Reflection and Refraction

Maxwell's equations lead to definition for the velocity of electromagnetic radiation in a vacuum:

$$c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}$$

where

ε_0 is the permittivity of free-space ($8.854\text{x}10^{-12}\ C^2 \cdot N^{-1} \cdot m^{-2}$)
μ_0 is the permeability of free-space ($4\pi\text{x}10^{-7}\ kg \cdot m \cdot C^{-2}$)

In a medium, velocity is reduced

$$v = \frac{1}{\sqrt{\varepsilon \mu}}$$

The ratio of the velocity in a medium to free-space is refractive index

$$\eta = \frac{c}{v} = \sqrt{\frac{\varepsilon \mu}{\varepsilon_0 \mu_0}} \qquad > 1.00 \text{ in a medium}$$

- η varies with wavelength
  - usually increases with frequency (called normal dispersion)
  - decreases with frequency in region of absorption (called anomalous dispersion)

λ (nm)	η
351	1.539
458	1.525
486	1.522
532	1.519
644	1.515
830	1.510

Important:

Frequency of radiation is fixed by source. Hence, wavelength of radiation in a medium must increase

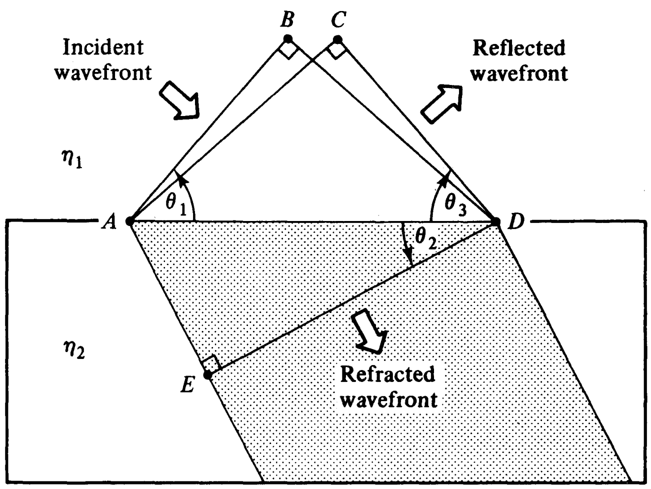
$$\lambda = \frac{c}{\eta \; \upsilon} \qquad \text{since } v = \upsilon \; \lambda$$

$$\lambda_{medium} > \lambda_{vacuum}$$

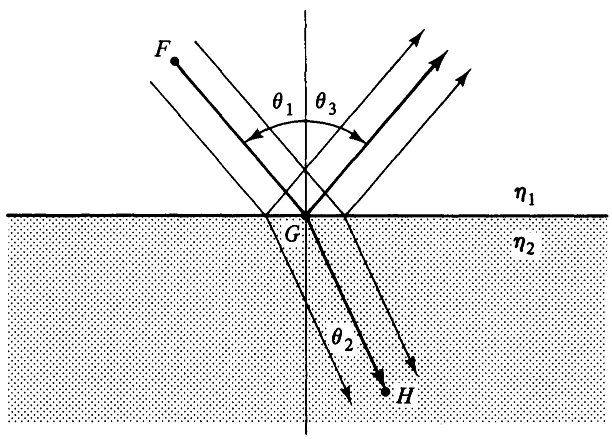
When a wave passes from medium with refractive index η_1, to medium of refractive index η_2, we can write

$$\frac{\lambda_2}{\lambda_1} = \frac{c}{\eta_2 \; \upsilon} \times \frac{\eta_2 \; \upsilon}{c} = \frac{\eta_1}{\eta_2}$$

Based on wave representation of electromagnetic radiation and geometry, we can quickly deduce the angle of reflection:



(a)



(b)

$\theta_i = \theta_3$ Law of specular reflectance

The refracted beam does not travel at same velocity as the incident beam ($v_2 = v_1 \cdot \eta_1/\eta_2$):

- first part of the wavefront to strike the interface is retarded preferentially

- light beam bends towards the interface normal when $\eta_2 > \eta_1$

$$\eta_1 \sin\theta_1 = \eta_2 \sin\theta_2$$ Snell's law of refraction

- no refraction when $\theta_1 = 0°$

- no transmittance when $\theta_1 > \theta_c$ (critical angle)

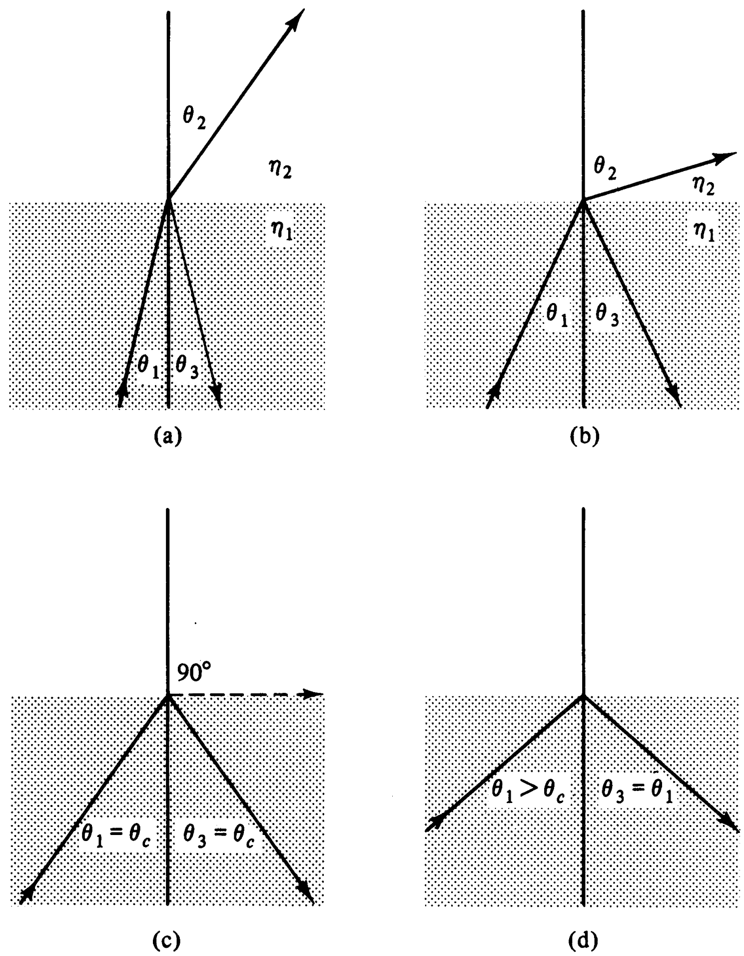
  total internal reflection

$$\sin\theta_1 = \left(\frac{\eta_2}{\eta_1}\right)\sin\theta_2$$ Snell's law

when $\sin\theta_2 = 90°$

$$\theta_i = \theta_c = \sin^{-1}\left(\frac{\eta_2}{\eta_1}\right)$$

For air/glass $\theta_c \approx 42°$



θ2
η2
η1
θ1
θ3
(a)
θ2
η2
η1
θ1
θ3
(b)
90°
θ1 = θc
θ3 = θc
(c)
θ1 > θc
θ3 = θ1
(d)

Fresnel Equations

Reflectance losses occur at all at interfaces

$$\alpha(\lambda) + T(\lambda) + \rho(\lambda) = 1 \qquad \text{Conservation Law}$$

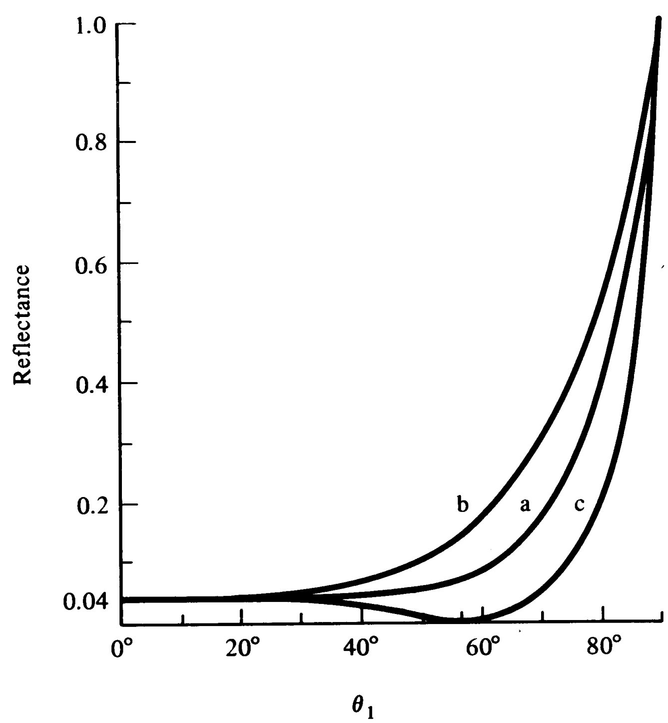
- magnitude increases as the *difference* in the refractive indices increases
- dependent on incidence angle

Equation describing the reflectance $\rho(\lambda)$ is the Fresnel equation

$$\rho(\lambda) = \frac{1}{2}\left[\frac{\sin^2(\theta_i - \theta_r)}{\sin^2(\theta_i + \theta_r)} + \frac{\tan^2(\theta_i - \theta_r)}{\tan^2(\theta_i + \theta_r)}\right]$$

- where θ_i is incidence angle and θ_r is refraction angle

For the air/glass at 589 nm, reflectance is about 0.04 or 4 % per interface



- $\rho(\lambda)$ constant for small angles
- $\rho(\lambda)$ increases rapidly at large angles (grazing incidence)

Prisms

Serves several purposes in a spectrometer

- change the direction of a beam
- change the polarization of a beam
- split a beam into two
- disperse the beam

A variety of shapes and materials are available to perform these functions.

Dispersing prism

According to Snell's Law,

$$\sin\theta_1 = \left(\frac{\eta_2}{\eta_1}\right)\sin\theta_2 \qquad \text{Snell's law}$$

there will be no dispersion if $\eta(\lambda)$ is constant

- dispersion in prism occurs because of the change in refractive index of the prism material as a function of wavelength
- if prism material exhibits normal dispersion, higher frequency (shorter wavelength) light experiences a higher refractive index than lower frequency (longer wavelength) light

Light of different wavelengths become divergent and become separated in space

angle between incident and refracted beam is called the deviation

The variation in deviation with wavelength is called the angular dispersion

$$D_A = \frac{d\theta}{d\lambda} = \frac{d\theta}{d\eta} \underbrace{\frac{d\eta}{d\lambda}}_{\substack{\text{prism} \\ \text{dispersion}}}$$

- first term depends on size and shape of the prism and the incidence angle
- second term (prism dispersion) depends on the material of the prism and the wavelength

$$\frac{d\eta}{d\lambda}(\text{glass@357 nm}) = 1.94\text{x}10^{-4}\ \text{nm}^{-1}$$

$$\frac{d\eta}{d\lambda}(\text{glass@825 nm}) = 1.78\text{x}10^{-5}\ \text{nm}^{-1}$$

Prisms not often used as dispersion elements because of non-constant D_A with wavelength

- produces *non-constant bandwidth*
- means range of λ's projected onto exit slit varies with λ

Electromagnetic radiation

An electromagnetic wave is a transverse wave: electric and magnetic fields perpendicular to the propagation direction

Plane (linearly) polarized beam has constant plane containing the electric and magnetic vectors (often called unpolarized)

The time-dependent electric field is

$$E = E_0 \sin(\omega\ t - \varphi)$$

where

E_0 is the maximum electric field strength
ω is the angular frequency ($2\pi\upsilon$)
t is time
φ is the (angular) phase

The angular phase is (φ_0+$2\pi x/\lambda$) where x is distance and φ_0 is the phase at x=0

$2\pi/\lambda$ is number of waves per unit length

If two waves maintain the same relative phase difference over

(i) extended period of time

(ii) length

they are said to be coherent

Superposition:

The superposition of two waves states two plane polarized waves can be algebraically summed to produce a resultant wave

If waves have same frequency

$$E = E_1 + E_2$$
$$= E_{0,1}\sin(\omega t + \varphi_1) + E_{0,2}\sin(\omega t + \varphi_2)$$

Amplitude (intensity) of wave is E^2

$$E^2 = (E_1 + E_2)^2$$
$$= E_1^2 + E_2^2 + E_1\ E_2$$
$$= E_{0,1}^2 + E_{0,2}^2 + \underbrace{2E_{0,1}\ E_{0,2}\cos(\varphi_2 - \varphi_1)}_{\text{interference term}}$$

If $(\varphi_1\text{-}\varphi_2) = 0, 2\pi, 4\pi\ldots$

- $\cos(0, 2\pi, 4\pi\ldots) = 1$
- wave amplitude will be reinforced (constructive interference)

If $(\varphi_1\text{-}\varphi_2) = \pi, 3\pi, 5\pi\ldots$

- $\cos(\pi, 3\pi, 5\pi\ldots) = -1$
- wave amplitude will be reduced to zero (destructive interference)

Interference can result from difference in pathlength

If the waves initially start out with same phase, the difference in phase, δ, due to different paths is

$$\delta = (\varphi_1 - \varphi_2)$$
$$= \frac{2\pi\ x_1}{\lambda} - \frac{2\pi\ x_2}{\lambda}$$
$$\frac{2\pi(x_1 - x_2)}{\lambda}$$

where

x_1 and x_2 are the lengths to the measurement point from source

$2\pi/\lambda$ is the number of a complete waves per unit length

Thus, when $\delta = 0, 2\pi$... (an integral number of wavelengths)

$$m\ 2\pi = \frac{2\pi(x_1 - x_2)}{\lambda}$$

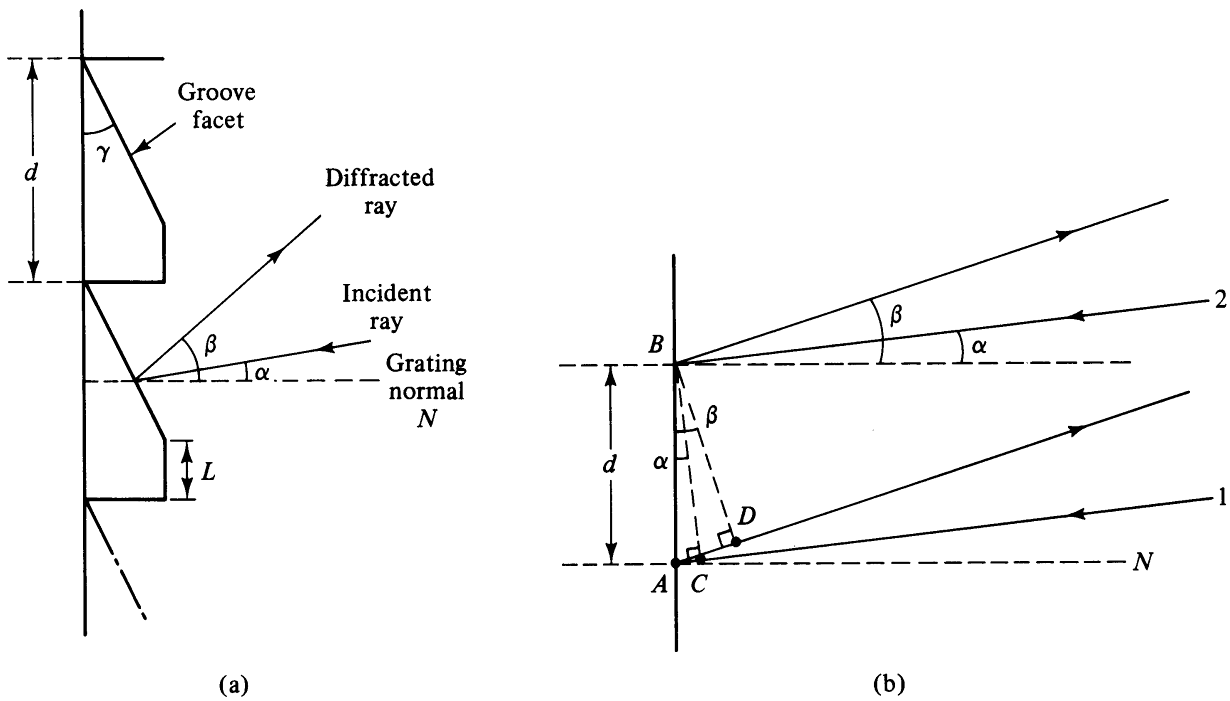
$$m \quad \lambda = \frac{\delta}{2\pi} \qquad \text{constructive interference}$$

when $\delta = \pi, 3\pi$... (an integral number of wavelengths+1/2)

$$\left(\frac{2m+1}{2}\right)\lambda = \frac{\delta}{2\pi} \qquad \text{destructive interference}$$

Diffraction (Eschellete) gratings

Parallel grooves etched (blazed) onto reflective surface - asymmetric in profile



Incident light striking long facet is reflected in specular direction with respect to the *groove* normal

- light from neighboring grooves travels different distances and so interference occurs in outgoing beam

Note: angles α and β are defined with respect to the *grating* normal, not the *groove* normal

Constructive interference occurs when the pathlength difference is an integral number of wavelengths

- extra pathlength associated with the incident beam is AC

$$AC = d \sin \alpha$$

- extra pathlength associated with the outgoing beam is AD

$$AD = d \sin \beta$$

The total pathlength difference is AC + AD:

$$AC + AD = d(\sin\alpha + \sin\beta)$$

$$m\lambda = d(\sin\alpha + \sin\beta) \qquad \text{Grating Formula}$$

(minimum value of d as λ/2, because the maximum value of (sinα + sinβ) is 2)

The first order (m = 1) diffraction angle can be calculated for any incidence angle by rearranging the grating formula

$$\frac{m\lambda}{d} = \sin\alpha + \sin\beta$$

$$\sin\beta = \frac{m\lambda}{d} - \sin\alpha$$

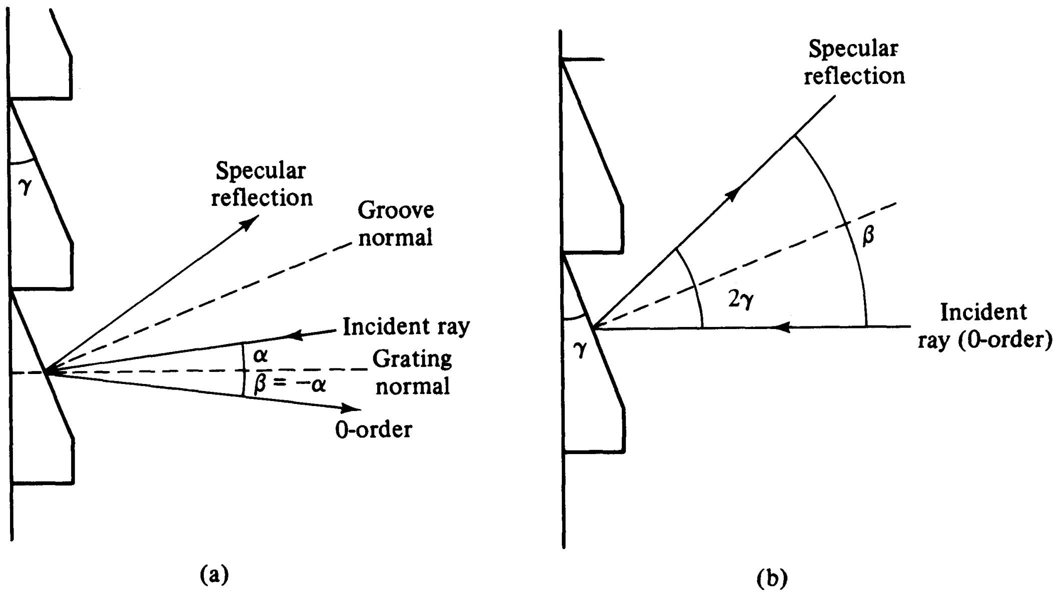
where d is found from the groove spacing

Important

- diffraction angle depends on d
- longer λ's diffracted more than shorter ones ($\beta_{600\ nm} > \beta_{500\ nm}$)
- When m=0 (zero order), sinα = -sinβ or α = -β. In this case, all λ's are diffracted at the same angle

  If blaze was parallel to the grating plane (γ = 0°), the zero order beam would also appear in the specular direction (most of the reflected light not dispersed)

  If blaze angle ≠ 0°, specular and zero-order angles do not correspond and majority of the light is dispersed



In the special case when incident beam is along the surface normal, $\alpha=0$ and first-order beam is in specular direction

- in this case, β is twice the blaze angle, γ. The wavelength at this angle is called the blaze wavelength

$$m \lambda_{blaze} = d(\sin\alpha + \sin\beta)$$

$$\lambda_{blaze} = d\sin\beta$$

$$= d\sin 2\gamma$$

Dispersion

The angular dispersion D_A of the grating can be obtained by differentiating the grating formula with respect to wavelength

For constant incidence angle

$$m\lambda = d(\sin\alpha + \sin\beta) \qquad \text{Grating Formula}$$

$$D_A = \frac{d\beta}{d\lambda} = \frac{m}{d\cos\beta} \qquad \sin\alpha \text{ fixed}$$

$$= \frac{d(\sin\alpha + \sin\beta)}{d\lambda\cos\beta}$$

$$= \frac{\sin\alpha + \sin\beta}{\lambda\cos\beta}$$

For nearly normal incidence, α is small so β is small, and so $\cos\beta$ does not change much with λ

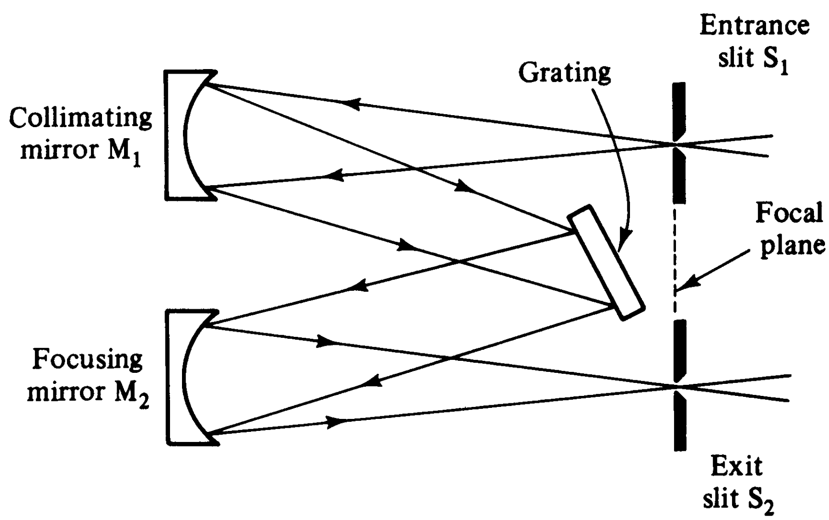
- D_A does not change much with wavelength
- much better dispersion element than prism

Monochromators

Comprised of

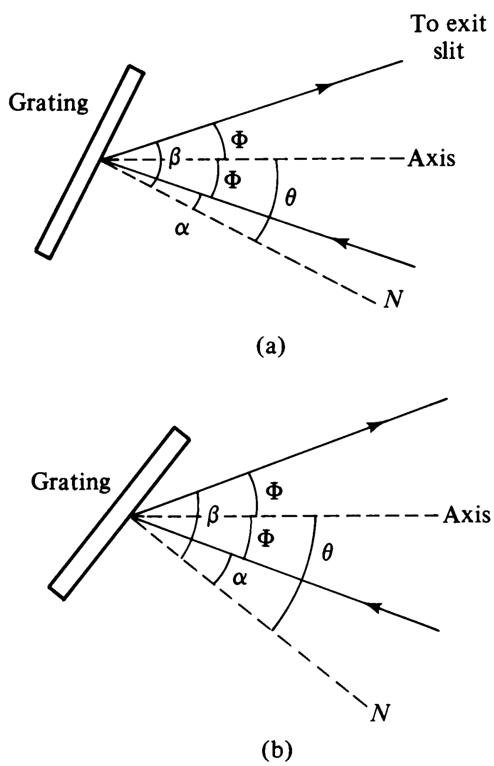
- dispersive element
- image transfer system (mirrors, lenses and adjustable slits)
  - an image of the entrance slit is transferred to the exit slit after dispersion

One of the most common arrangements is the Czerny-Turner monochromator:



Wavelength selection

Wavelength selection is accomplished by rotating the grating



Since angle between the entrance slit, grating and exit slit is fixed (2φ), grating formula can be expressed in terms of the grating rotation angle θ (between grating normal and optical axis)

Since $\alpha = \theta - \varphi$ and $\beta = \theta + \varphi$,

$$m\lambda = d[\sin(\theta - \varphi) + \sin(\theta + \varphi)]$$
$$= 2d\sin\theta\cos\varphi$$

(the trigonometric identity 1/2(sin(A+B)+sin(A-B)) is sinA·cosB)

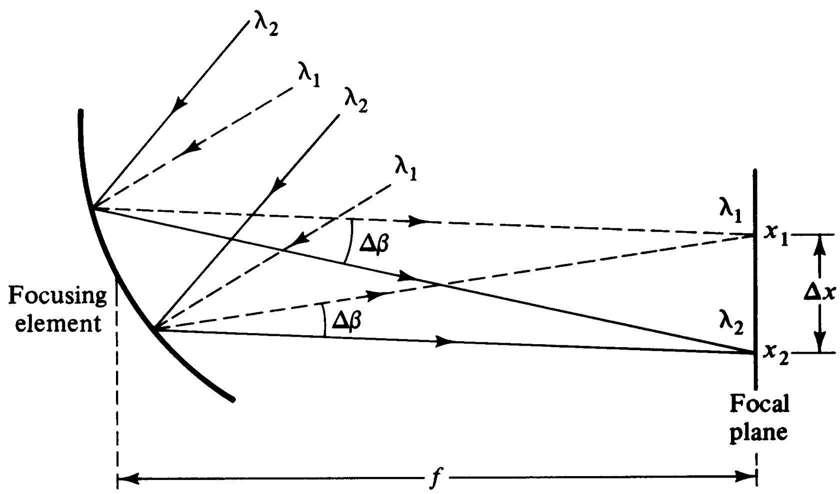
Grating formula now in experimental variables: θ (the grating rotation angle) and φ (half-angle between the entrance, grating and exit and slit)

Dispersive characteristics

Already mentioned the angular dispersion (rate of change of diffraction angle with wavelength) for a grating

$$D_A = \frac{d\beta}{d\lambda} \qquad \text{angular dispersion}$$

However, in monochromator much more interested in dispersion at focal plane (exit slit), defined by the linear dispersion, D_l,



$$D_l = \frac{dx}{d\lambda} \qquad \text{linear dispersion}$$

- units of D_l are $mm \cdot nm^{-1}$ or similar

For a Czerny-Turner arrangement, the linear dispersion is:

$$D_l = f \; D_A$$

where

f is the focal length of the focusing (exit) optic

Sometimes the inverse linear dispersion, R_d, is used (units of nm·mm^{-1} or similar)

$$R_d = D_l^{-1} = \frac{d\lambda}{dx} \qquad \text{inverse linear dispersion}$$

$$D_A = \frac{\sin\alpha + \sin\beta}{\lambda\cos\beta}$$

$$R_d = \left(f \;\; D_A\right)^{-1}$$

$$= \frac{\lambda\cos\beta}{f(\sin\alpha + \sin\beta)}$$

Spectral bandpass and the slit function

The spectral bandpass (nm) is the half-width of the range of wavelengths passing through the exit slit

The geometric spectral bandpass

$$s_g = R_d \;\; W \qquad \text{geometric spectral bandpass}$$

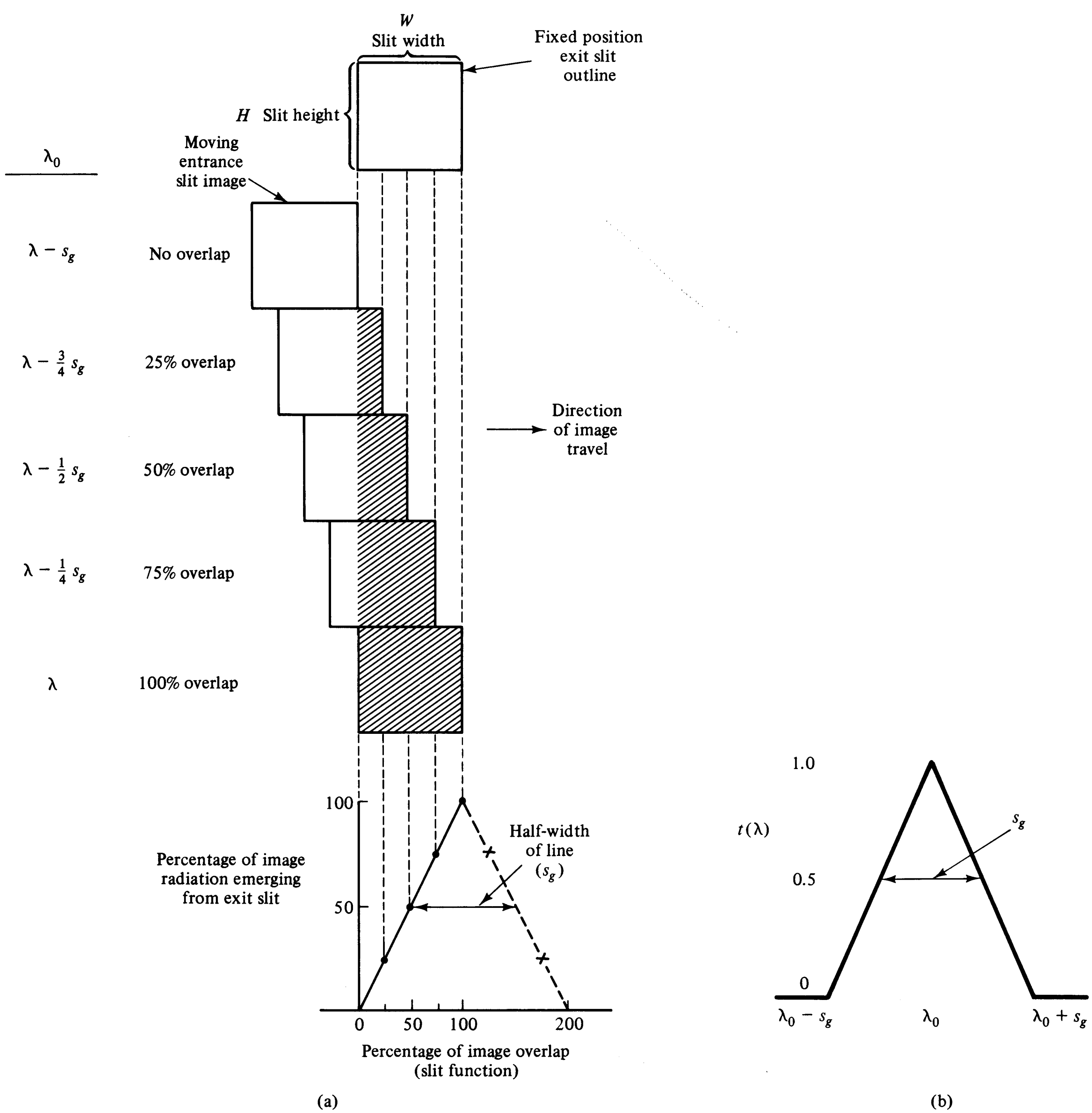
where

R_d is the inverse linear dispersion

W is slit width

In a monochromator, an image of entrance slit is focused at the exit slit:

- when input is polychromatic, a monochromated version of the image appears at the exit slit
- when input is monochromatic image, rotating the grating angle θ will sweep monochromatic image across the exit slit



The total intensity t(λ) measured at the exit slit as image is translated is called the slit function

- for equal entrance and exit slits, shape is triangular
- for unequal entrance and exit slits, shape is trapezoidal

with a base of s and half-width of s_g

Mathematically, the slit function is

$$t(\lambda) = 1 - \left(\frac{\lambda - \lambda_0}{s_g}\right) \qquad \lambda_0 - s_g \le \lambda \le \lambda_0 + s_g$$

$$t(\lambda) = 0 \qquad \text{elsewhere}$$

where

λ is the incident (monochromatic) wavelength at entrance slit

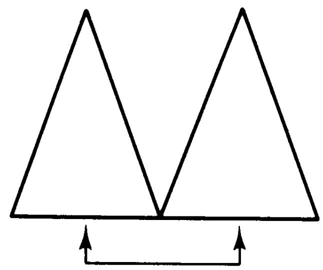
λ_0 is the wavelength setting of the monochromator (the wavelength directed to the center of the exit slit)

Resolution

Resolution quantifies how well separated two features are at the exit slit

- closely related to linear dispersion (D_l)

  (or angular dispersion (D_A), and physical dimensions of the monochromator (through f))
- slit width W



If the width of a single peak base is s (= $2s_g$), then two features will just be completely separated when the wavelength difference between them is s

$$\Delta\lambda_s = s = 2s_g = 2R_d W \qquad \text{slit-width-limited resolution}$$

Alternatively, we may adjust slit width to obtain resolution of two features separated by $\Delta\lambda_s$

$$W = \frac{\Delta\lambda_s}{2R_d}$$