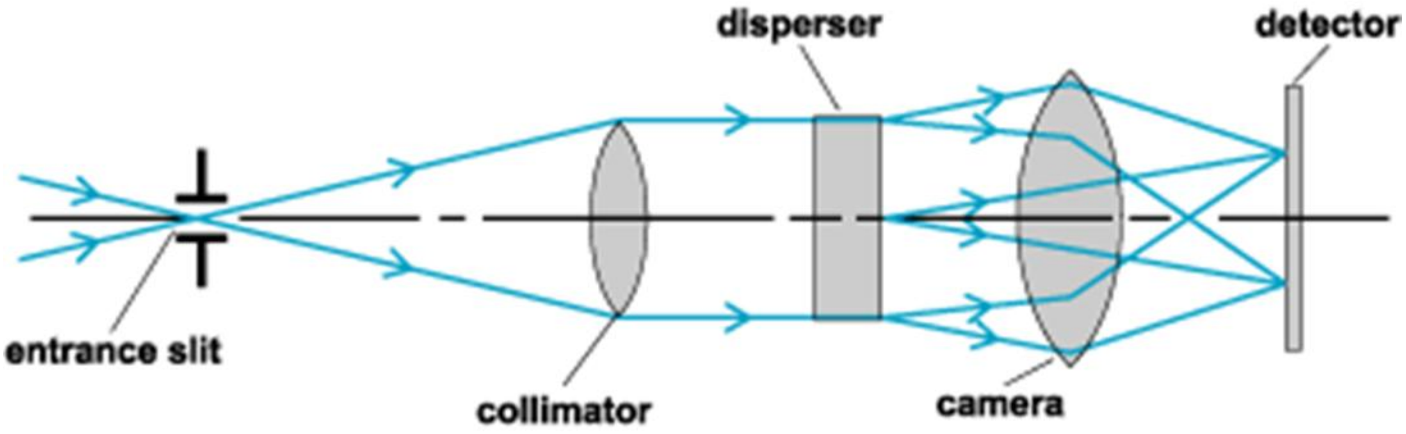
Spectral analysis is the source of most of our astrophysical knowledge.

Techniques of Spectroscopy

- At X-ray and gamma ray wavelengths detectors have intrinsic energy resolution.
- At lower energies we must use different techniques to separate radiation of different wavelength/energy/frequency spatially.
- These techniques are largely those of interference, so considering radiation as waves.

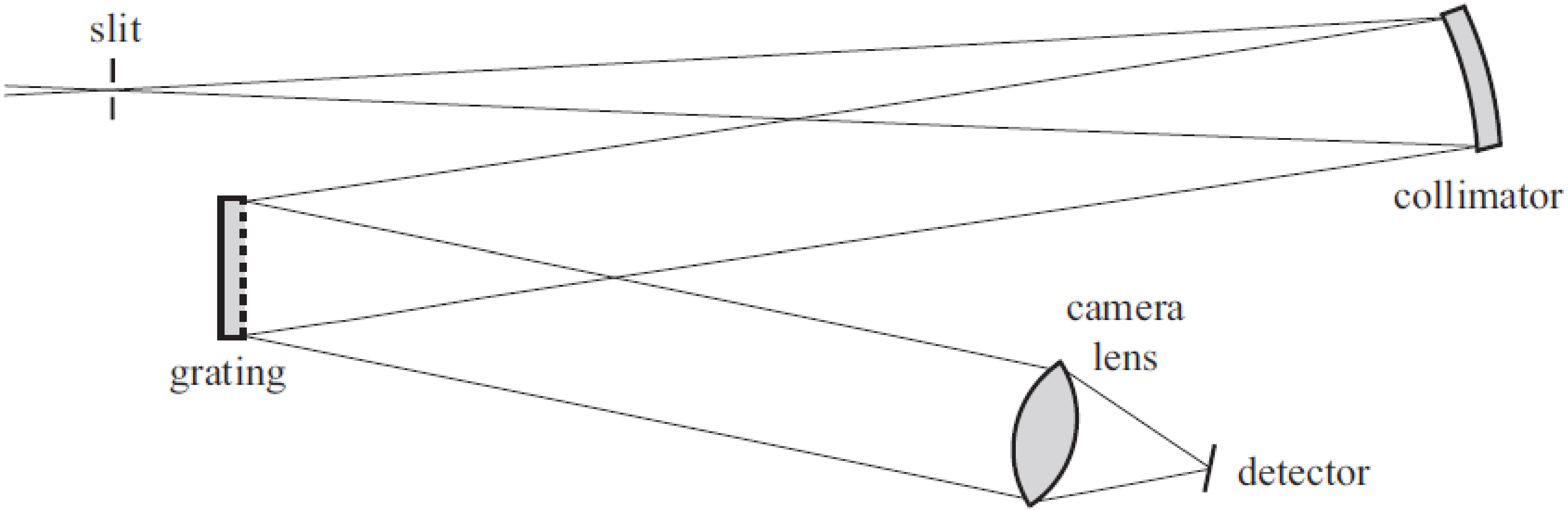
Spectrometers

- All spectrometers have essentially the same basic design, but many different implementations are possible depending on the constraints and choice of spectral disperser.



Spectrometers: main elements

- Entrance apertures at focal plane of telescope
- Collimator
- Disperser
- Camera



Spectrometers: main elements

- **Entrance aperture:** The image of a target is focused onto the slit. The slit is in the focal plane, and usually has an adjustable width w. The slit width must be matched to either the seeing conditions or the diffraction disk depending on the design and application. A narrower slit improves resolution $\sim 2 - 10\times$. The diverging beam continues to the collimator, which has focal length F_{coll}.
- **Collimator:** mirror or lens to convert diverging beam from telescope into parallel beam for input to disperser.
- **Disperser:** grating or prism, usually on rotating stage so can adjust central wavelength.
- **Camera:** to re-focus parallel output beam from disperser onto focal plane of detector

Diffraction Grating

- At optical, infra-red, ultra-violet and to some extent x-ray wavelengths the principal device used to generate interference is the diffraction grating.
- A diffraction grating is a set of multiple, identical slits (transmitting or reflecting) separated by a distance comparable to the wavelength of light. Plane or concave surface.
- Any interference device works by generating phase differences between contributions to the total amplitude at a particular point.

Diffraction Grating

- Each slit can be considered as radiating secondary waves (Huygens' secondary wavelets).
- The amplitude at any point on the image side of the slit can be calculated by summing the amplitude contributed by each set of secondary wavelets.

Diffraction Grating

- The theory of Fraunhofer diffraction from a plane grating predicts that the diffracted light is distributed as:

$$I(\vartheta) = I_0 \, f_1 \, f_2,$$

where I is the output intensity leaving the grating in direction θ with respect to the normal, I_0 is the input intensity at the grating, f_1 is the diffraction pattern for a single grating slit, and f_2 is the pattern for a set of N identical apertures.

Diffraction Grating

- The two patterns are given by:

$$f_1 = \frac{\sin^2(\pi\alpha)}{(\pi\alpha)^2}, \qquad \alpha = \frac{a\sin\theta}{\lambda}$$

$$f_2 = \frac{\sin^2(N\pi\delta)}{\sin^2(\pi\delta)}, \qquad \delta = \frac{d\sin\theta}{\lambda}.$$

where *a* is the linear width of the apertures (assumed rectangular) and *d* is the linear separation between them. We assume normal incidence of the incoming light here.

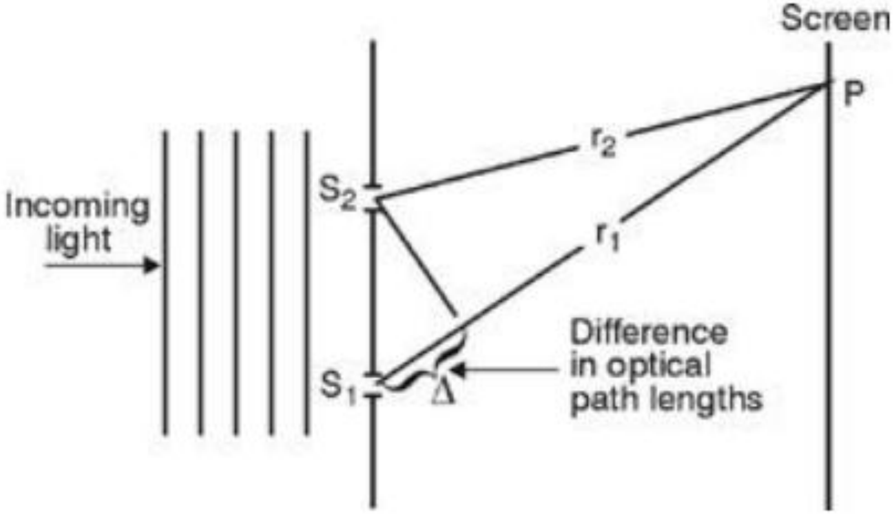
Diffraction Grating

- Consider monochromatic light. Maxima (“orders”) in the multislit pattern occur for $\delta = n$, where n is any integer. This implies the path difference Δ between adjacent slits will be n wavelengths

$$\Delta = d \sin i + d \sin \theta$$

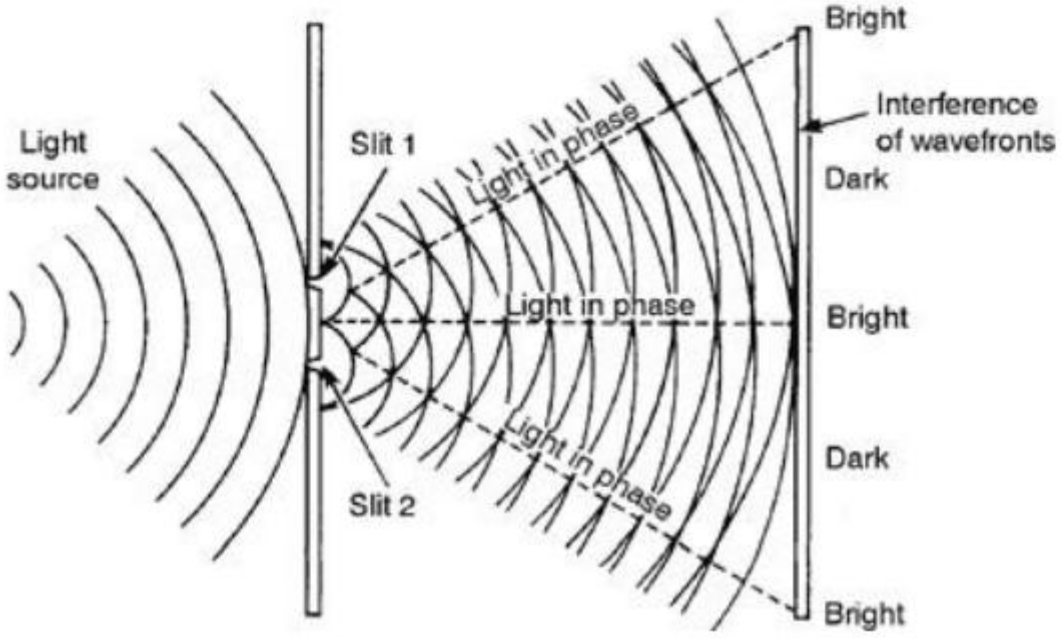
i – is the angle of incidence

θ – is the angle of diffraction



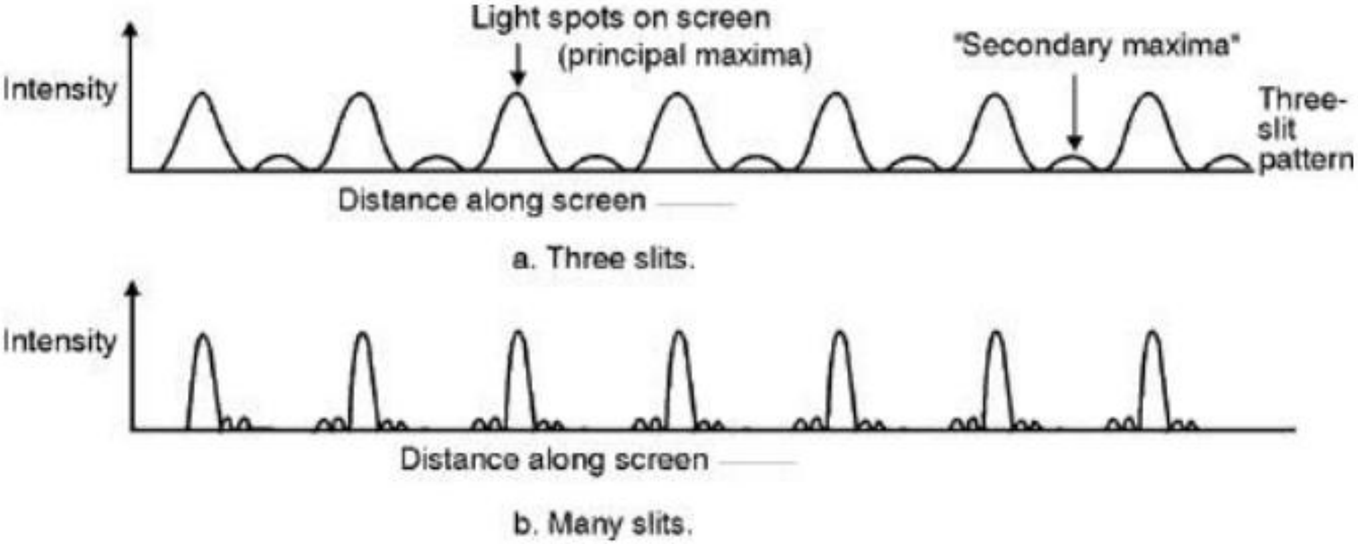
Diffraction Grating

- This produces constructive interference. Maxima in the output intensity occur at a sequence of angles $\sin \theta_n = n \lambda / d$.



Diffraction Grating

- The monochromatic multi-slit pattern for 3 slits and a large number of slits. Each peak corresponds to a particular order. The addition of slits increases the sharpness and brightness of the peaks but leaves the locations of the orders unchanged.



For a real grating, the single-aperture diffraction pattern would be superposed on the multi-slit pattern (here centered on $\theta = 0$).

Diffraction Grating

- Principal maxima are given by the general grating equation:

$$n \lambda = d\,(\sin i + \sin \theta)$$

n is an integer representing the order in which the grating is being used. n is called the order of diffraction.

Diffraction Grating

- The single slit diffraction pattern modifies this by affecting the heights of the maxima, the strongest maximum is that at $n = 0$.
- This maximum is of no use to us, because it does not provide any discrimination in wavelength, it is at the same angle for any λ.
- Gratings are designed to concentrate radiation in orders with $n \neq 0$ (note that positive and negative n are equivalent).

Diffraction Grating: Resolution

- In a given order, redder light is diffracted to larger angles than blue light. The maxima for adjacent wavelengths in a given order are offset slightly.
- Spectral resolution for order n is determined by the wavelength shift needed to place the diffraction pattern maximum for λ + δλ on the first minimum in the pattern for λ. The spectral resolution is

  $$R = \frac{\lambda}{\delta\lambda} = nN$$

  it depends both on the order and on the total number of slits illuminated on the grating.

Diffraction Grating: Resolution

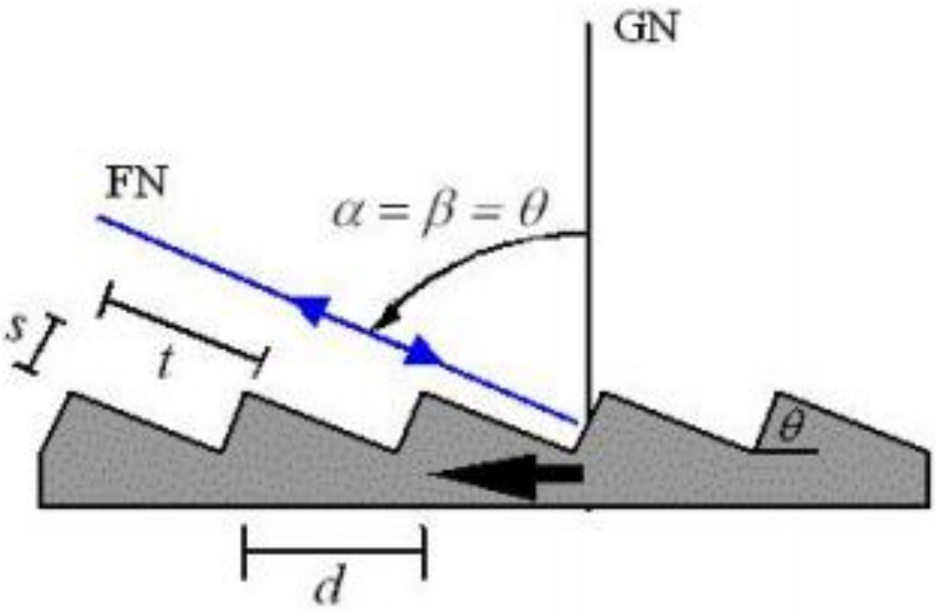
- Angular dispersion (AD): the rate of change of the dispersed angle θ of the beam with respect to wavelength λ:

$$AD = \frac{\delta\theta}{\delta\lambda} = \frac{n}{d\cos\theta}$$

"Higher" dispersion corresponds to larger values of this quantity. Echelles take advantage of both n and θ dependence to maximize dispersion.

Diffraction Grating: Resolution

- "Echelle" gratings: Achieve very high resolutions by operating at large n ~ 50 – 100 and angle of incidence $\theta_1 \sim 90^\circ$. Yield $R > 10^5$.



Diffraction Grating: Resolution

- Astronomers often use the word "dispersion" to refer to $d\lambda/dx$ in the spectrograph focal plane, usually quoted in Å per mm. This is more properly called the "linear reciprocal dispersion" (K). It is inversely related to the angular dispersion, so lower values correspond to higher wavelength dispersion.
- In K units, "low" dispersion corresponds to >200 Å/mm and "high" to < 10 Å/mm.

Reflection gratings

- Most practical gratings are reflection gratings, they are not composed of a screen with equally spaced slits, but of alternating reflecting and non-reflecting strips, made by ruling on a reflecting surface. For a reflecting grating the grating equation derived still holds.

Grating Advantages

- Dispersion same for all wavelengths in given order
- Large dispersions/resolutions possible (large n)
- Transmission or reflection gratings available; plane or curved
- High UV throughputs possible (depending on reflection coating)
- Grating technology highly developed, extensive customization possible

Grating Disadvantages

- **Size limited** by capacity of ruling engine
- **Order superposition:** red light of a given order is spatially coincident with blue light from a higher order. Wavelength λ_m in order n is superposed on light from wavelength λ_n in order n if

$$\lambda_m = \frac{n\lambda_n}{m}$$

For instance, λ_1 = 10000Å, λ_2 = 5000Å, and λ_3 = 3330Å are coincident.

Solution: Use "order separating" filters to block out the unwanted orders (through this becomes difficult for large n). In case of high order echelle spectrographs, use a second grating as a "cross-disperser".

Grating Disadvantages

- **Low efficiency:** Gratings distribute light across a large number of orders (including the zeroth order, which has no dispersion). Flux decreases rapidly with order, $\sim n^{-2}$ for $n \geq 1$.
- Solution: "Blazed" reflection gratings, in which the facets of the slits are cut at an angle that places the maximum of the single-aperture pattern at a chosen wavelength and order.

Blazed Gratings

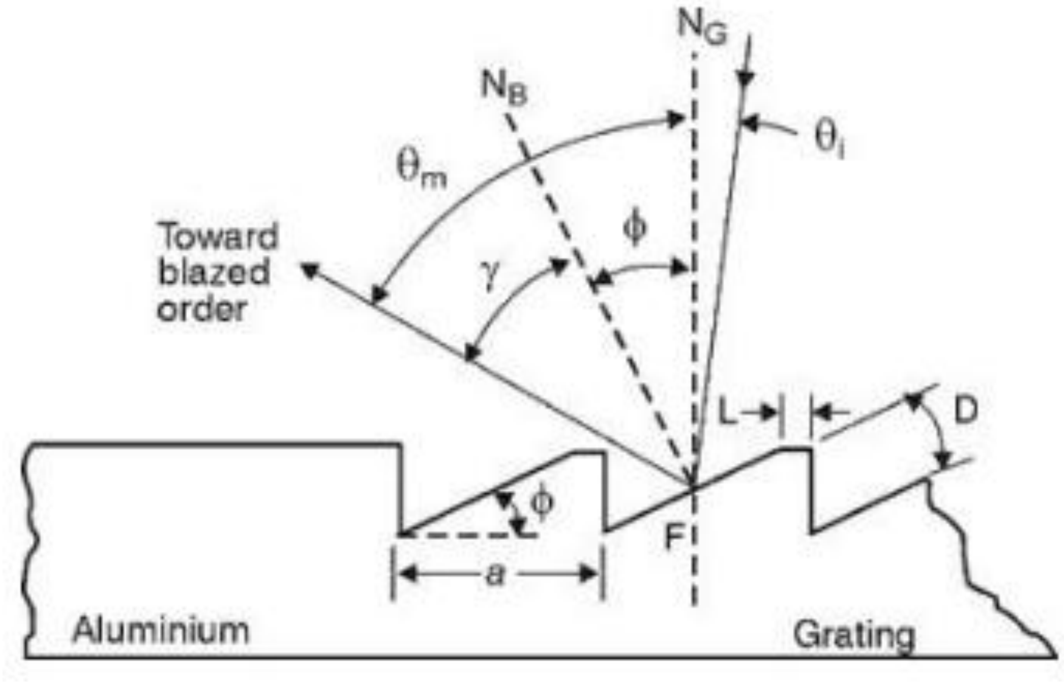
- To concentrate light away from zero order to higher orders, gratings are blazed.
- The reflecting surfaces are now oriented at some angle with respect to the surface of the grating, reflecting light preferentially in that direction.
- An additional advantage is that the whole surface can now be reflecting, since the step where two facets join provides a phase difference to allow diffraction to occur.

Blazed Gratings

- Blaze shifts the peak of the grating efficiency envelope towards higher orders.
- But a grating is blazed not in an order, or at a wavelength but at a particular angle.
- If a grating is blazed to be efficient at a particular wavelength with $n=1$, then it is also efficient at half that wavelength with $n=2$.
- In fact those wavelengths are diffracted by the same amount, this is called order overlap.

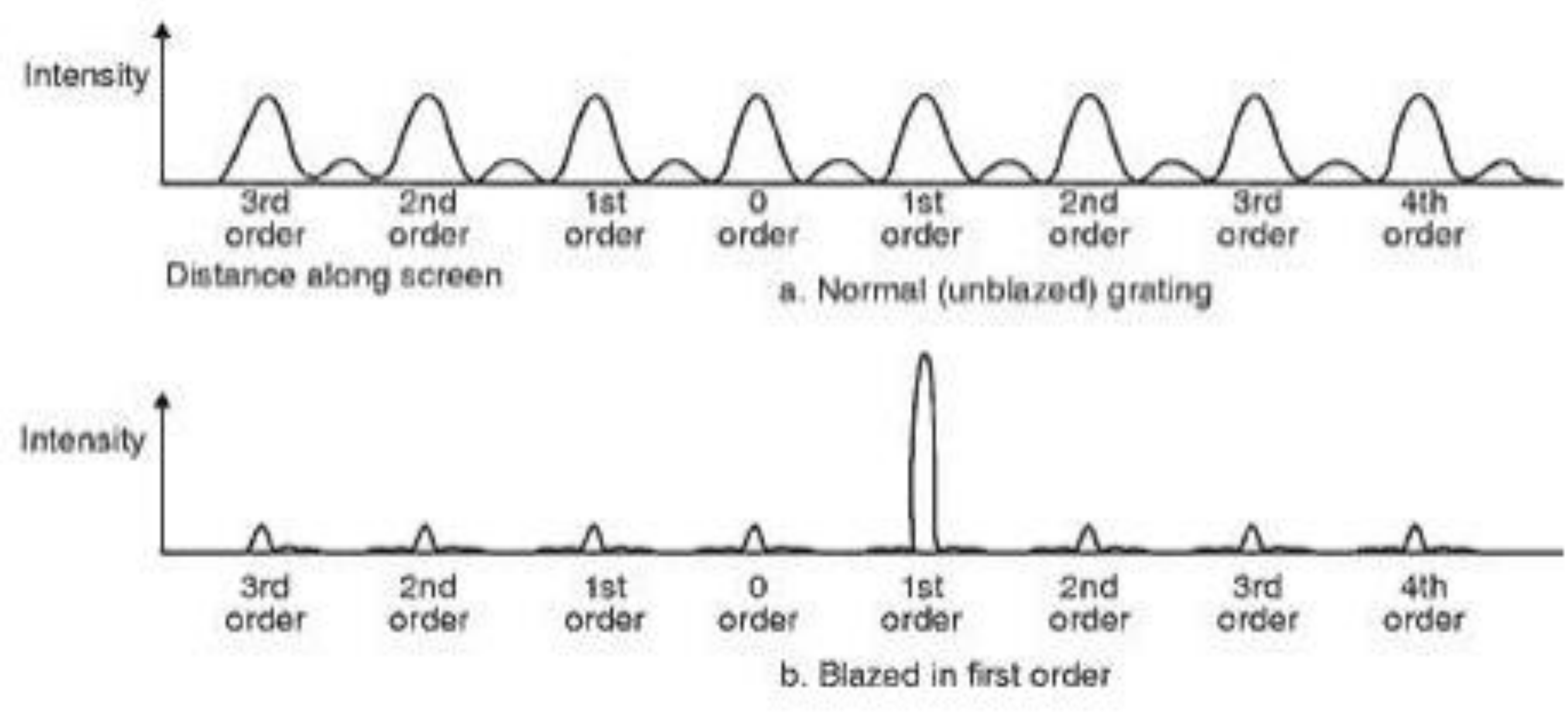
Blazed Gratings

- For the grating in the diagram below, the "wavelength of the blaze" is $\lambda BL = d/n \sin 2\varphi$:

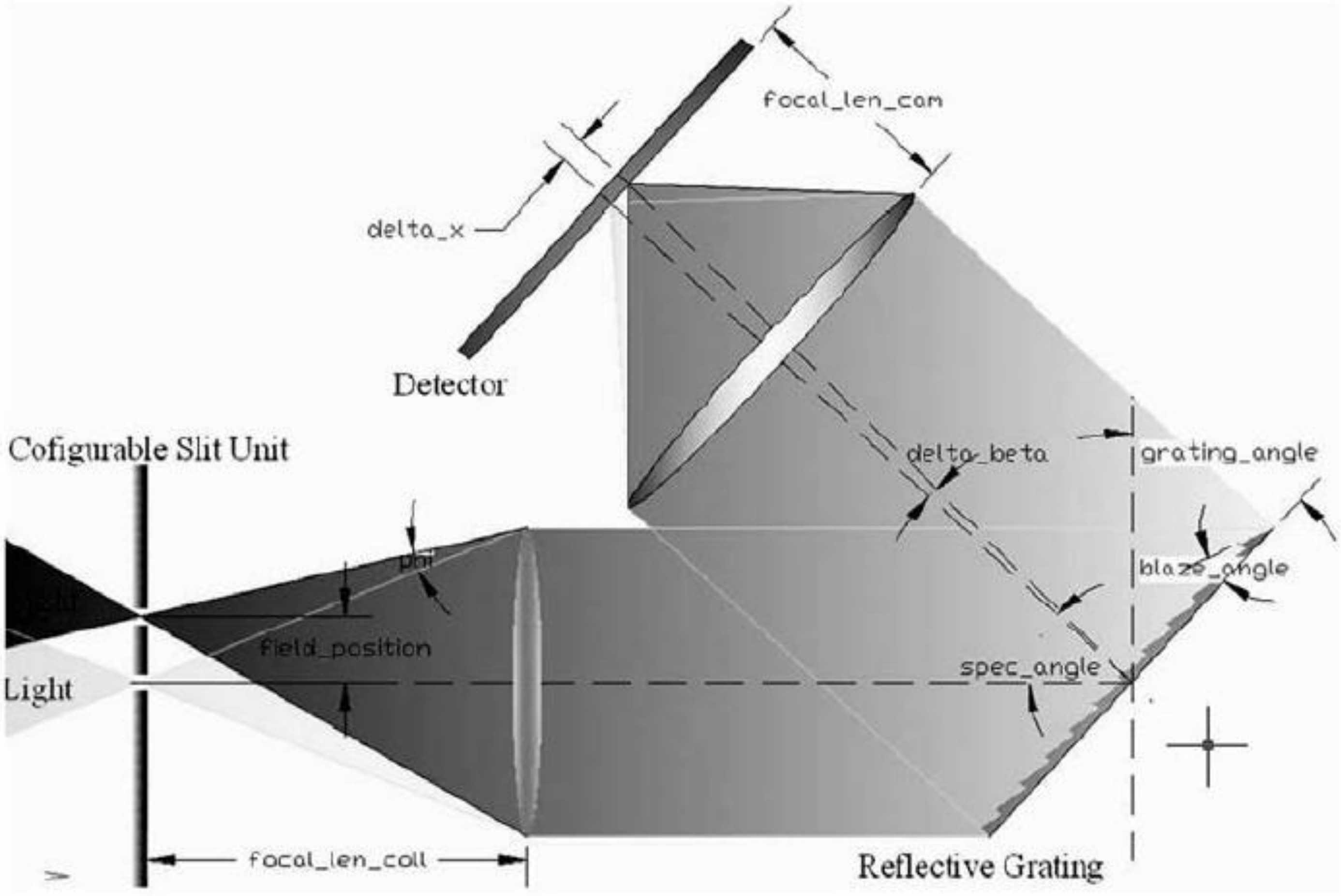


Blazed Gratings

- The effect of a blaze on the diffraction pattern in monochromatic light:



Blazed Gratings

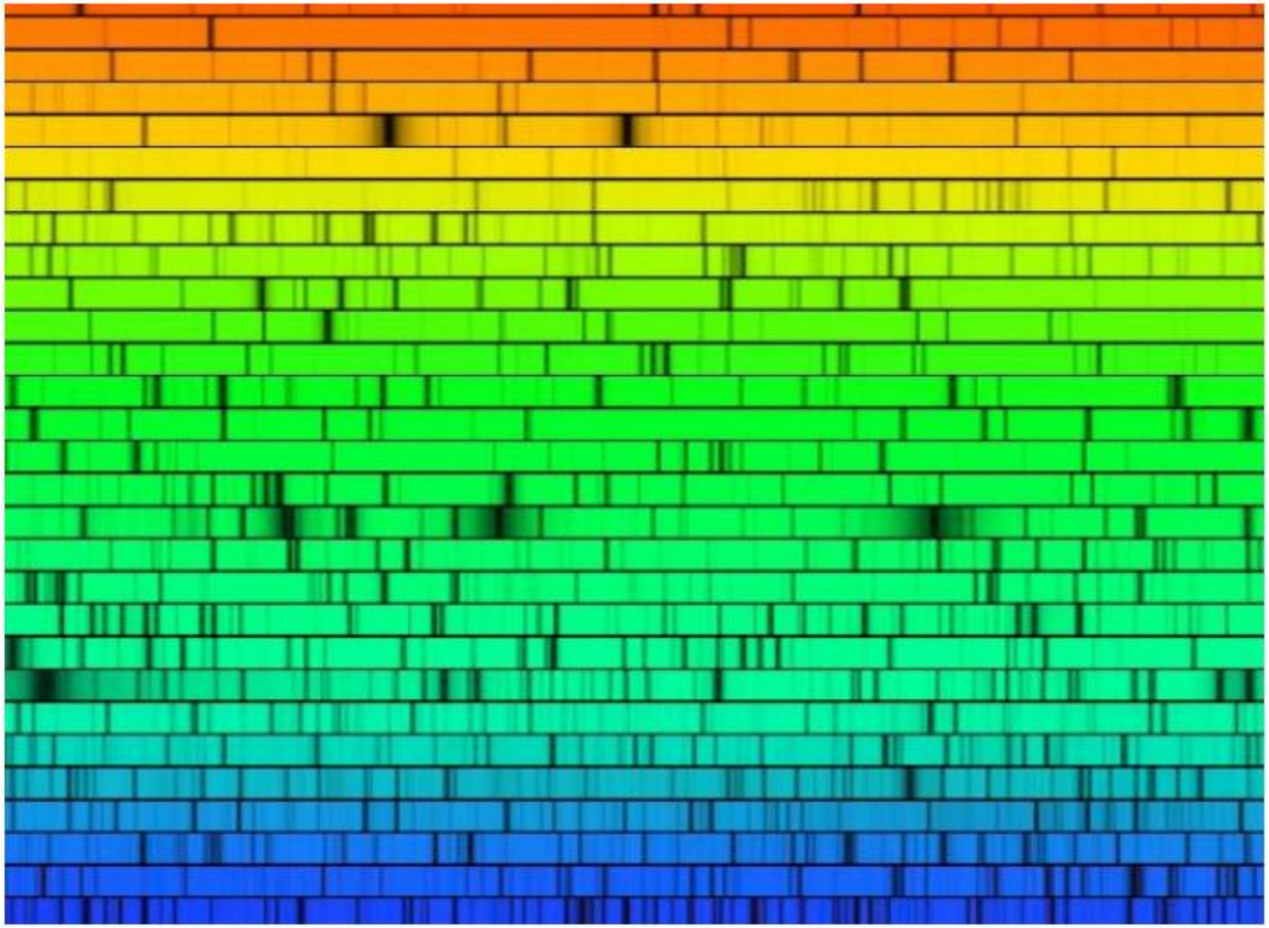


Echelle gratings

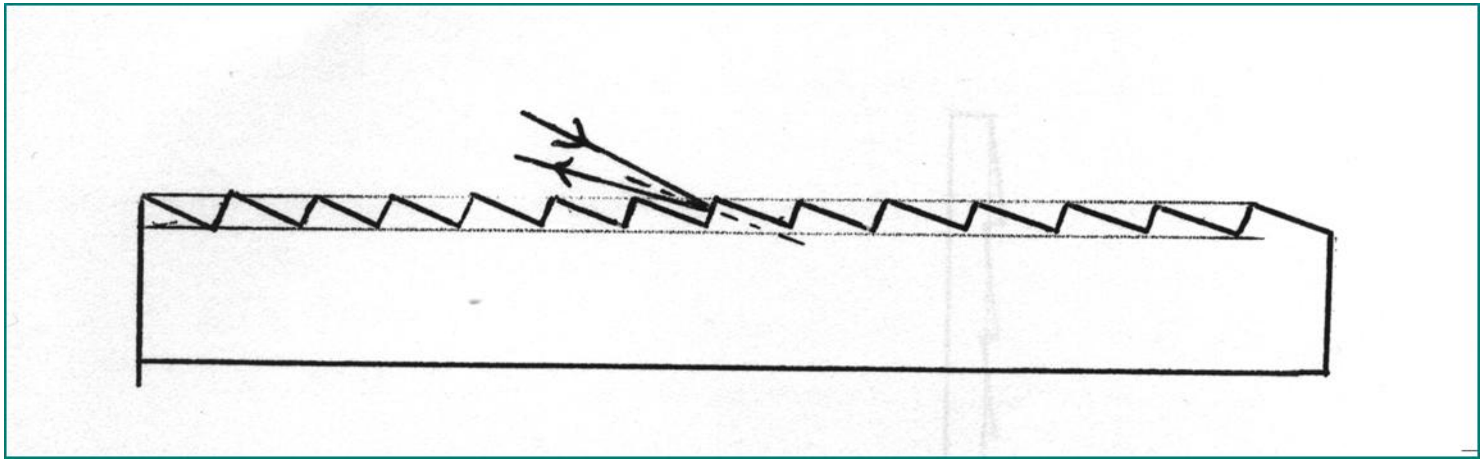
- Echelle grating is more extremely blazed, to high angles and therefore high order n.
- Order overlap is much worse, because adjacent orders differ in wavelength by small amounts (e.g. Order 6 @ 500nm is coincident with order 5 @ 600nm, order 7 @ 429nm, order 8 @ 375nm etc)
- Must separate these orders by cross-dispersion, usually dispersing with a prism at right angles to the grating dispersion.
- Echelle spectrum consists of a number of spectral orders arranged side by side on the detector.

Echelle gratings

High resolution, optical band solar spectrum



Echelle gratings

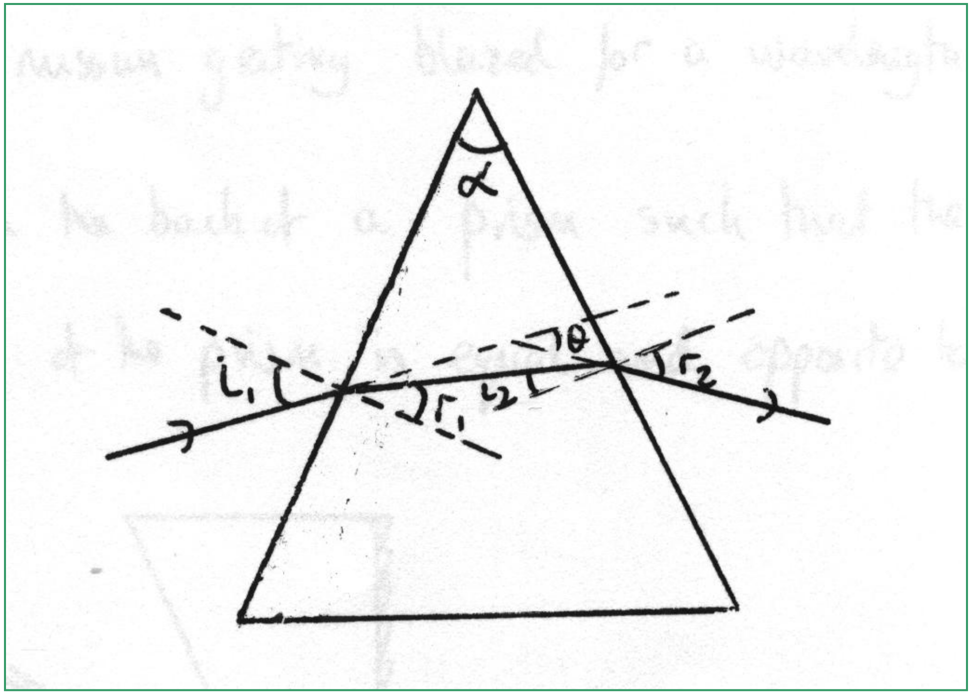


Echelle grating showing the high blaze angle, and also that the camera angle (angle between incident and diffracted rays) must be small in order to avoid light being lost due to groove shadowing.

Echelle Spectrographs

- Order *n* in a large stellar echelle spectrograph can be several hundred. The image on the detector consists of a number of separate orders side by side.
- Echelles can only be used for point sources (stars and quasars) or for small objects, otherwise the light from different orders still overlaps.

Prismatic Dispersion



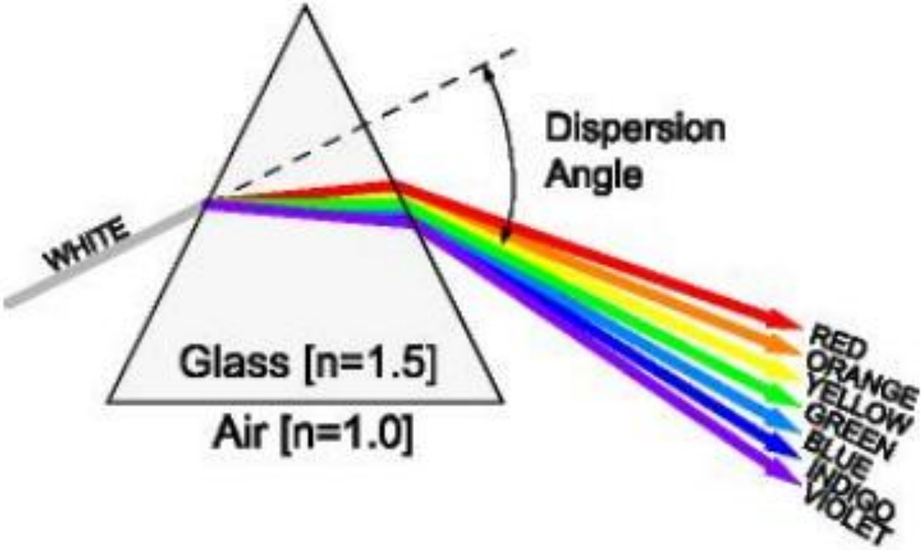
- Prismatic dispersion is a function of the angle of the prism, α, and the material the prism is made from.

Prismatic Dispersion

- The spectral resolution of this type of prism is

$$R = B\frac{dn}{\delta\lambda},$$

where B is the length of the prism base, and n is the index of refraction.



Advantages and Disadvantages of prism spectrographs

- Advantages:
    - High throughput; useful for faint-object spectroscopy
    - Wide field possible for multi-object samples
    - Cheap, simple; predominant in early astronomical spectroscopy
- Disadvantages:
    - R can be a strong function of wavelength
    - Wide band coverage difficult
    - Internal absorption limits use in UV
    - More complex data reduction because of variable dispersion

Prisms

- Prisms are rarely used on their own in spectrographs, although there is still some use in the infrared.
- Used in conjunction with gratings:
  - As cross-dispersers for echelle gratings
  - In conjunction with a transmission grating as a grism.

Transmission gratings and grisms

- Transmission gratings are hard to make with small ruling spacings, and even harder to make blazed. Spacings smaller than 2 μm are rare, and these gratings are usually inefficient.
- More often used in combination with a prism for low resolution applications.
- Grating is replicated on the surface of a prism. Prism bends the light so the deviations caused by refraction and diffraction cancel for some optimum wavelength.
- Grism spectrograph can thus have a straight through optical path.

Transmission gratings and grisms

- A very popular way to convert a camera into a spectrograph is to deposit a transmission grating on the hypotenuse of a right-angled prism and use the deviation of the prism to bring the first order of diffraction on axis. Such a device is called a “grism".
- The advantage of a grism is that it can be placed in a filter wheel and treated like another filter.

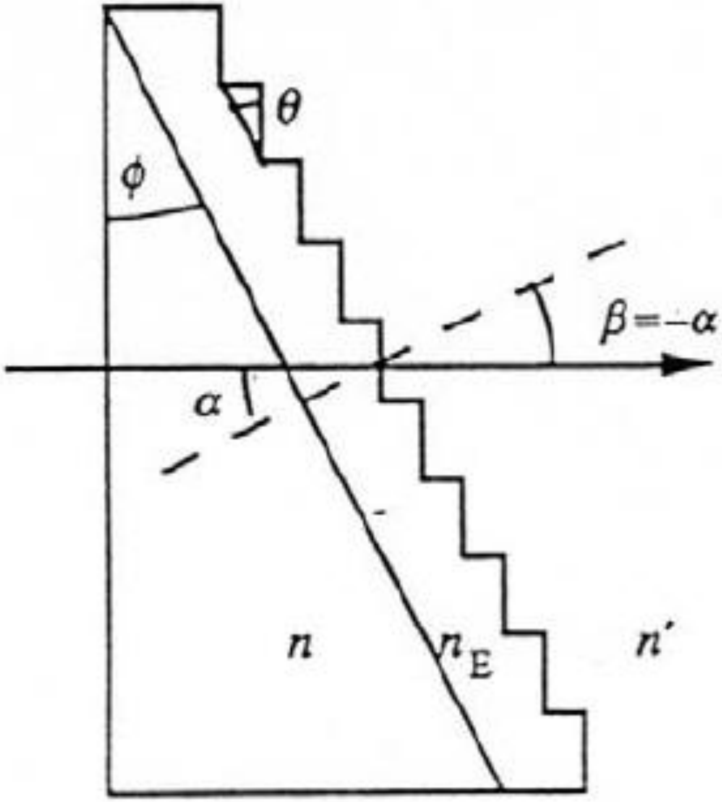
Grisms

- ☐ The basic relationships required to design a grism are

$$m\,\lambda_c T = (n-1)\sin\varphi$$

$$R = \frac{EFL}{2\,dpix}(n-1)\tan\varphi$$

where λ_c is the central wavelength, T(=1/d) is the number of lines per millimeter of the grating; n is the refractive index of the prism material; φ is the prism apex angle; EFL is the effective focal length of the camera system and d_{pix} is the pixel size. Resolving powers (two pixels) of R ~ 500 – 2000 are practical.



Practical spectroscopy

- The purposes of spectroscopy are:
  - To measure accurate wavelengths of emission and absorption lines.
  - To measure the relative strengths of emission lines.
  - To measure equivalent widths of absorption lines.
  - To measure the spectral energy distribution of the continuum radiation.

Calibrations

- The first stage of calibration is to calibrate the detector, and the steps in doing this are exactly the same as for photometric observations.
  - Subtract off the CCD bias signal, either as a constant value or as a frame. This step is not needed for photon counting detectors
  - Subtract off the dark current, either as a constant value or as a frame. As spectroscopic exposure times are longer than photometric exposure times, this step is now more often needed.
  - Divide by the flat field frame to correct for variations in the sensitivity of the detector.

Calibrations

- **Wavelength calibration** – a comparison spectrum usually of a hollow cathode discharge lamp, gives a series of emission lines of the gas in the lamp, plus the metal or metals that the cathode is made from.
- Typically the gas is a noble gas (helium, argon, neon etc.) and the metal is copper, iron or thorium.
- Using the laboratory determined wavelengths of these lines a functional fit of wavelength against position on the detector is made.
- In principal this is a two dimensional fit, although in practice the dispersion direction is usually accurately aligned with one of the principal axes of the detector (usually vertical on a CCD), so this reduces to a series of one dimensional fits, one per CCD column.

Calibrations

- **Spectrophotometric calibration or Flux calibration**. This is a calibration of sensitivity and efficiency, and is carried out in the same way as the photometric calibration, by observing a number of standard stars whose flux as a function of wavelength is accurately known, at a variety of airmass values. There is one extra quite serious problem.
  - The slit size α is set so that the size projected on the detector p is of order 2 detector pixels, this gives the maximum spectral resolution. α is normally smaller than the resolution set by seeing, so light is lost at the entrance slit.
  - The amount of light lost varies between exposures, making an absolute flux calibration very difficult.
  - The amount of light lost is also wavelength dependent, due to the weak dependence of seeing on wavelength, and due to atmospheric dispersion.

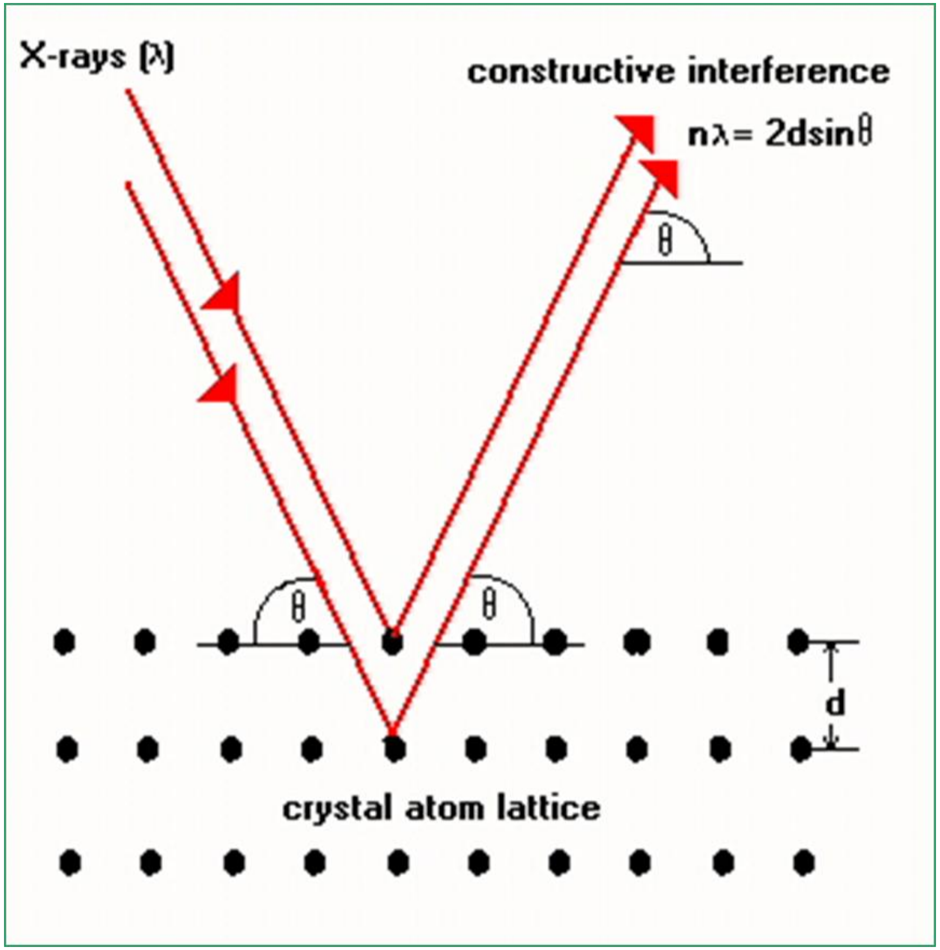
Calibrations

- Atmospheric dispersion occurs because the refractive index of air is wavelength dependent, so unless your telescope is looking straight up, the atmosphere acts as a prism. It can be compensated for in two ways:
    - Some telescopes have an atmospheric dispersion compensator, which is a pair of prisms which can be rotated. At any orientation of the telescope, the prisms can be rotated so that their combined dispersion is equal and opposite to that of the atmosphere.
    - The slit can be oriented at the parallactic angle for all observations. This is the angle on the sky which corresponds to the slit being perpendicular to the horizon, and is different for different telescope orientation. The atmospheric dispersion is then along rather than across the slit, so light is not lost to the system, but simply dispersed into different pixels on the detector.

Bragg diffraction

- Bragg diffraction was used in the early 20th century to study the structure of crystals. X-rays are diffracted by the planes of atoms in a crystal structure, and light is only diffracted when the Bragg condition is met, and this caused by constructive interference between rays reflected by different crystal planes.

Bragg diffraction



Bragg diffraction

- Successive crystal planes reflect radiation with a phase difference:

$$\delta = (4\pi\, d_s \sin\theta) / \lambda$$

where d_s is the crystal plane spacing. We can sum the amplitudes from the individual planes in the same way that we did for the slits in the conventional grating, and find that constructive interference occurs when radiation is reflected at the Bragg angle θ, where:

$$m\lambda = 2\, d_s \sin\theta$$

Bragg diffraction

- A crystal in a collimated beam acts as a reflecting monochromater, so only one wavelength is reflected, and this wavelength changes as the crystal is rotated.