Optical Spectrometers

- Prism Spectrometers
- Grating Spectrometers
- Interferential Spectrometers
- Hyperspectral Spectrometers

Experimental Methods in Physics [2011-2012]

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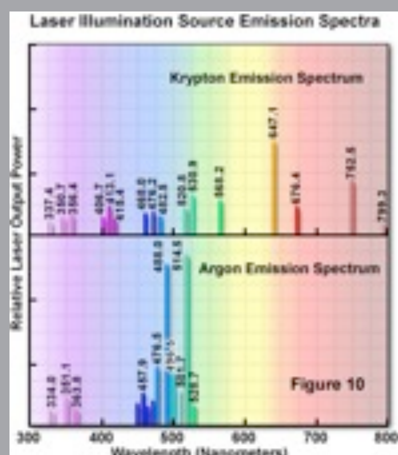
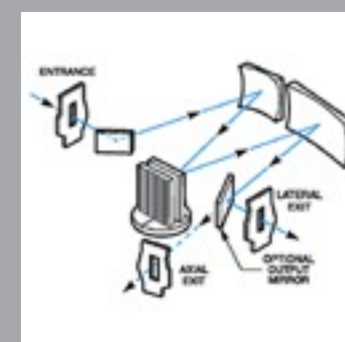
Optical spectroscopy

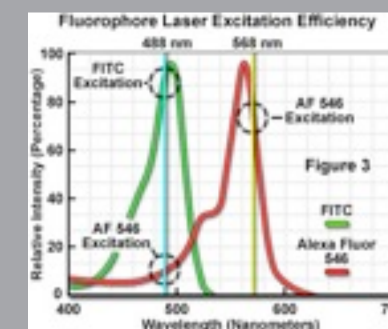


light source

sample



light analyzer



light detector

Content

Optical spectroscopy

General properties of dispersive apparatus

- Resolvance (resolving power)
- Luminosity

Classification of dispersive apparatus

- Prism spectrometer
- Grating spectrometer
- Interferential spectrometer
- Fourier spectrometer
- Hyperspectral spectrometer

Optical spectroscopy

Definition

The emission spectrum of a source, primary or secondary, is characterized by its luminance L (ν).

The absorption spectrum is characterized by the absorption factor *A* (ν).

The role of dispersive devices (prism, grating, interferential) is to determine the functions *A* (ν) and L (ν) with the greatest precision.

Optical spectroscopy

Keep in mind that the important physical parameter is .... the frequency, ν , ... even if we measure the wavelength !

in the vacuum:

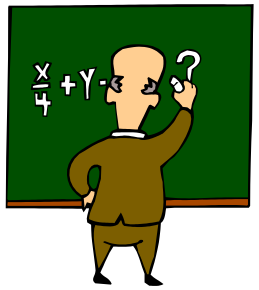
$$\lambda_v = \frac{c}{\upsilon}$$

in a medium of index n:

$$\lambda_n = \frac{c}{n \cdot \upsilon}$$

$$\lambda_v - \lambda_n = (n-1)\cdot\lambda_v$$

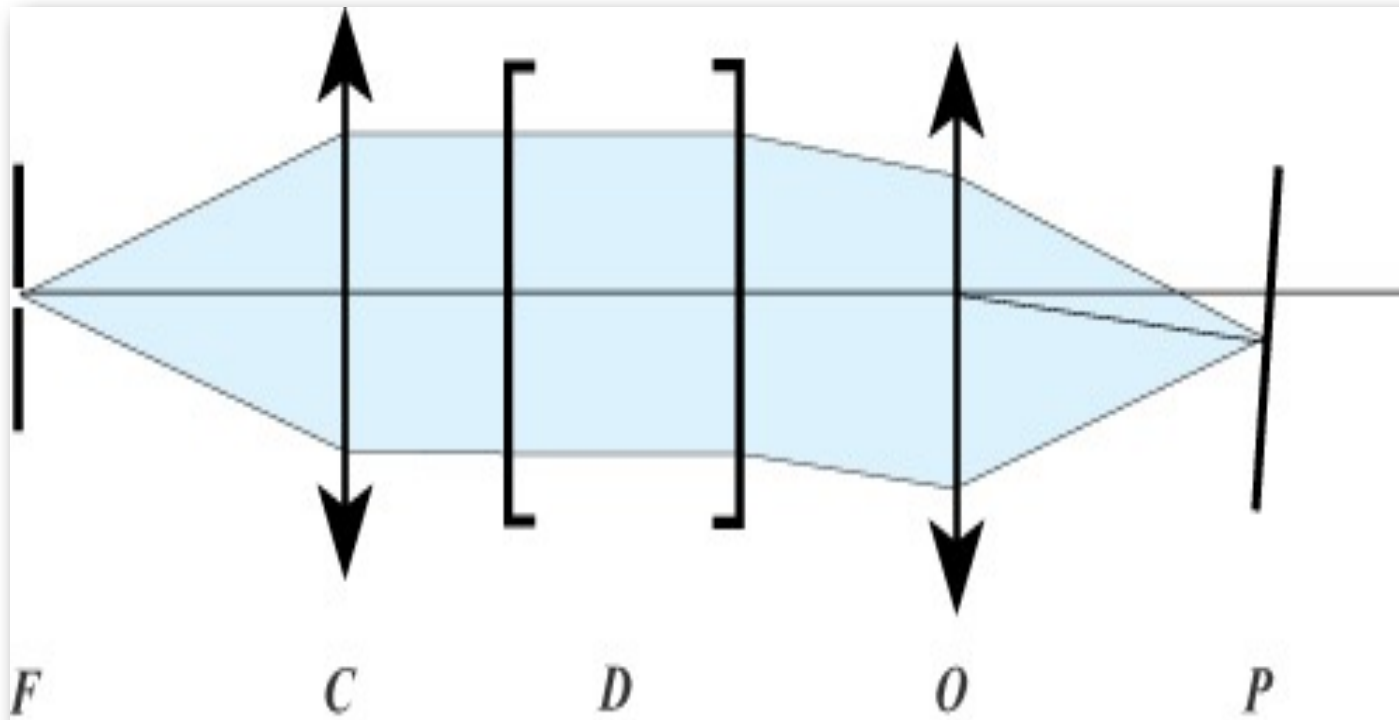
Often in the air, it makes no difference between λ_n and λ_v



In fact, in the visible range, the error is not negligible (1-2 Å)

Dispersive apparatus

General properties



F: entrance slit
C: collimator (objective, mirror, ...)
D: dispersive element (prism, grating, ...)
O: objective (mirror)
P: image plane (photodetector, CCD, ...)

Figures of merit

- Resolving power or resolvance

$$\Re = \frac{\lambda}{\Delta\lambda}$$

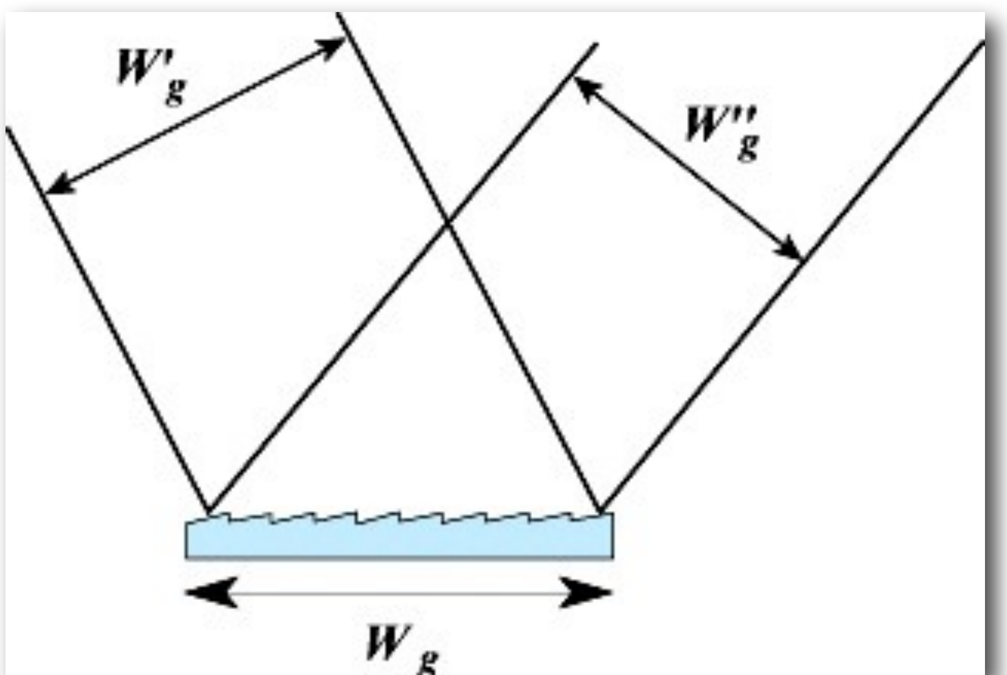
- Luminosity

$$L = \frac{E_M}{L_s}$$

Resolvance

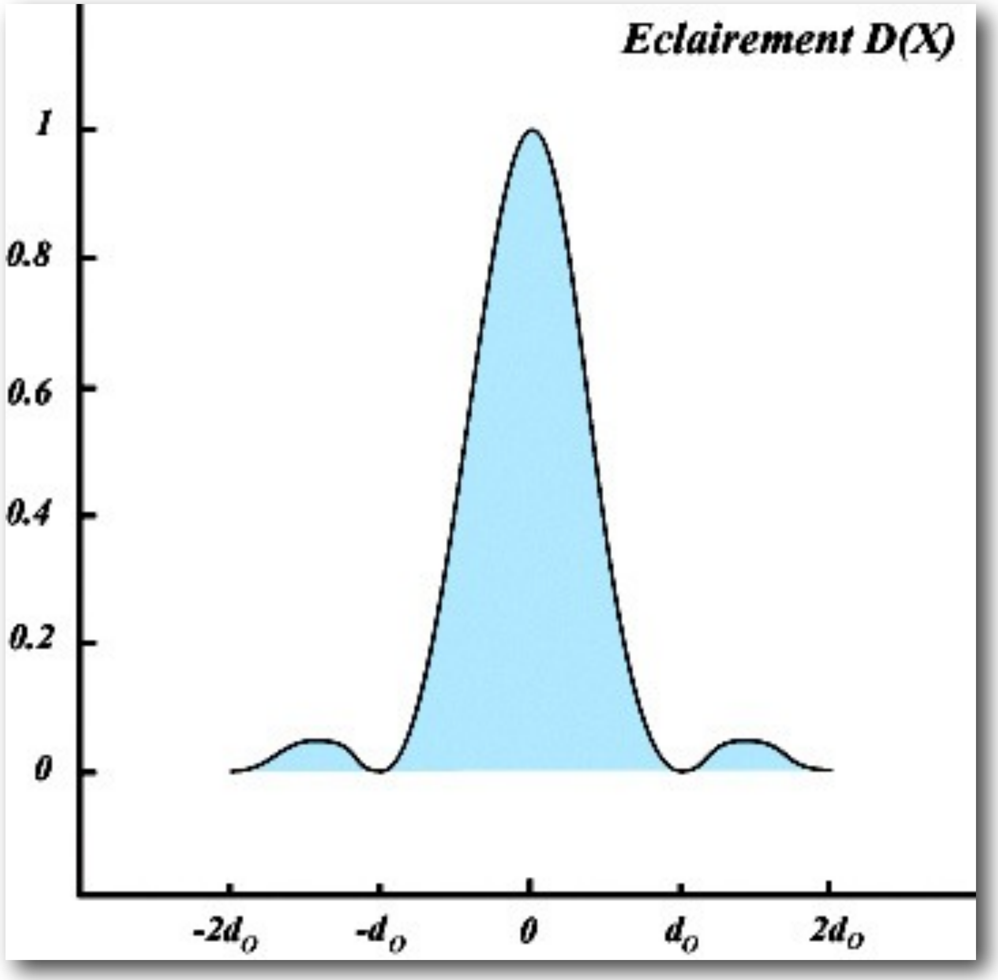
Ideal case: punctual source (eventually slit)

The size of the image, in the plane P, is limited by the diffraction ...



this is the projection of the contour of the dispersive element in a plane which is perpendicular to a direction that follows the dispersion that is important for calculating the size of the image.

Ideal case: incoherent punctual source



$$D(x) = \left[\frac{\sin(\pi \cdot x / d_o)}{(\pi \cdot x / d_o)}\right]^2$$

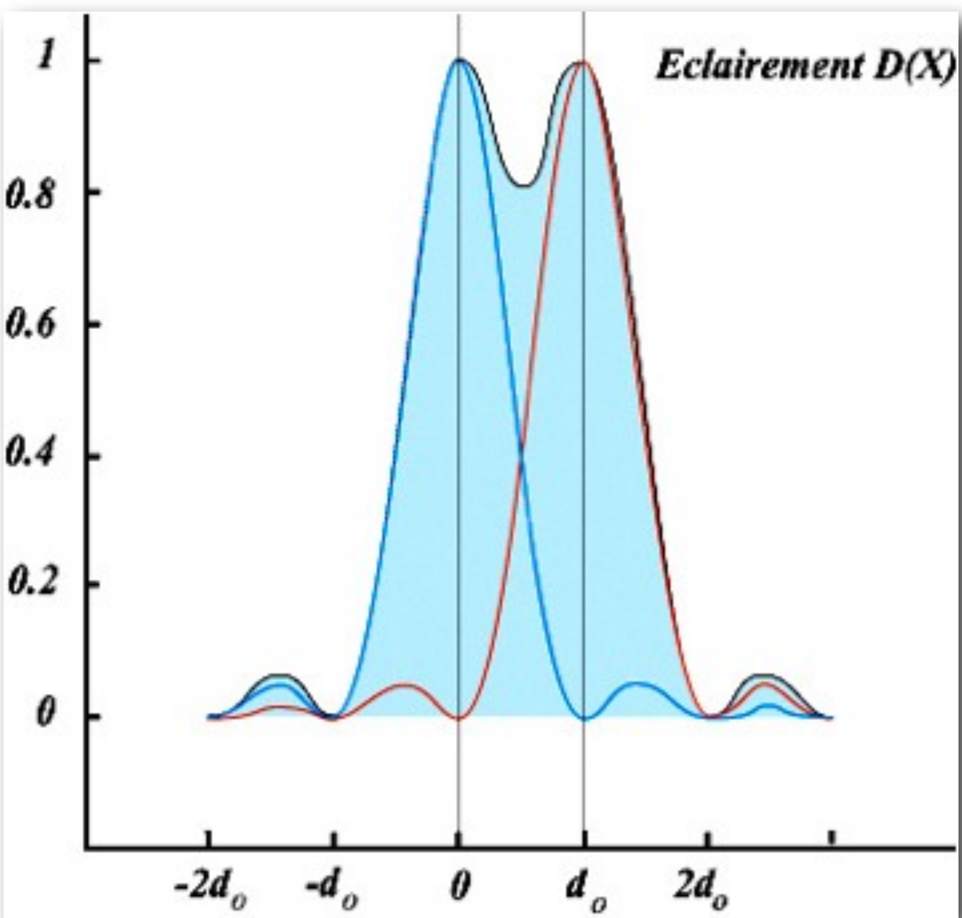
$$d_o = f \cdot \frac{\lambda}{w_g''}$$

Resolvance

Rayleigh criterium:

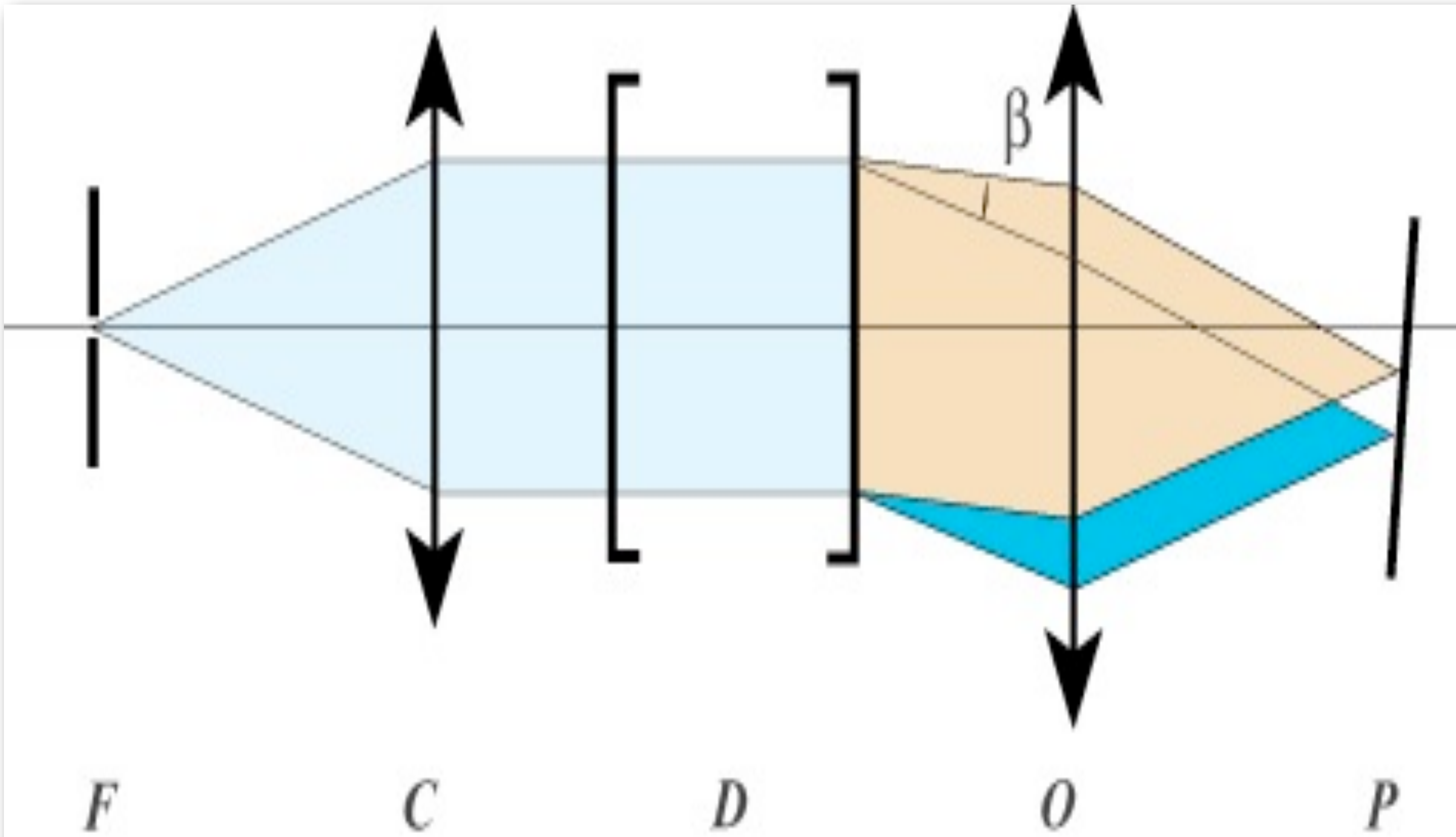
Ideal case:

2 punctual sources emitting at two different wavelengths (λ and [$\lambda + \Delta\lambda$])



We consider that both wavelengths, λ and [$\lambda + \Delta\lambda$] are resolved if the centers of their diffraction pattern are separated by at least d_0

Resolvance



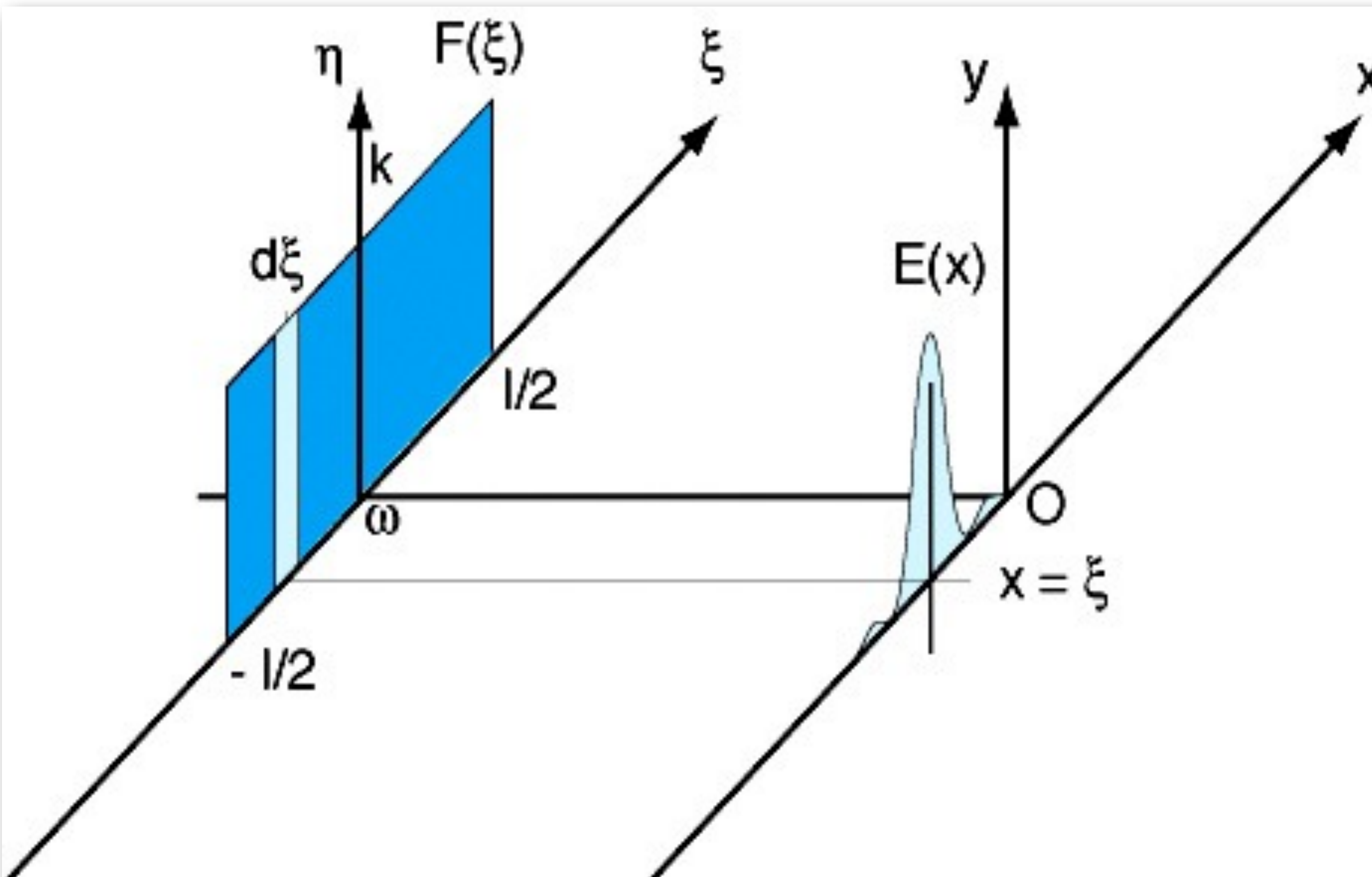
Resolvance

$$\Re_o = \frac{\lambda}{\Delta\lambda} = w_g'' \cdot \frac{d\beta}{d\lambda}$$

The intrinsic resolvance of the system is limited by the size of the dispersive element (or rather by it's projection ….), i.e. by the diffraction

Resolvance

Influence of the width of the entrance slit



Resolvance

Influence of the width of the entrance slit

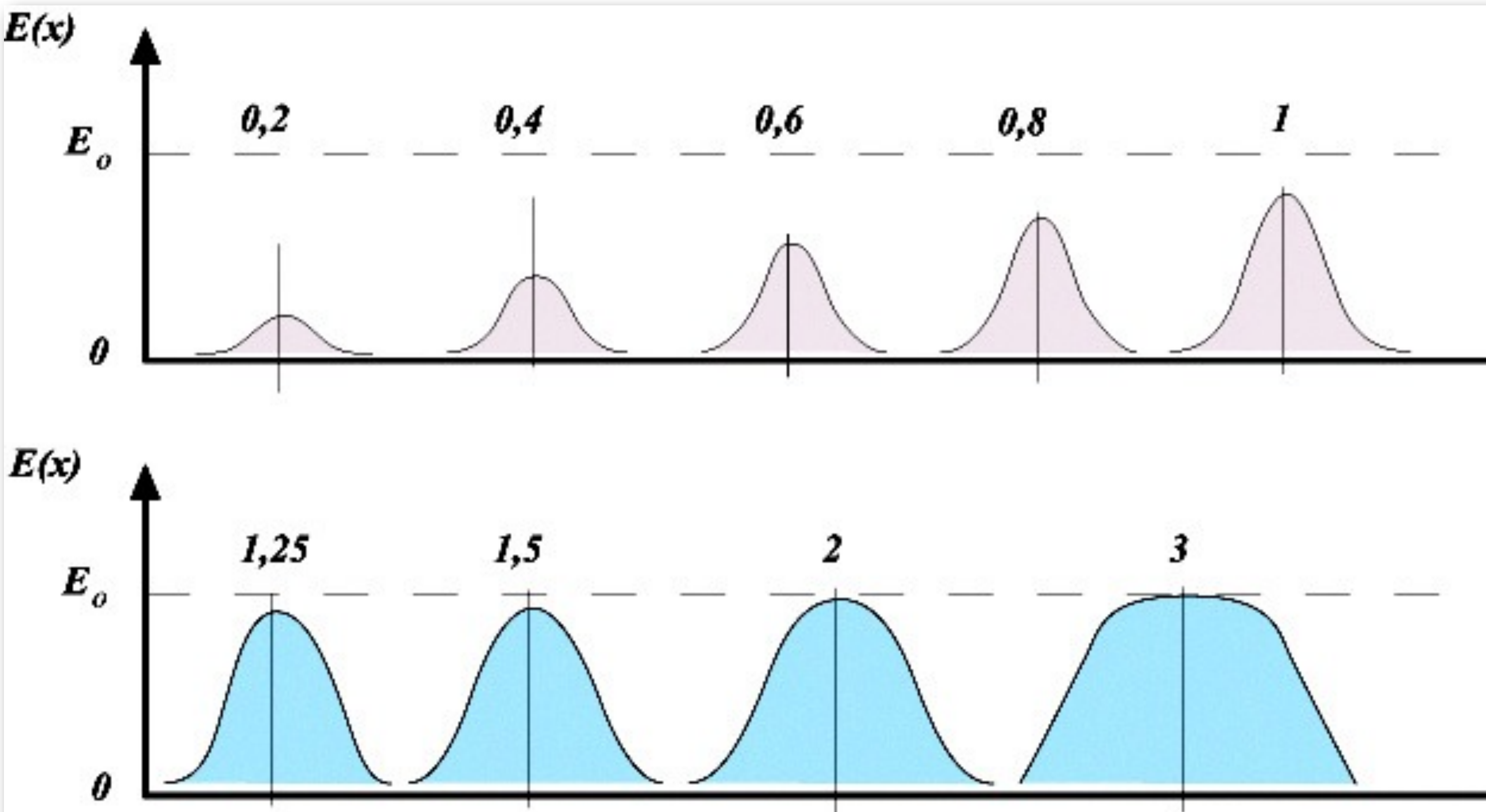
$$E(x) = \int F(\zeta) \cdot D(x-\zeta) d\zeta$$

$$E = F \otimes D$$

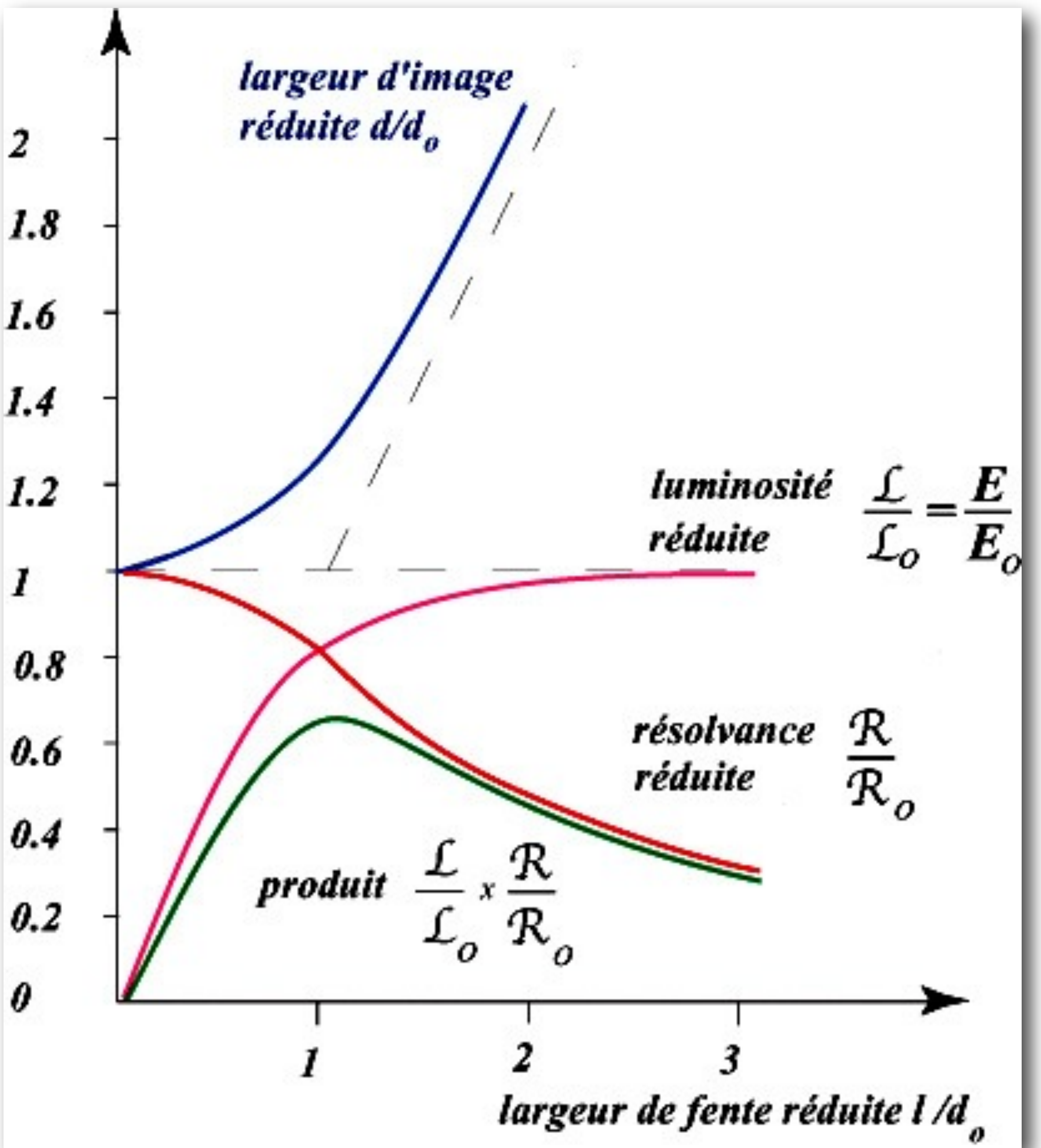
where F is the function "slit", and D(x) the diffracted intensity in the image plane, of an infinitely thin slit.

Resolvance

Influence of the entrance slit width



Luminosity versus resolvance - a compromise



Monochromator or spectrometer ?

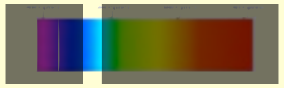
Dispersive instruments

. prism
. grating
. interferential

Monochromator

Bandpass filter - monochromator

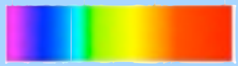
Monochromatic light source



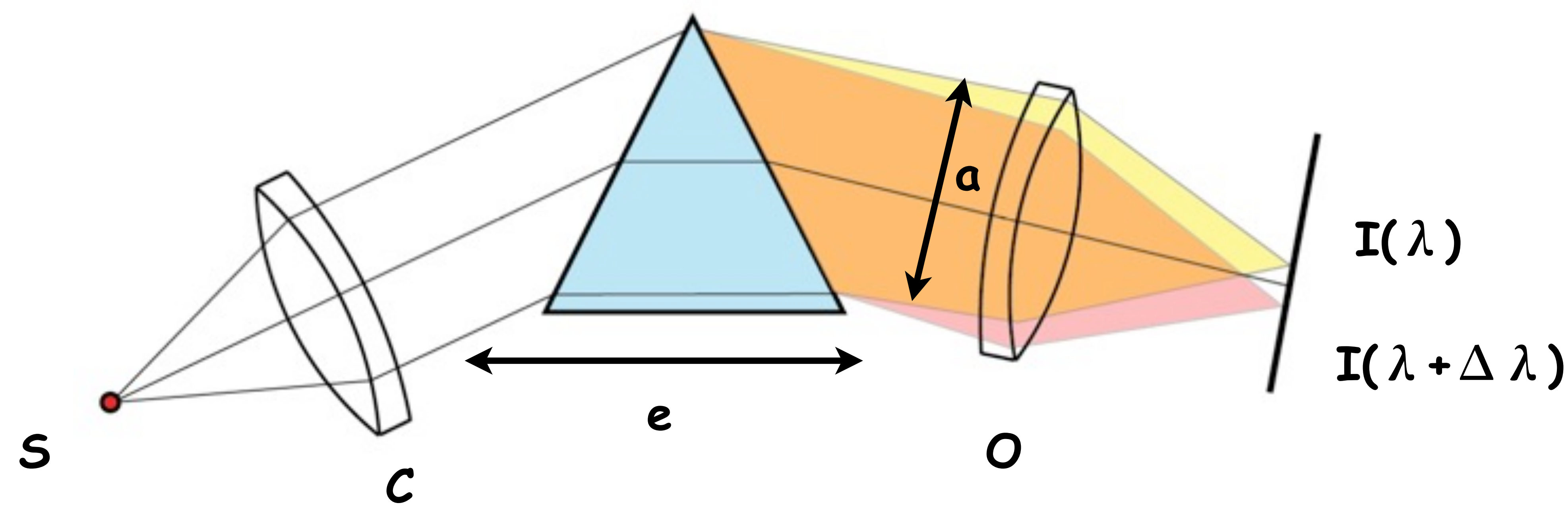
Monochromator + detector

Spectroscope
Spectrometer
Spectrograph

Spectral signature

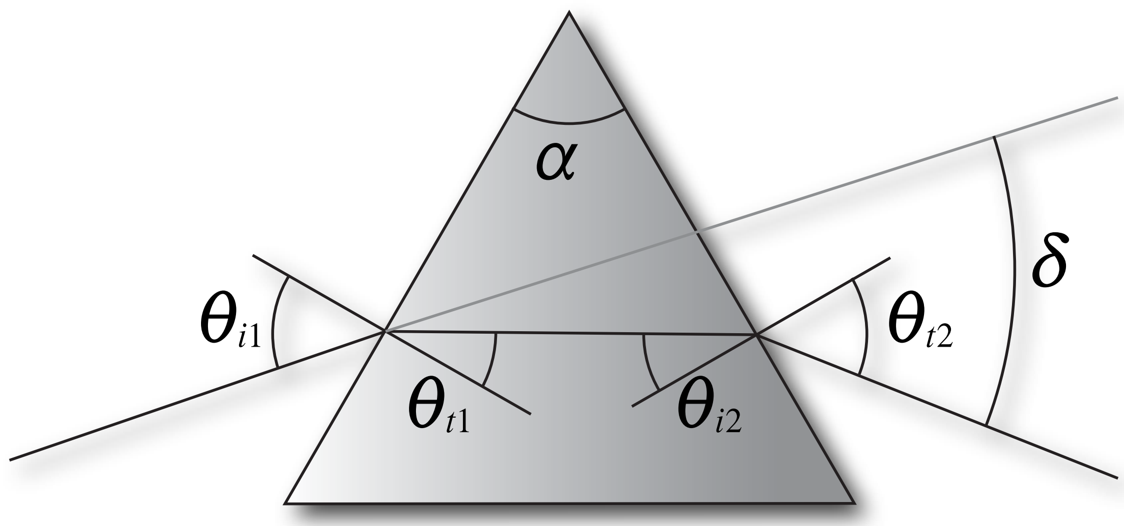


The prism spectrometer



S: ponctual source
C: collimator
O: objectif

The prism spectrometer



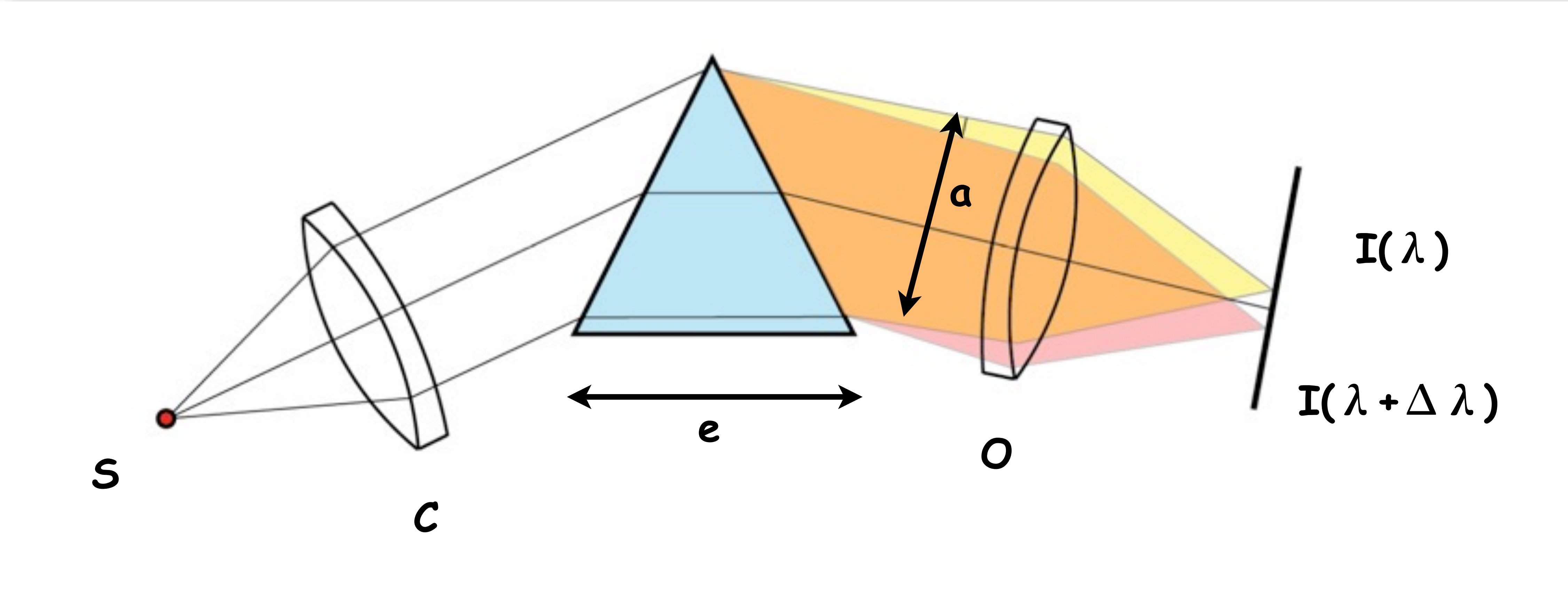
Snell's law

$$n = \frac{\sin(\theta_{i1})}{\sin(\theta_{t1})} = \frac{\sin(\theta_{t2})}{\sin(\theta_{i2})}$$

If the angle of deviation, δ , is minimum

$$n = \frac{\sin(\frac{\alpha+\delta}{2})}{\sin(\frac{\alpha}{2})}$$

The prism spectrometer



the resolving power is given by:

$$\Re = \frac{\lambda}{\Delta\lambda} = a\frac{d\beta}{d\lambda} = e\frac{dn}{d\lambda}$$

The prism spectrometer

Example:

To estimate the resolving power, we consider the case of a prism spectrometer working around 0.5 µm (green light).

$$\Re = e\frac{dn}{d\lambda} \approx \frac{n_r - n_b}{\lambda_r - \lambda_b} = \nu_{abbe}(n_y - 1)\frac{e}{170\ [nm]}$$

e = 25 mm →

$$\Re \approx \begin{matrix} 1100 & Crown \\ 3400 & Flint \end{matrix}$$

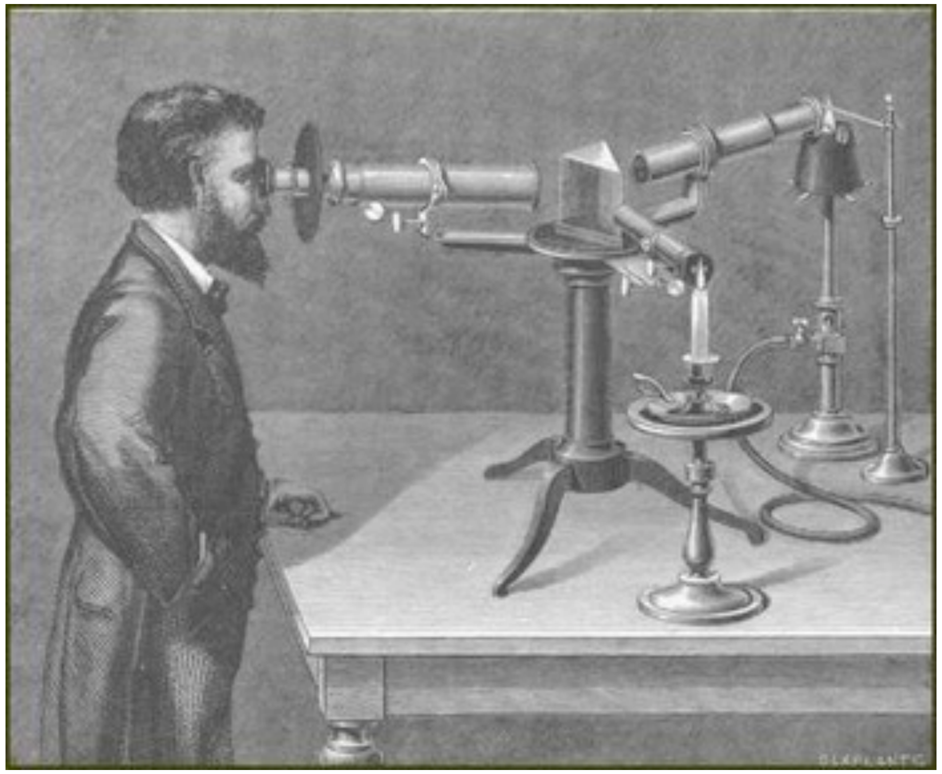
↓

$$0.17\ nm \lesssim \ \Delta\lambda \ \lesseqgtr \lesssim 0.5\ nm$$

The prism spectrometer

Advantages

- low sensitivity to polarization
- no overlap between different orders
- uniform efficiency over the whole spectrum
- heavy duty, high damage threshold
- scanning and imaging modes

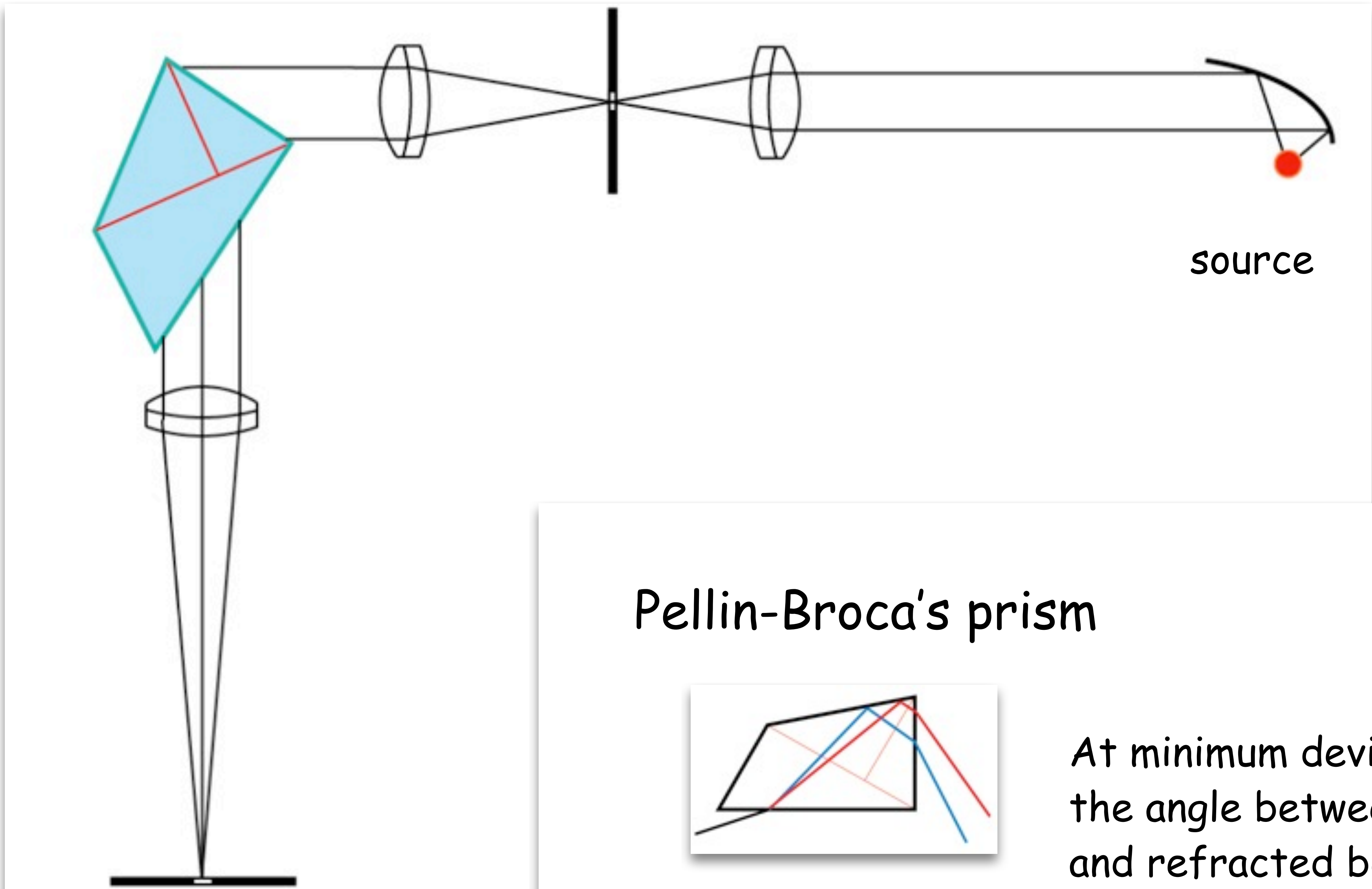


credit: www.antique-microscopes.com/chemistry/

Disadvantages

- $n = n(\lambda)$ non-linear dependance
- material has to be transparent over the whole spectrum
- relatively low resolving power, compared to grating instruments (for similar luminosity ...)
- need for costly achromatic optics
- need to control several angles ...

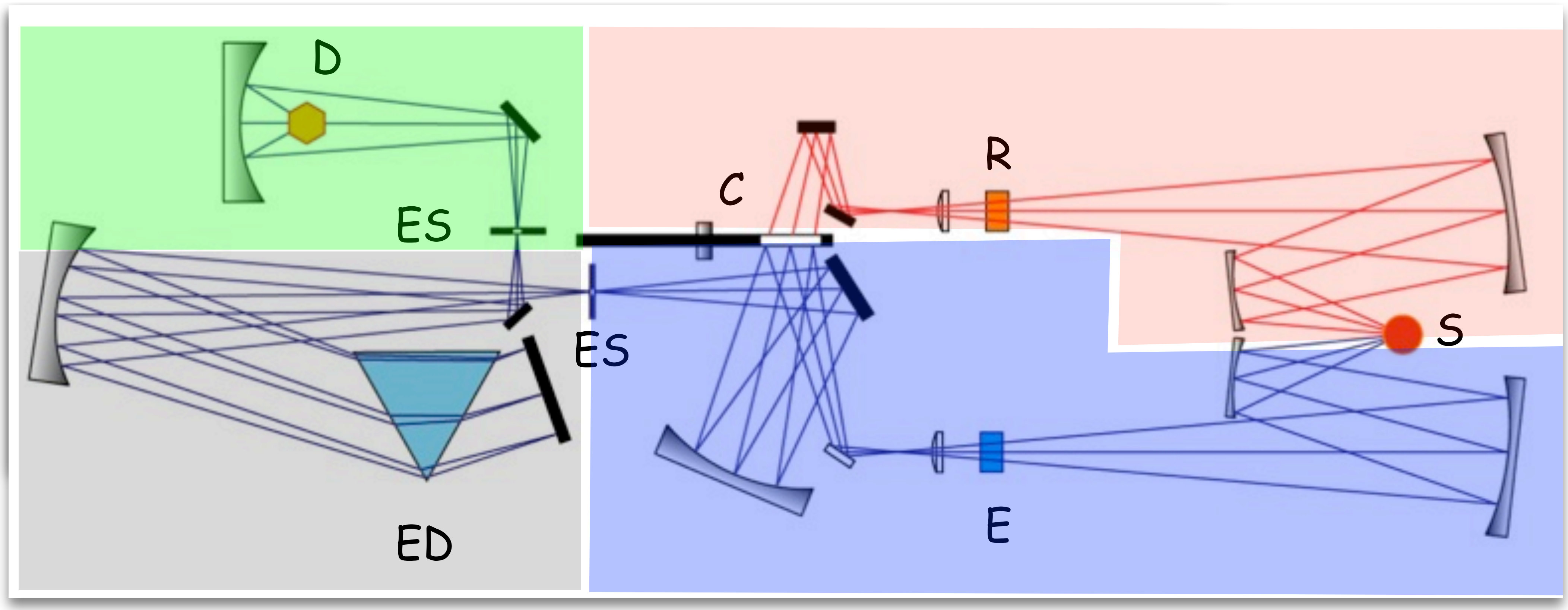
The prism spectrometer



Pellin-Broca's prism

At minimum deviation angle, the angle between incident and refracted beam is precisely 90 °

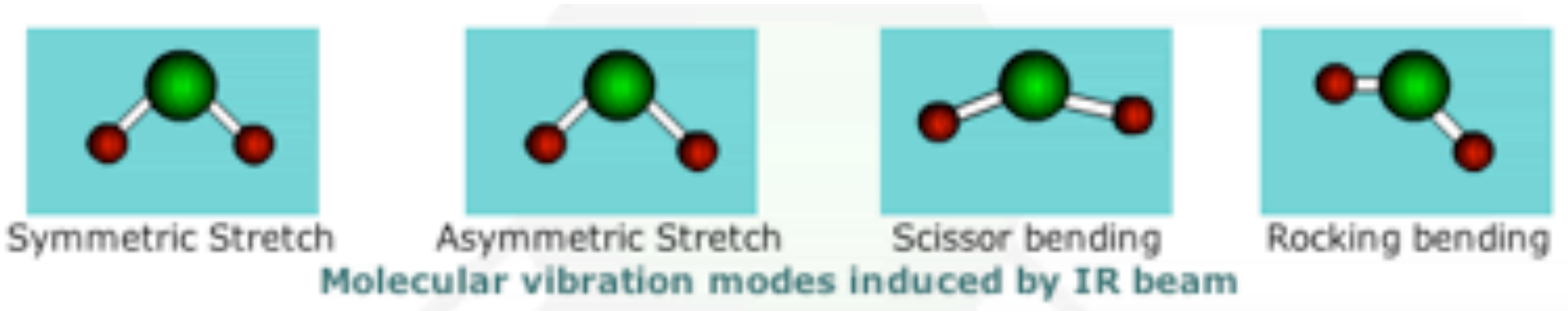
The prism spectrometer in the NIR

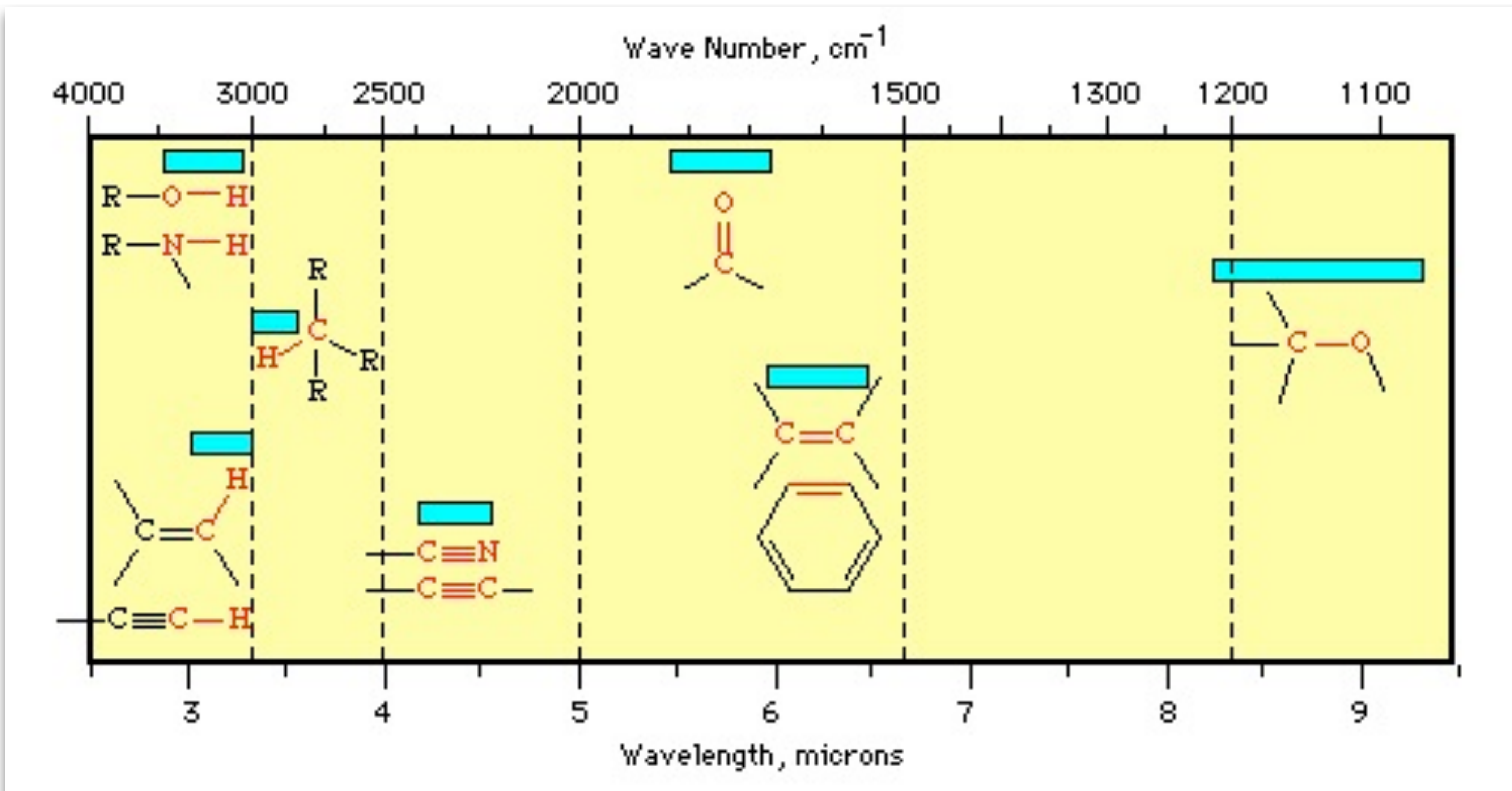


S: “white“ light source
R: reference
E: sample
C: chopper

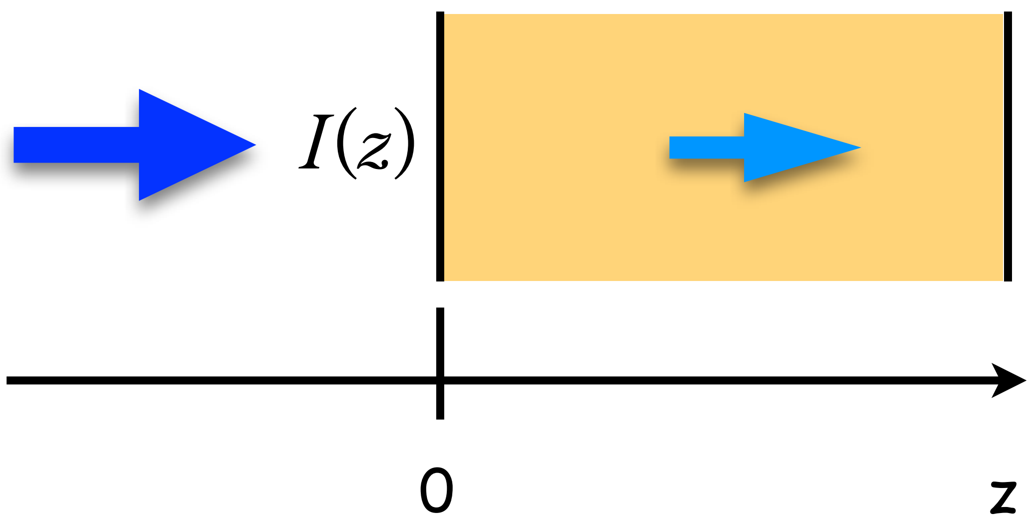
ES: entrance slit of the spectrometer
ED: dispersive element
ES: exit slit of the spectrometer
D: detector

The prism spectrometer in the NIR





The prism spectrometer in the NIR



Beer's law

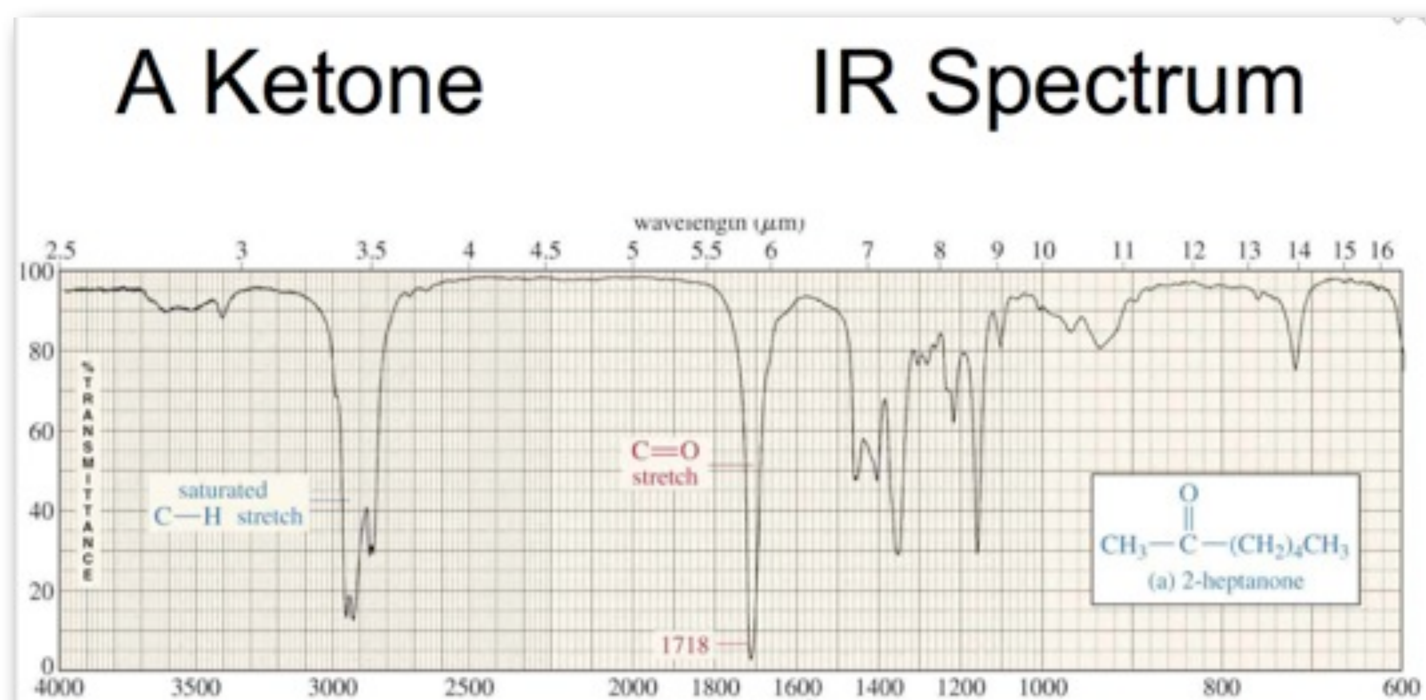
$$I(z) = I_0 \exp(-\alpha z)$$

Transmittance

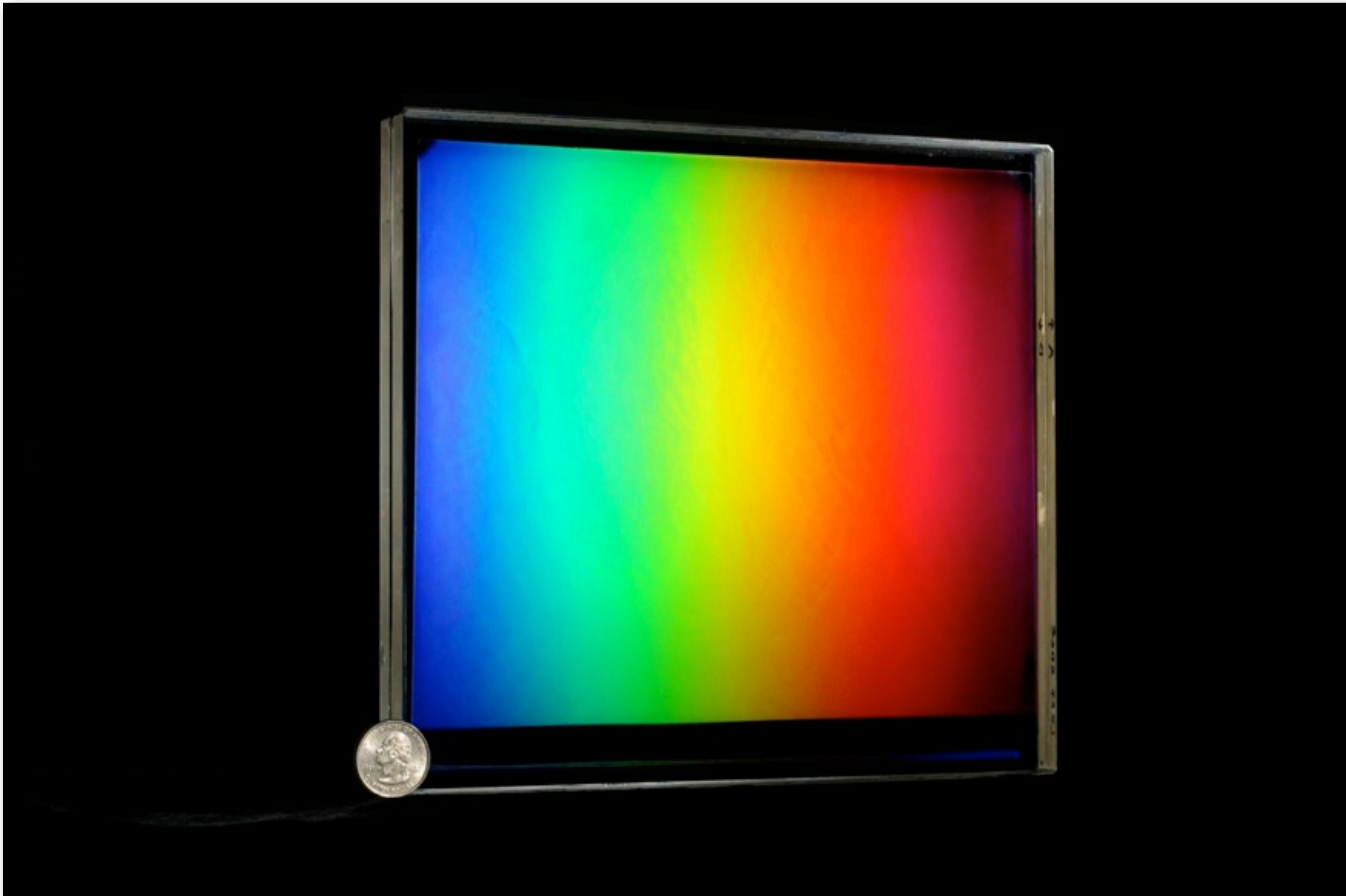
$$\%T = \frac{I}{I_0} \cdot 100$$

Absorbance

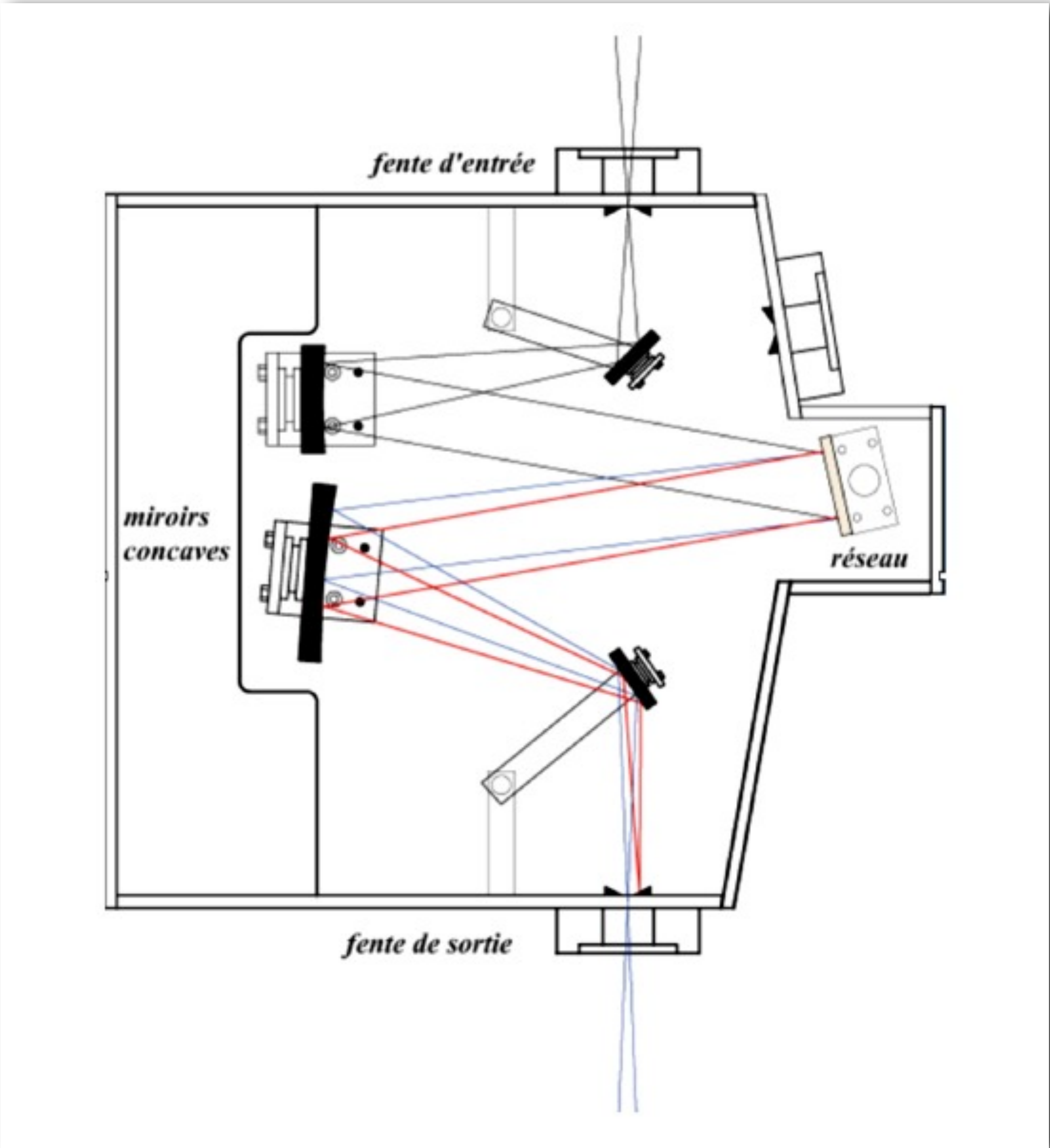
$$A = -\log T = \log\left(\frac{I_0}{I}\right)$$



The grating spectrometer



The grating spectrometer



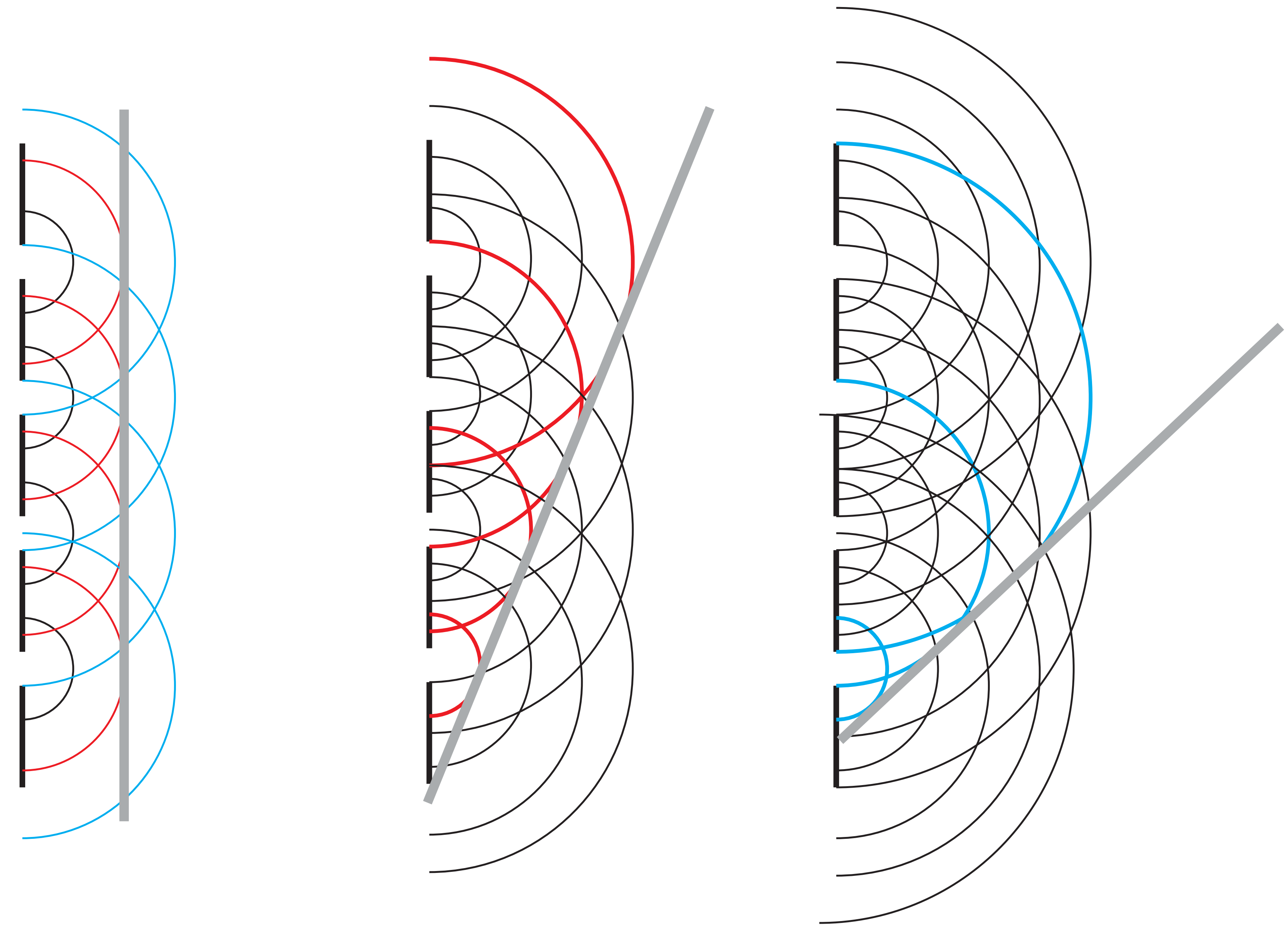
The dispersive element is a grating instead of a prism

collimator and objective are replaced by mirror optics (achromatic over a wide spectral range)

imaging mode possible using an image detector (CCD or CMOS array) placed in the exit plane

Grating .... intuitive feeling

Huygens' principle



$\Delta \phi = 0$

0^{th} order

$\Delta \phi = 2\pi$

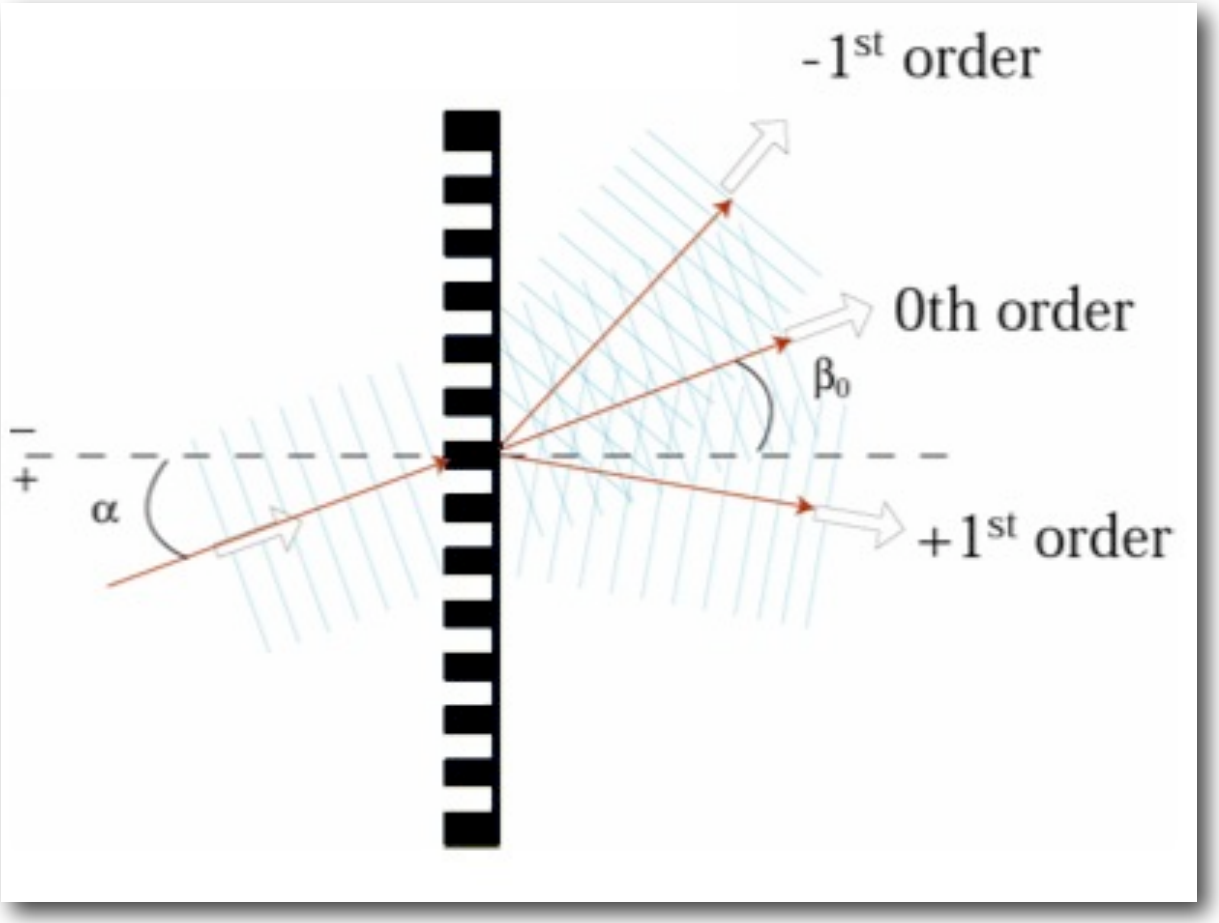
1^{st} order

$\Delta \phi = 4\pi$

2^{nd} order

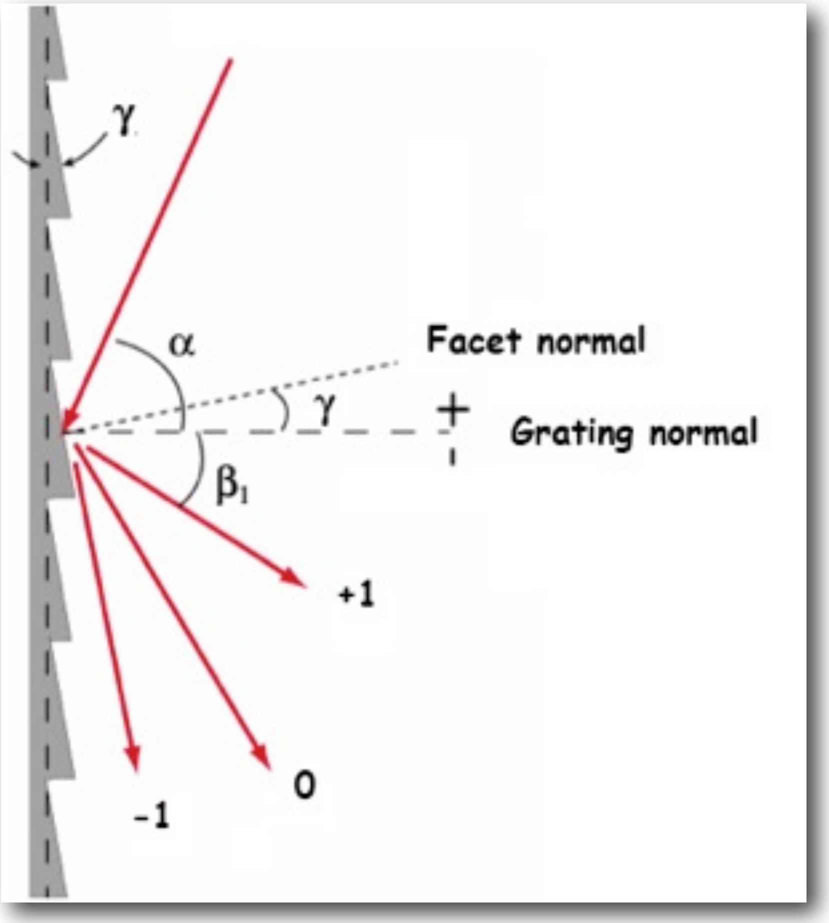
Transmission or reflection gratings ?

transmission grating



refractive index modulations within a thin layer of material sandwiched between two glass substrates

reflection grating



ruled gratings
holographic gratings

Grating spectrometer - basic equations

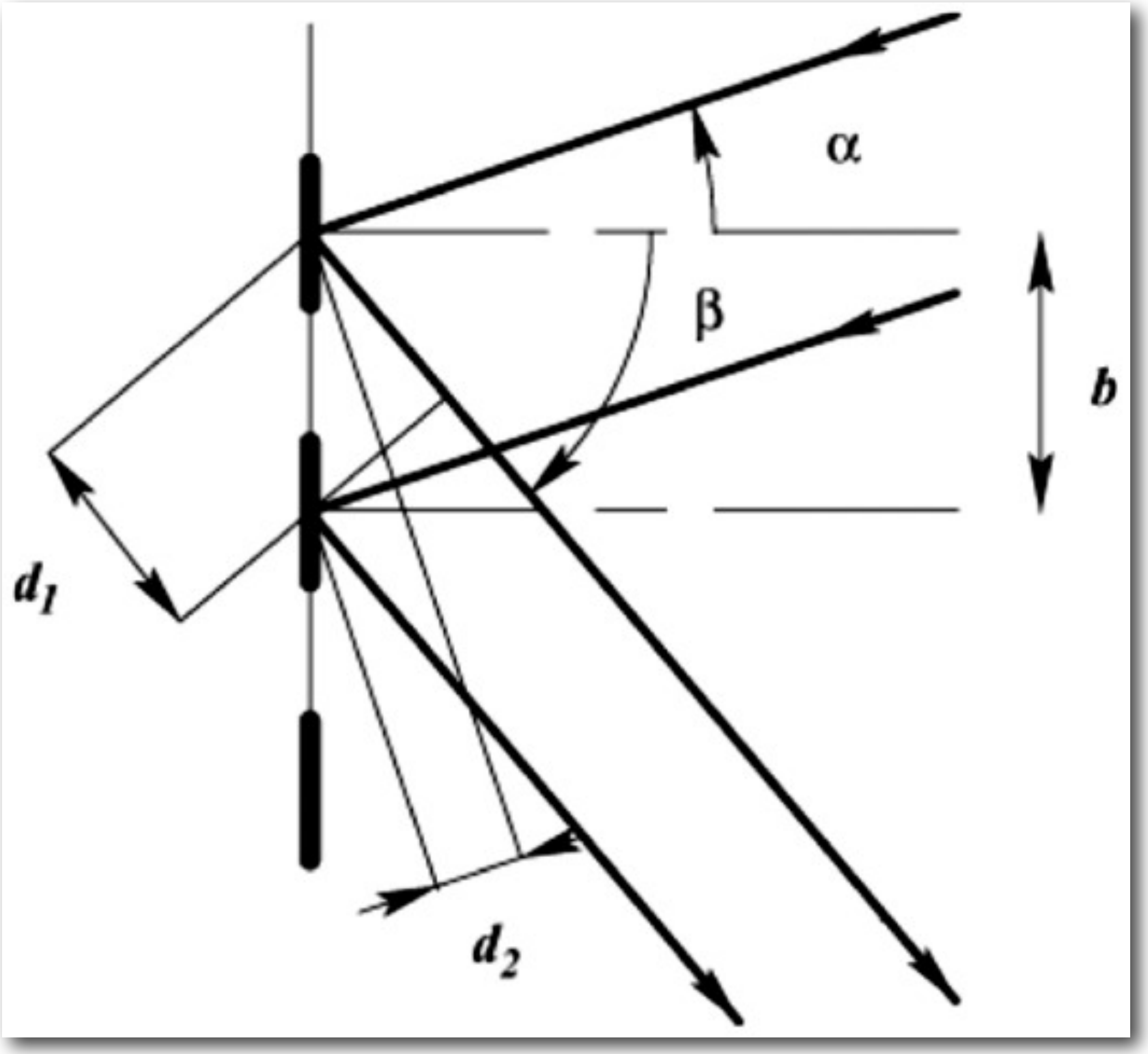
Notations

α = incident angle

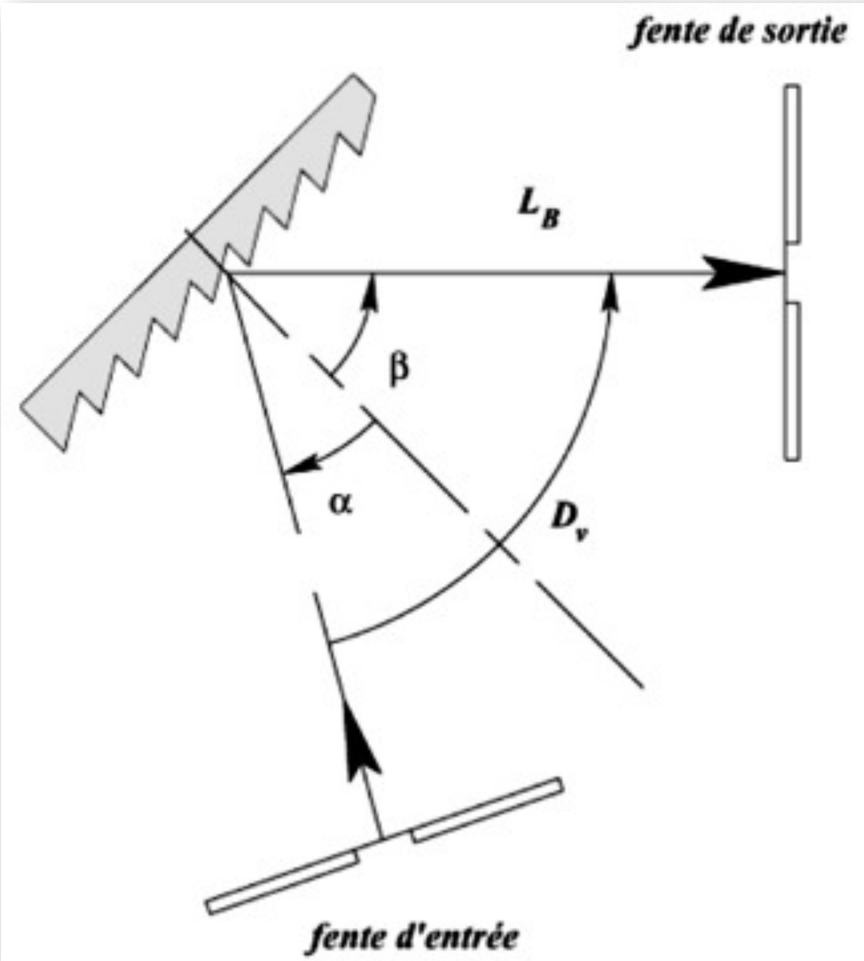
β = diffraction angle

k = diffraction order
N = total number of grooves
n = grooves density [grooves/mm]
λ = wavelength [nm]

b = grating step
$D_V = \alpha + \beta$ = total deviation angle



Grating spectrometer-basic equations



$$D_V = \beta - \alpha$$

D_V is fixed by the geometry

k = diffraction order

n = grooves density

$$\sin(\alpha) + \sin(\beta) = 2 \cdot \sin\left(\frac{\alpha+\beta}{2}\right) \cdot \cos\left(\frac{\beta-\alpha}{2}\right) = 10^{-6} \cdot k \cdot n \cdot \lambda$$

Grating spectrometer-basic equations

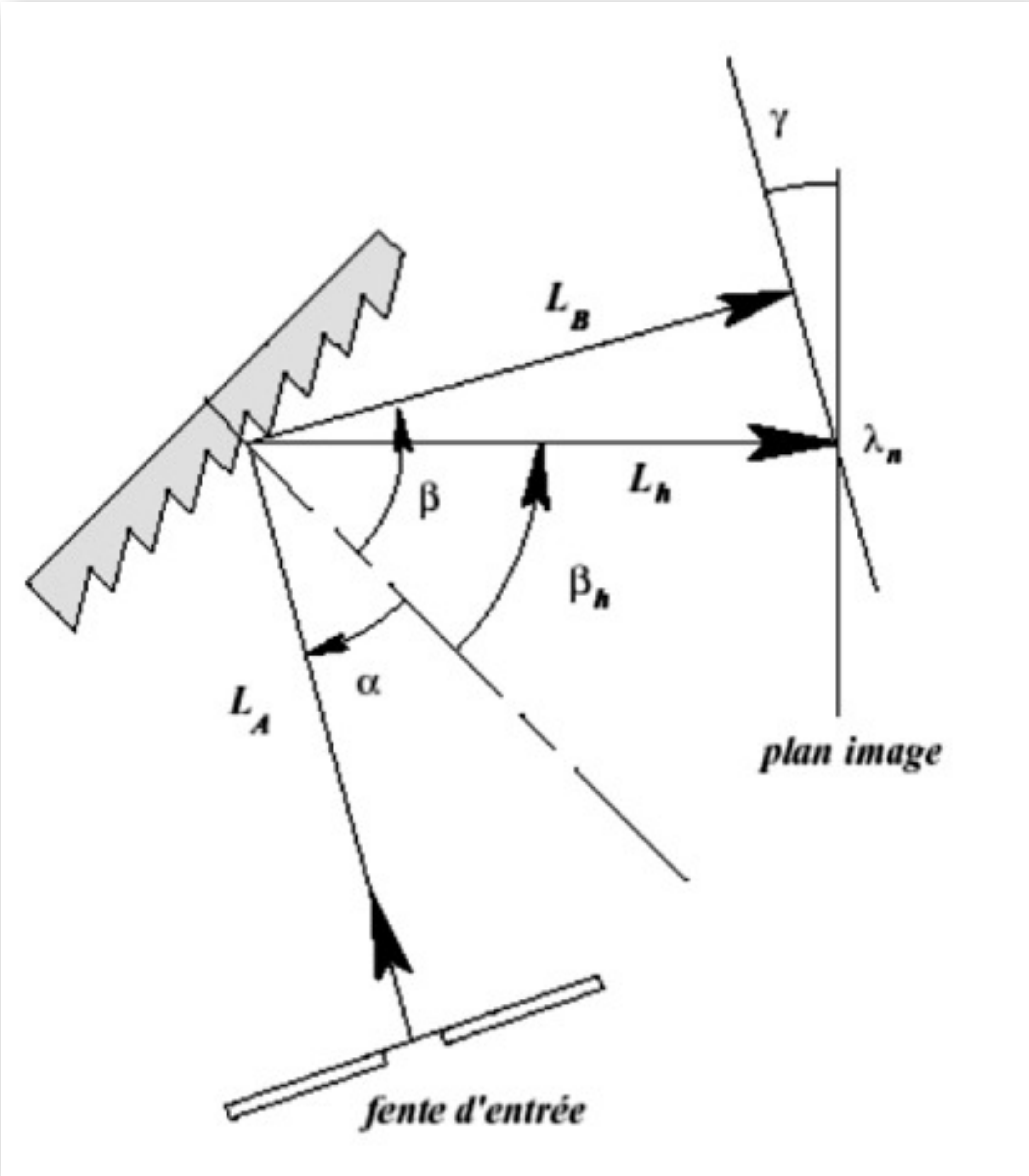
example of configuration

Table 1		D_V	α	β	
variation de l'angle d'incidence, α, et de l'angle de diffraction, β, en fonction de l'angle de déviation D_v (réseau de 1200 l/mm, k = 0 et λ = 500 nm)		0	17.458	17.458	littrow
		10	12.526	22.526	
		20	7.736	27.736	
		24	5.861	29.861	
		30	3.094	33.094	
		40	-1.382	38.618	
		50	-5.670	44.330	

Grating spectrometer

imaging mode

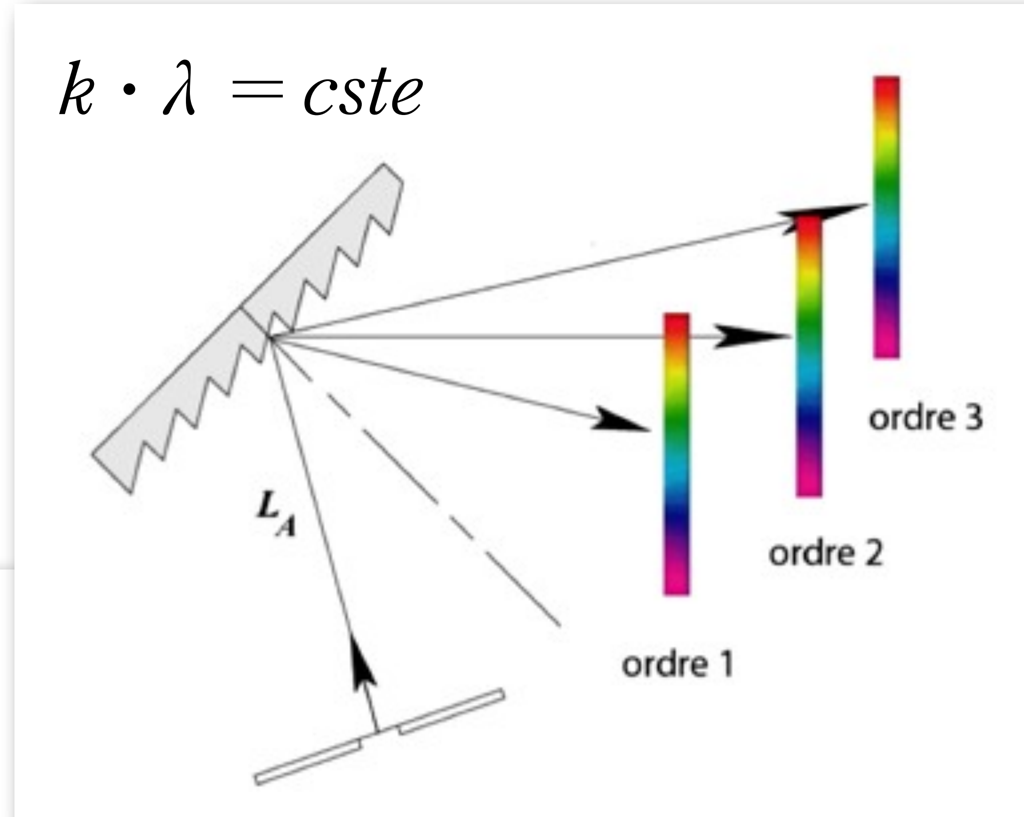
The image detector is placed in a plane which is not perpendicular to the axis defined by the central wavelength (to minimize the infuence of the aberrations).

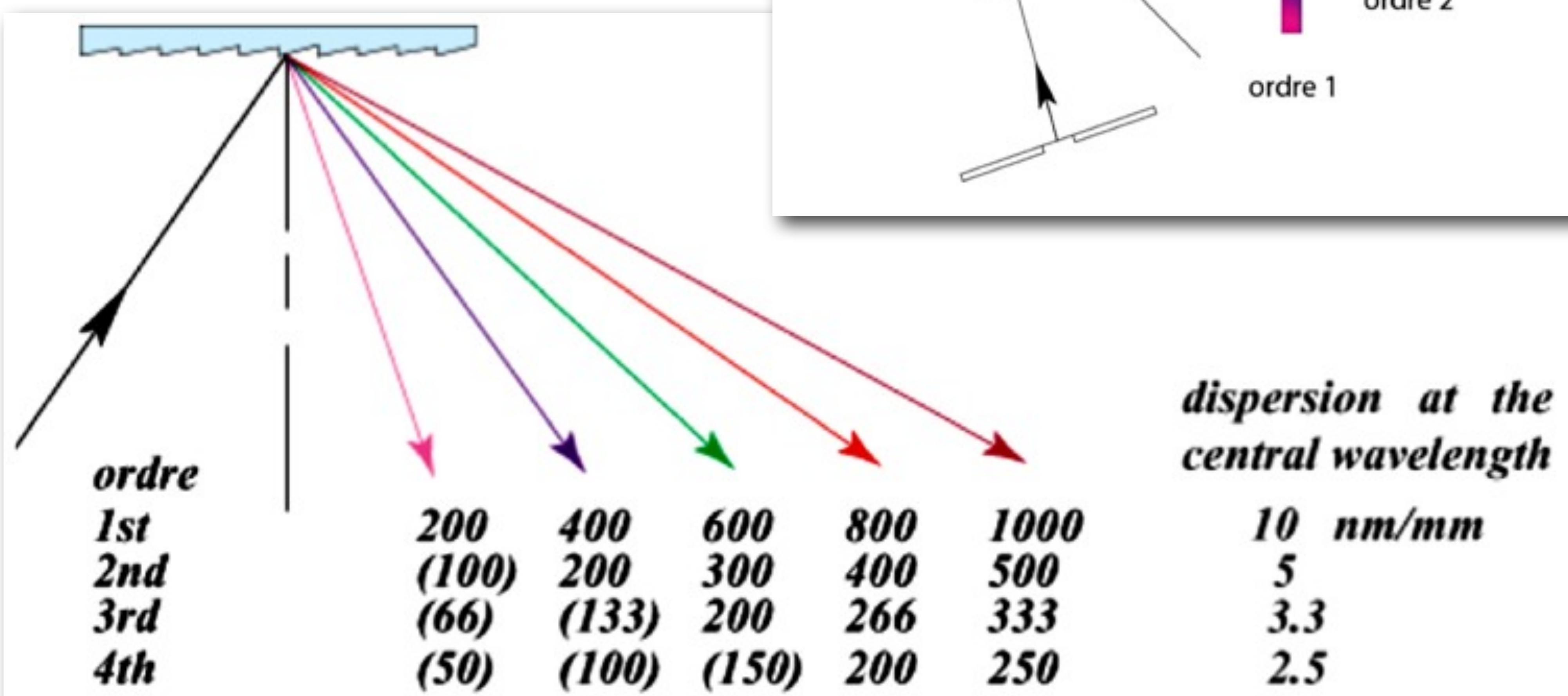


Grating spectrometer

Superposition of the different orders of diffraction

- cannot be avoided
- the use of blocking filter can help





ordre						dispersion at the central wavelength
1st	200	400	600	800	1000	10 nm/mm
2nd	(100)	200	300	400	500	5
3rd	(66)	(133)	200	266	333	3.3
4th	(50)	(100)	(150)	200	250	2.5

Grating spectrometer

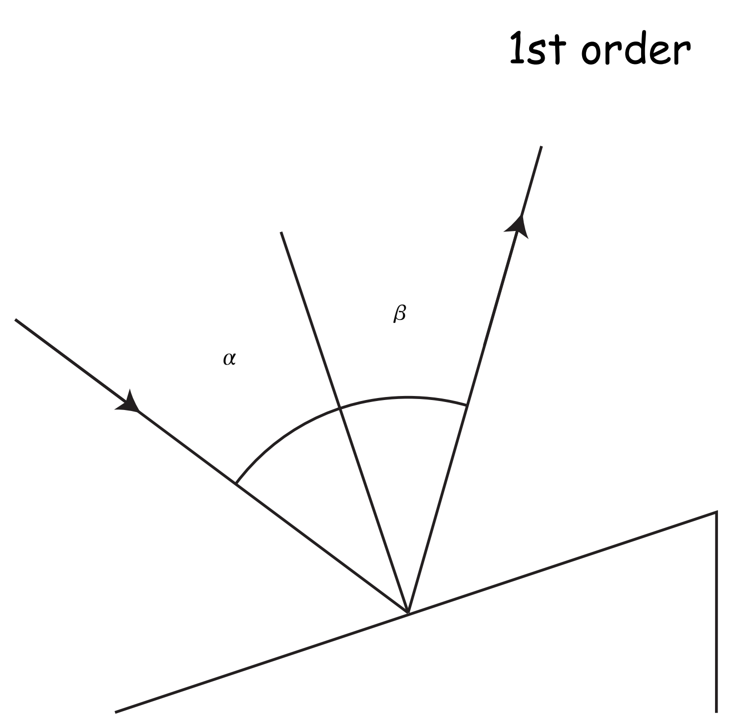
angular dispersion and intrinsic resolvance

$$\Re_0 = \frac{\lambda}{\Delta\lambda} = w_g'' \frac{d\beta}{d\lambda}$$

$$\Re_0 = \frac{\lambda}{\Delta\lambda} = w_g'' \frac{k \cdot n \cdot 10^{-6}}{\cos\beta} = w_g \cdot k \cdot n = k \cdot N$$

$$\Re_0 = \frac{\lambda}{\Delta\lambda} = w_g \cdot \frac{\sin(\alpha) + \sin(\beta)}{10^{-6} \cdot \lambda}$$

blazed gratings

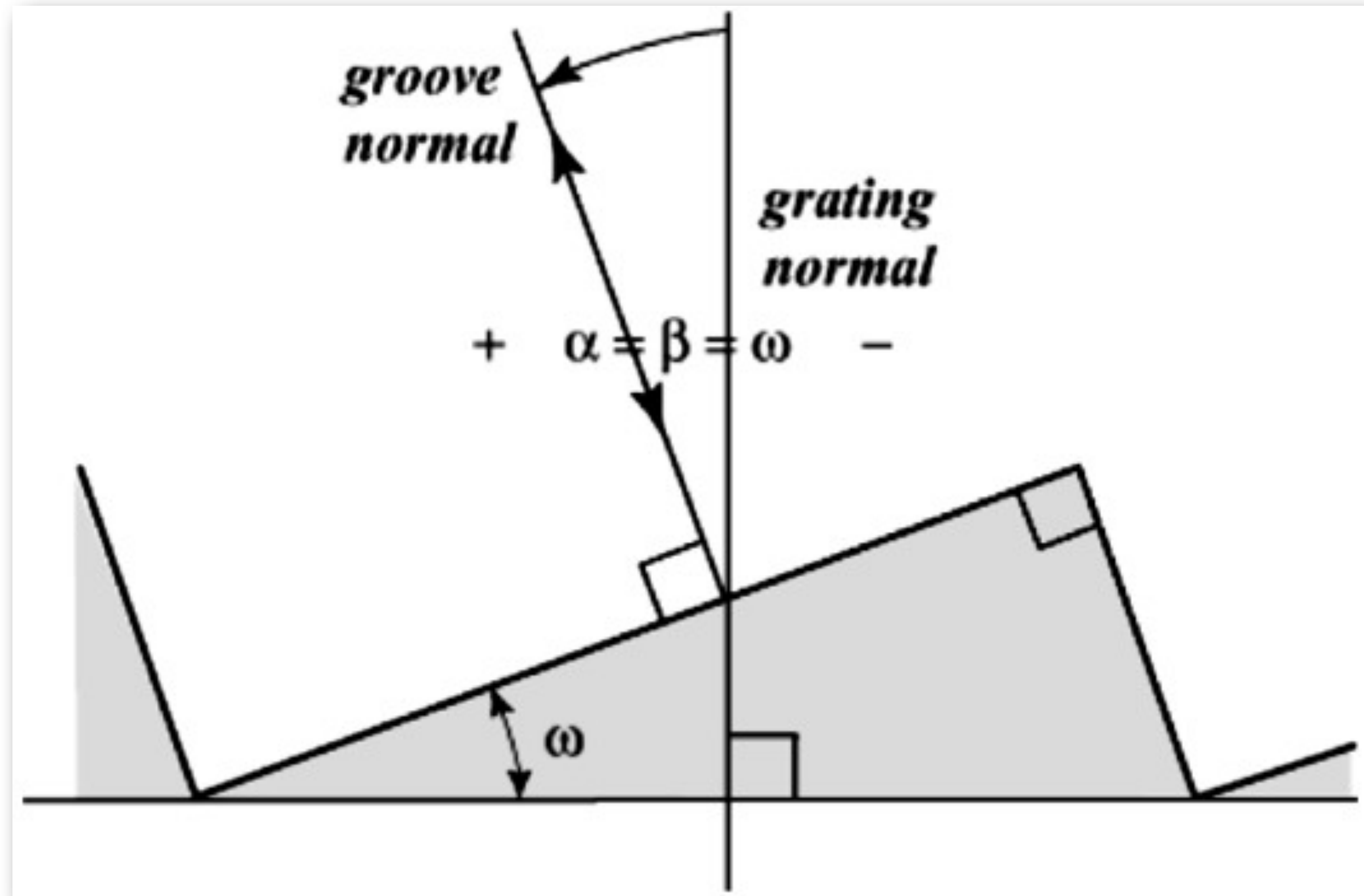


it is possible to concentrate most of the diffracted energy in the first order for a given wavelength if $|\alpha| = |\beta|$

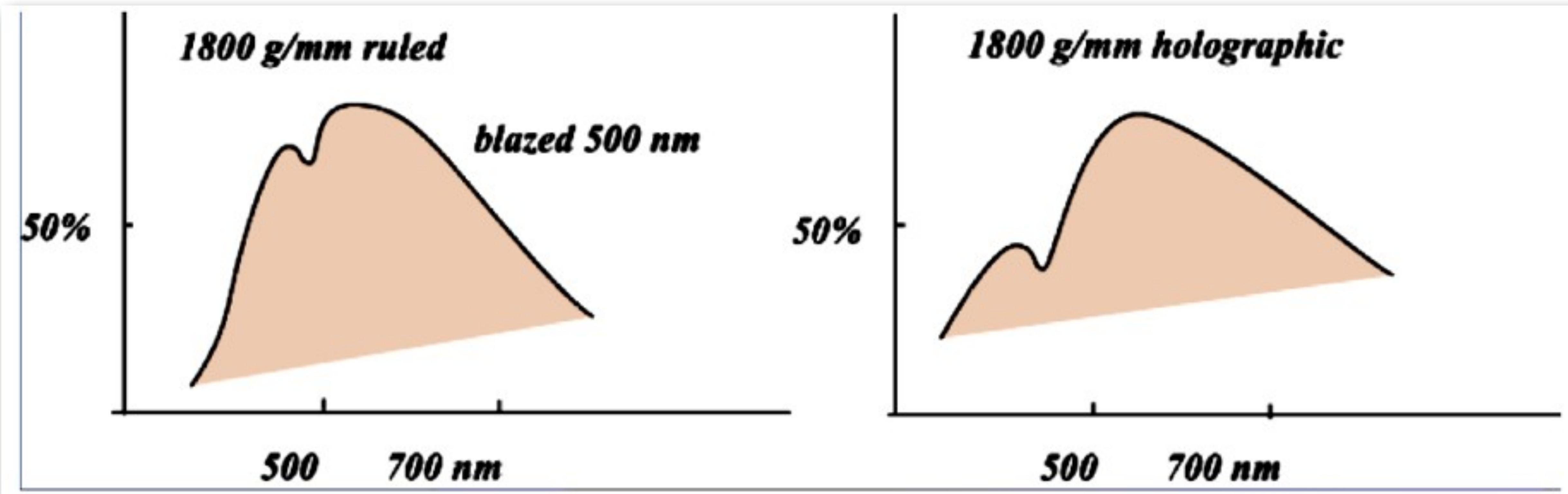
The grating equation shows that the angles of the diffracted orders only depend on the grooves' period, and not on their shape. By controlling the cross-sectional profile of the grooves, it is possible to concentrate most of the diffracted energy in a particular order for a given wavelength. A triangular profile is commonly used. This technique is called blazing

blazed gratings

Usually the blazed angle is defined for a Littrow configuration to be independent of the angle of total deflection (D_V is imposed by the geometry of the monochromator)



blazed gratings



Grating spectrometer

Ebert- Fastie design

- one concave mirror
- one planar grating
- slits are placed in the focal
- plane of the mirror

advantages

simple

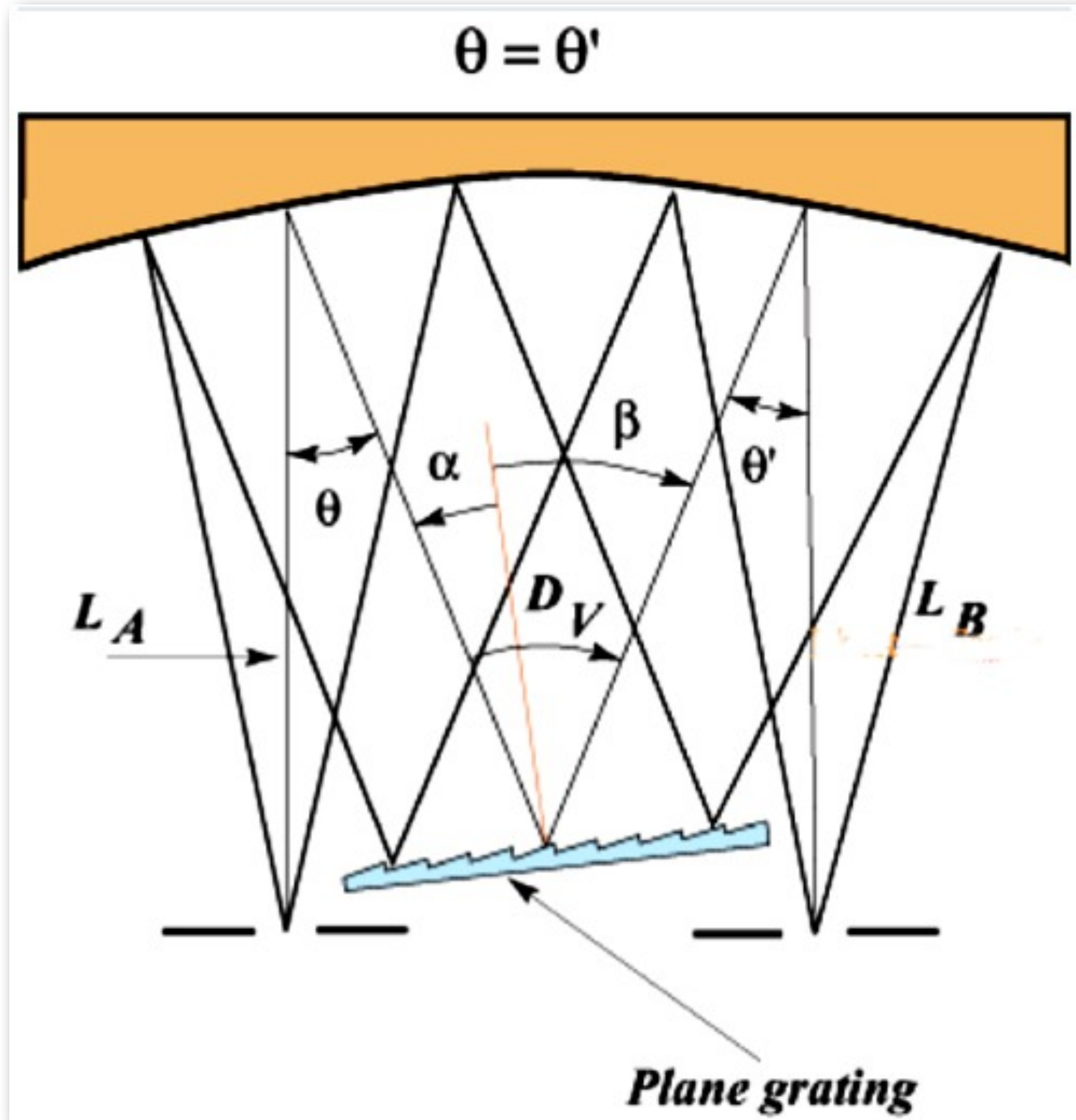
inexpensive

disadvantages

off-axis configuration,

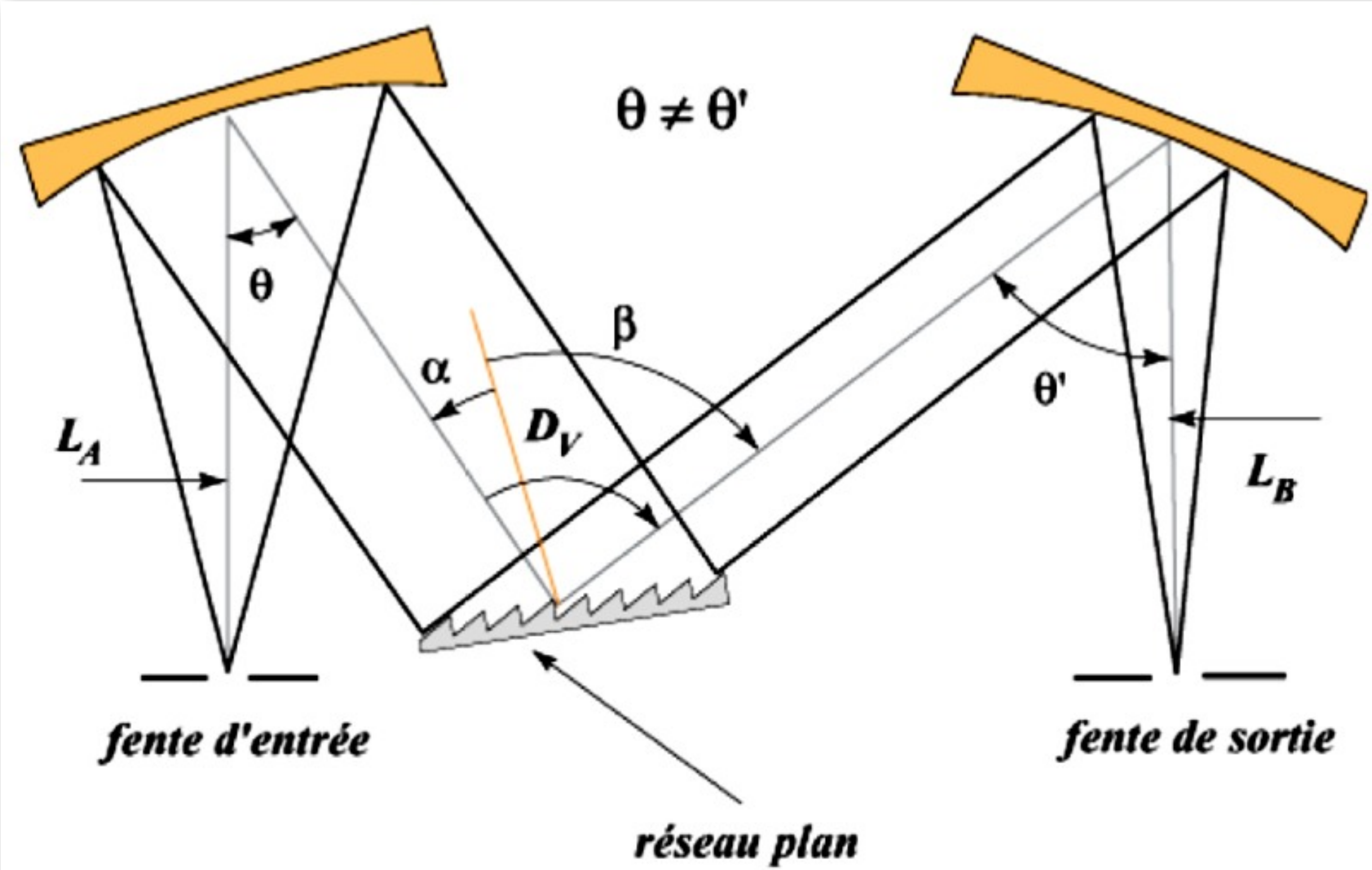
performances strongly limited

by aberrations



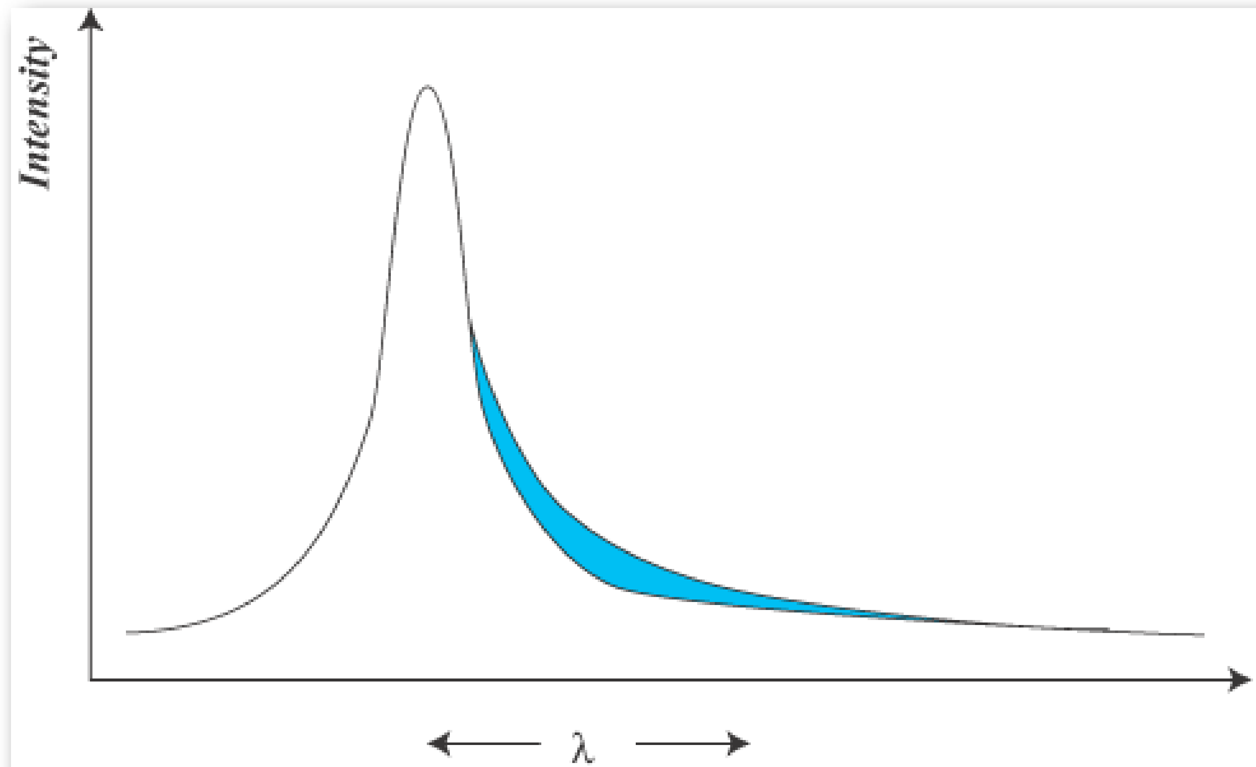
Grating spectrometer

Czerny - Turner

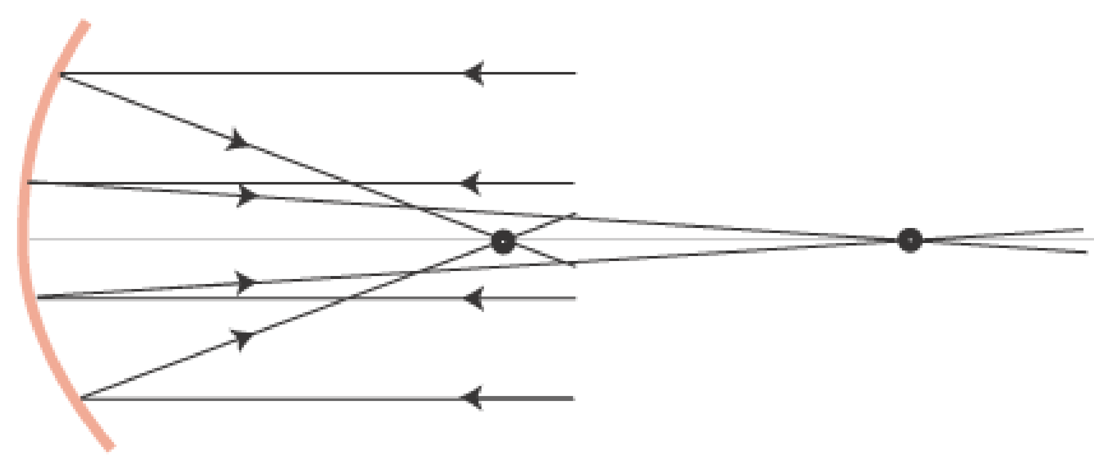


Grating spectrometer

Aberration in PGS systems

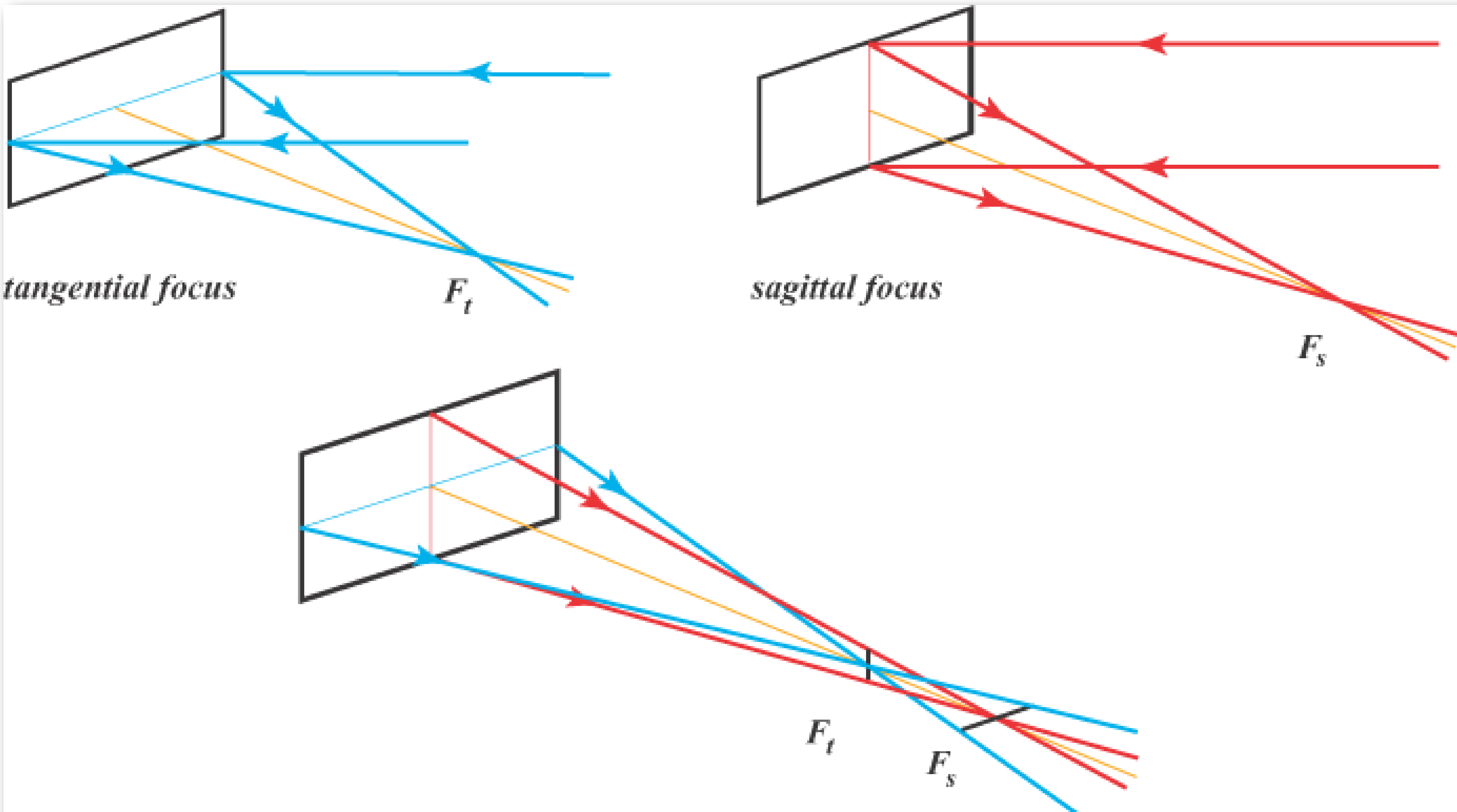


The effect of the Coma

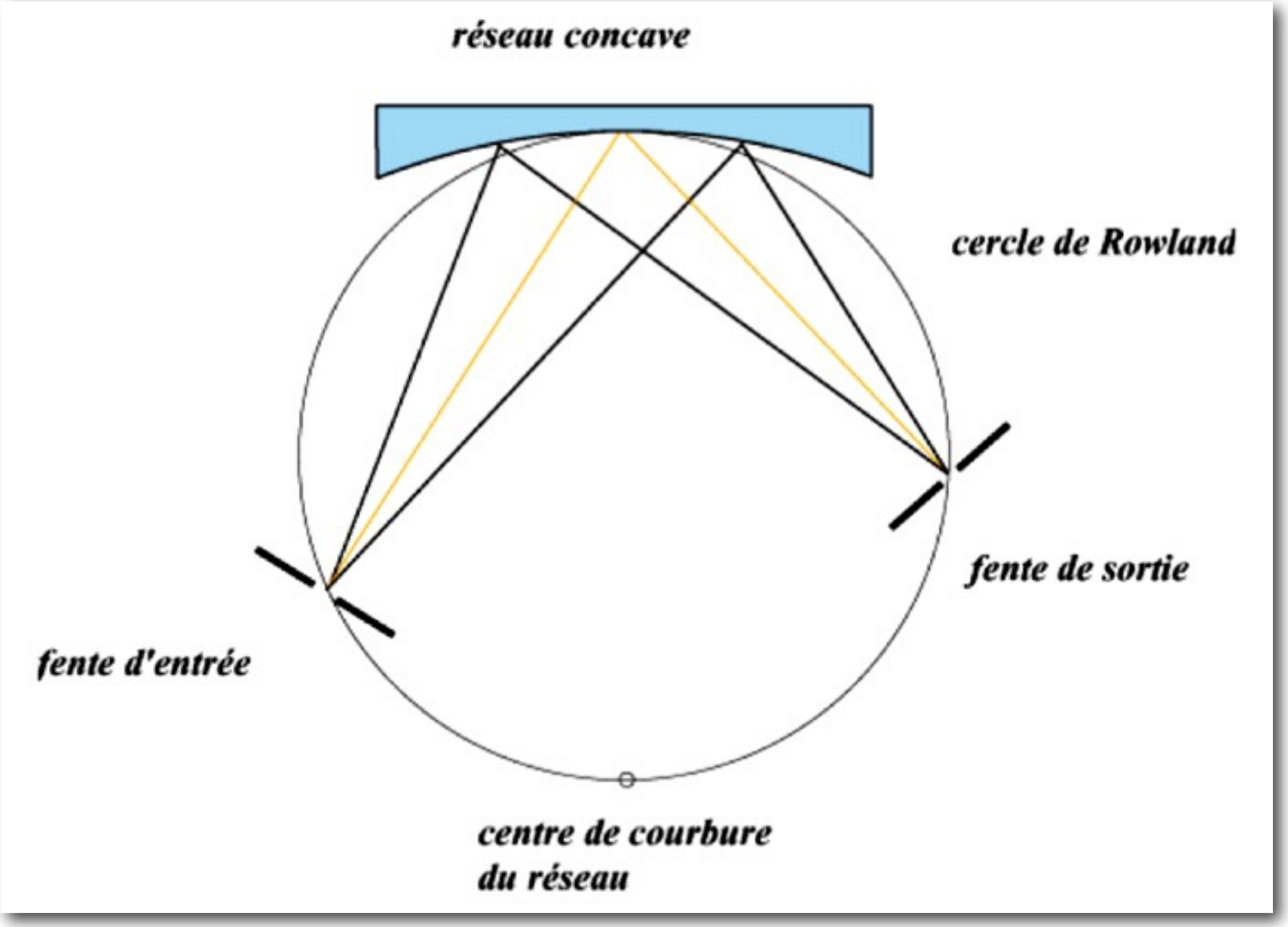


The effect of Spherical Aberration

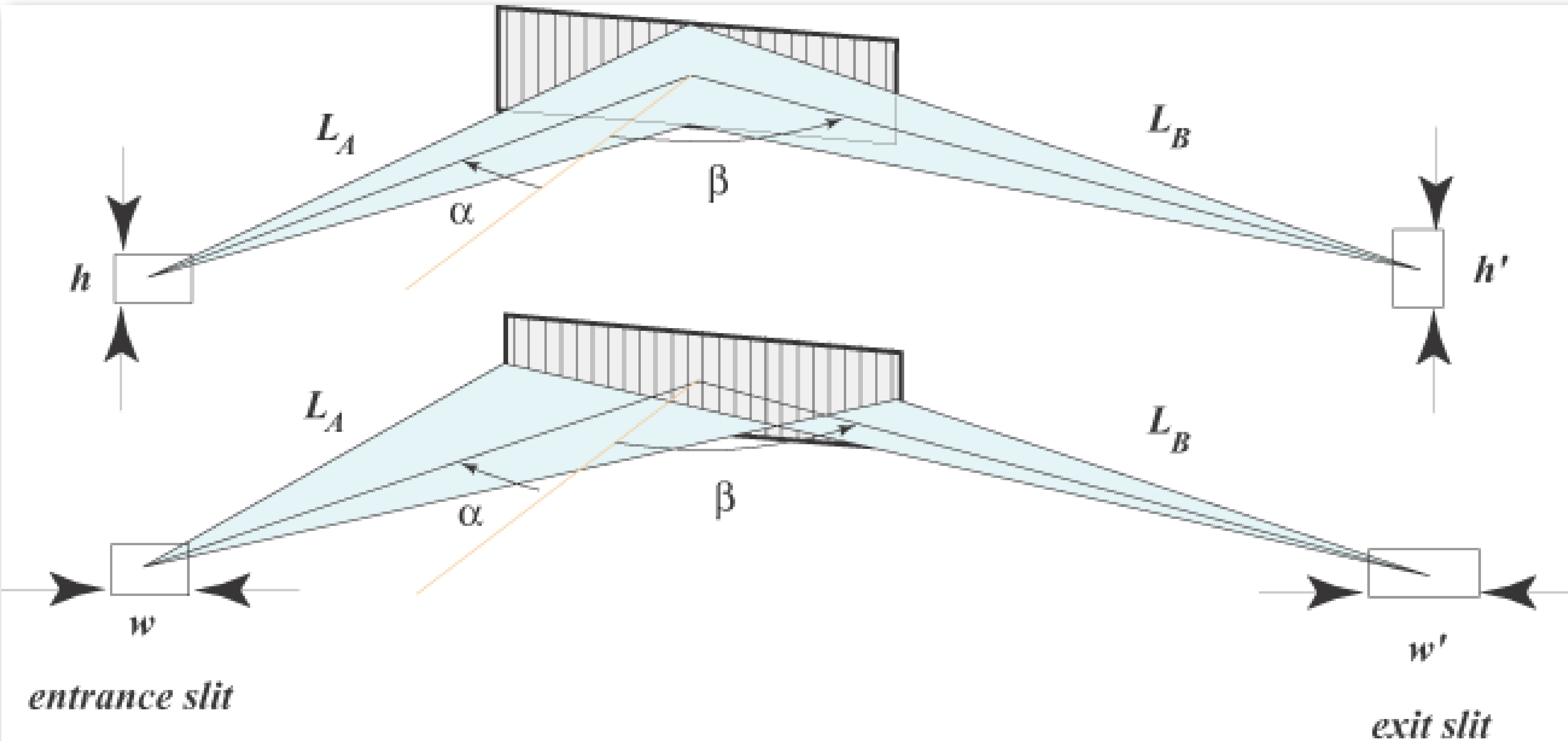
Aberration in PGS systems



Concave gratings (ACGH)

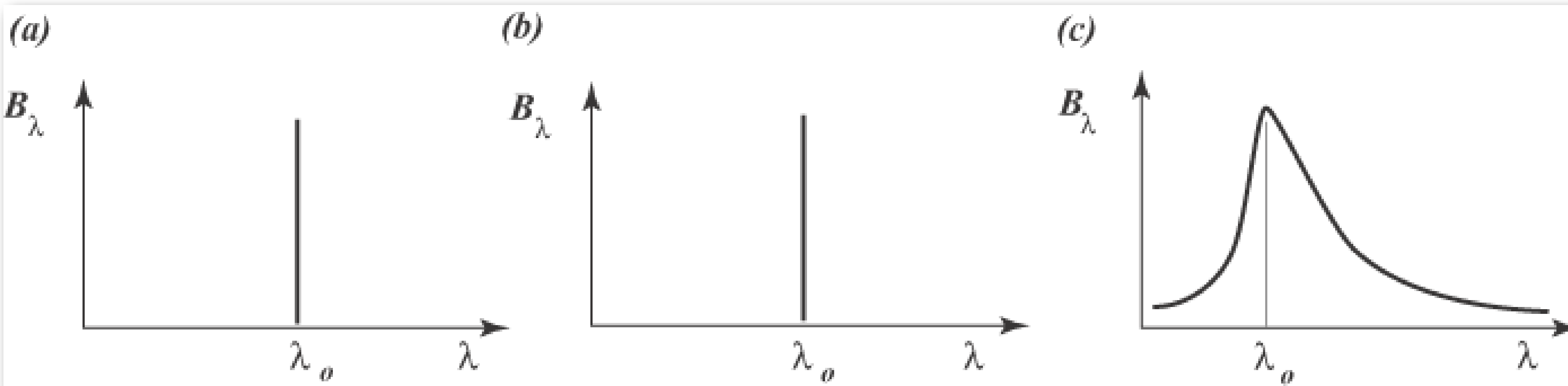


Anamorphism



Grating spectrometer

Bandpass and resolution

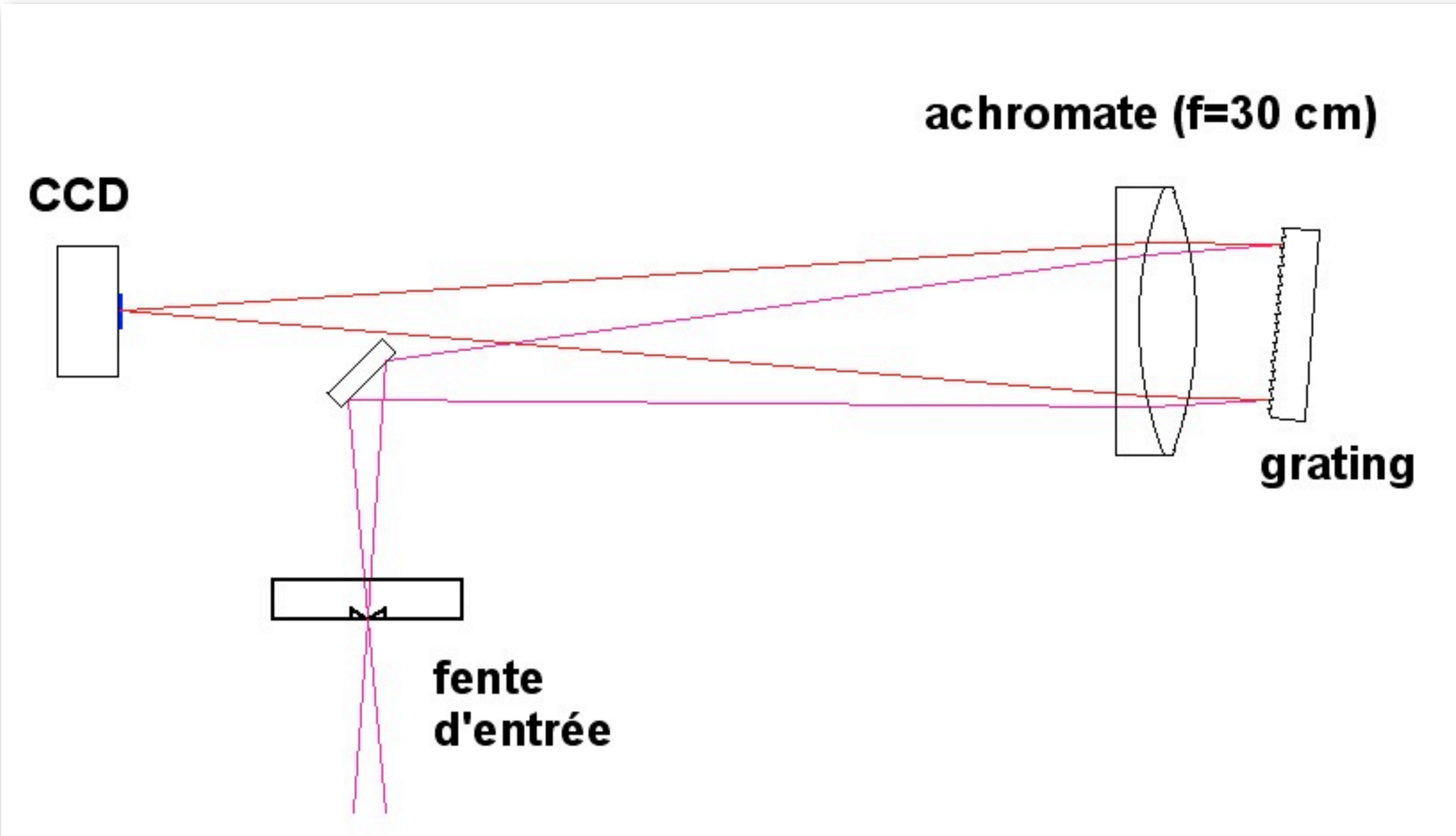


$$F(\lambda) = B(\lambda) \otimes P(\lambda)$$

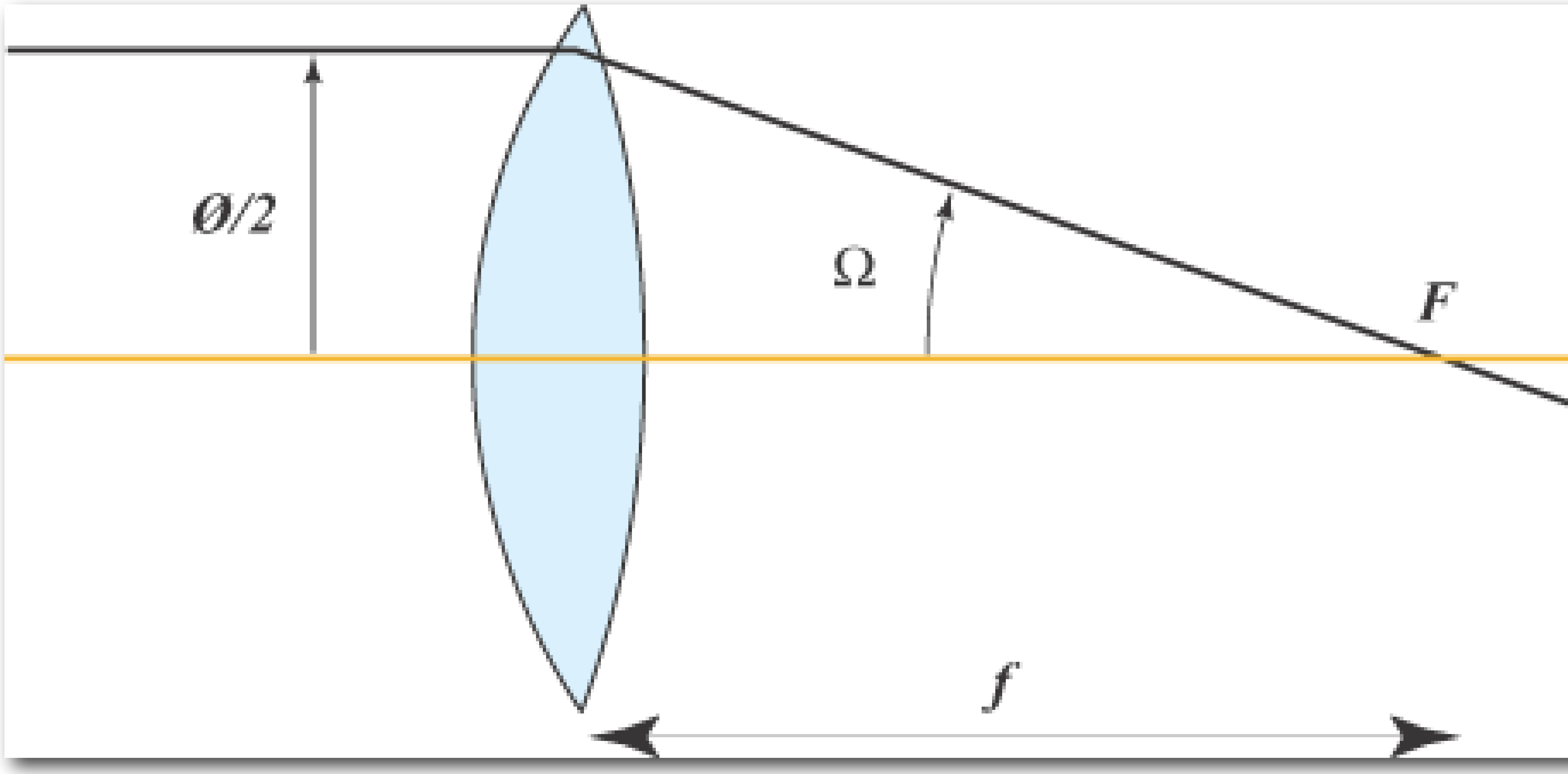
$$P(\lambda) = P_1(\lambda) \otimes P_2(\lambda) \otimes P_3(\lambda) \otimes P_4(\lambda) \otimes \ldots$$

Grating spectrometer

Quasi-littrow configuration



F - value

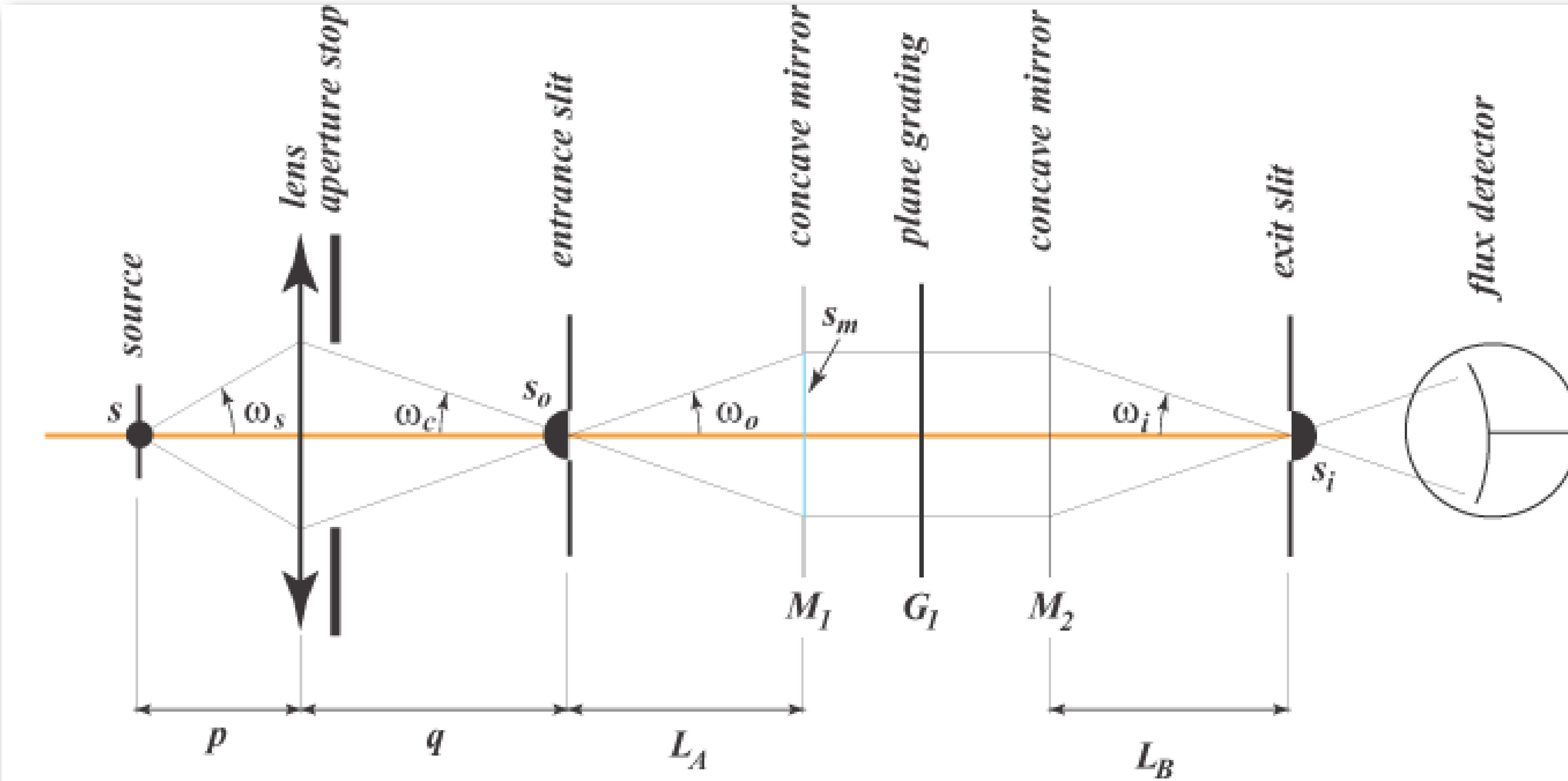


$$N.A. = \sin \Omega$$

$$f/value = \frac{1}{2\ NA}$$

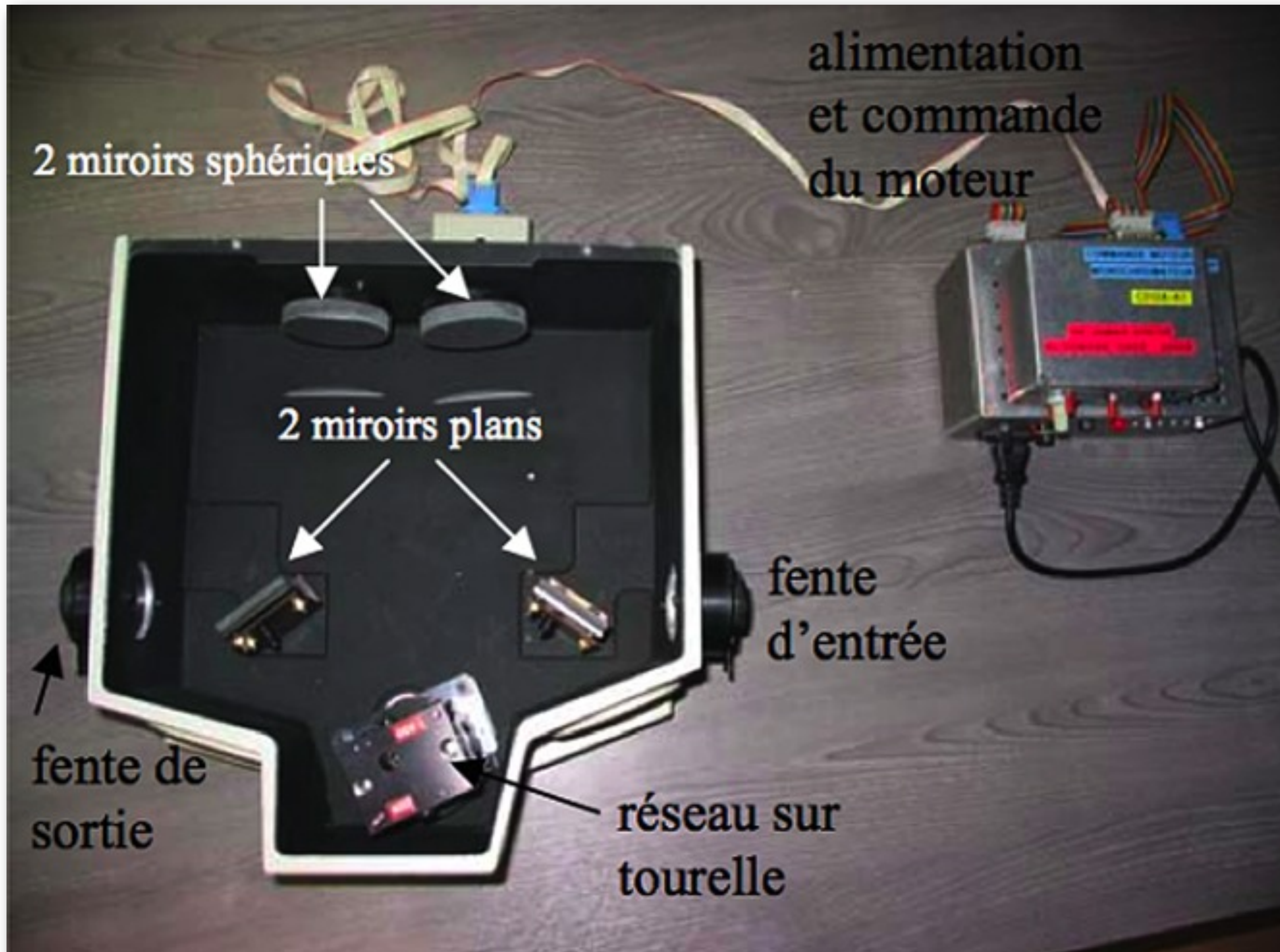
Grating spectrometer

Radiometry and spectrometry ... geometry extent



Grating spectrometer

One example: Jobin-Yvon HR 250



Grating spectrometer

Examples: Triax Series

Specifications

TRIAX180:

Imaging Monochromator/Spectrograph

1 entrance port, 1 exit port

Focal length: 190 mm, f number: F/3.9

Dispersion: 3.6 nm/mm

Resolution: 0.3 nm

TRIAX190:

Imaging Monochromator/Spectrograph

1 entrance port, 2 exit ports

Focal length: 190 mm, F number: F/3.9

Dispersion: 3.6 nm/mm

Resolution: 0.3 nm

TRIAX320:

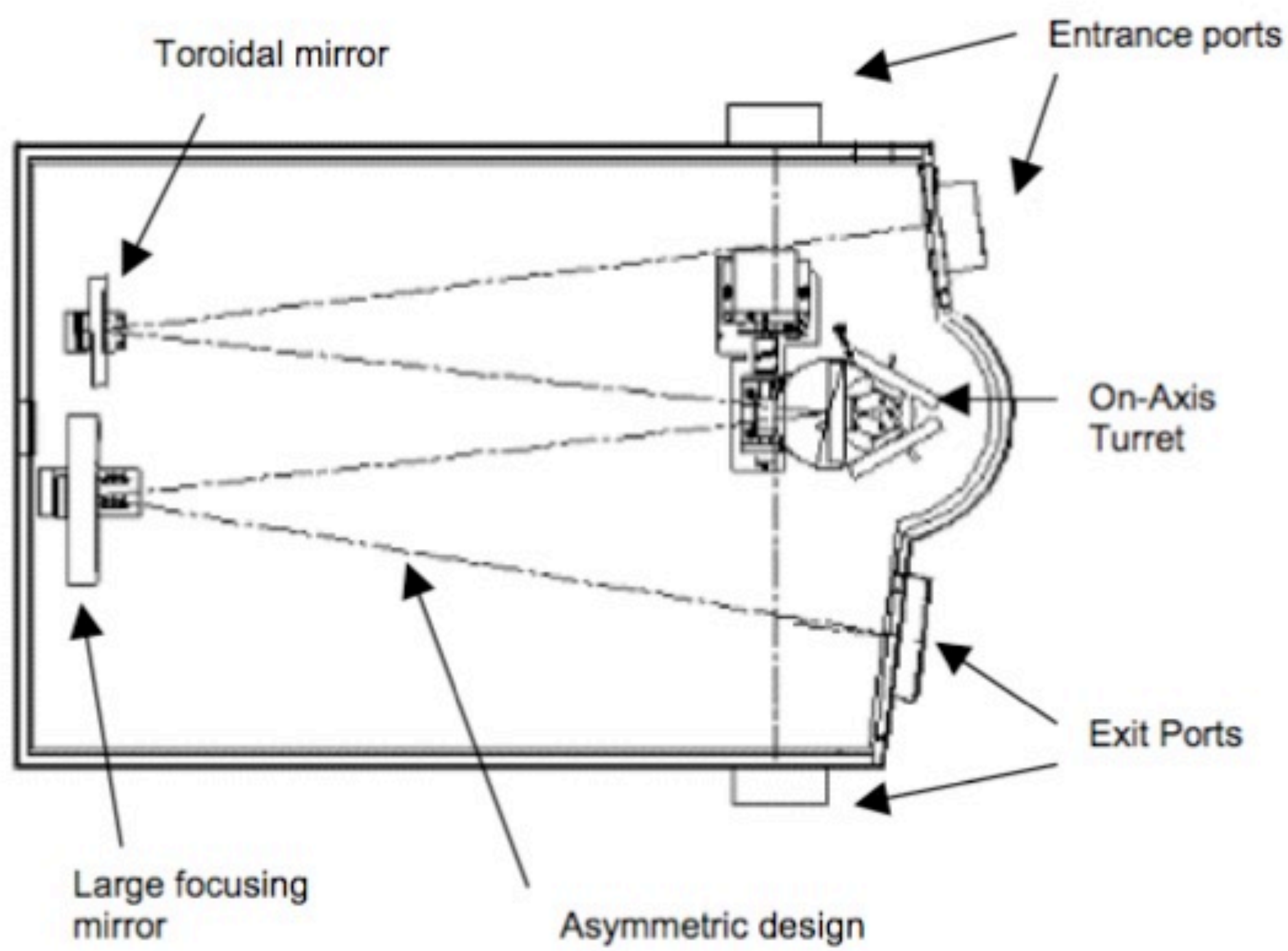
Imaging Monochromator/Spectrograph

Up to 2 entrance ports, 2 exit ports

Focal length: 320 mm, F number: F/4.1

Dispersion: 2.64 nm/mm

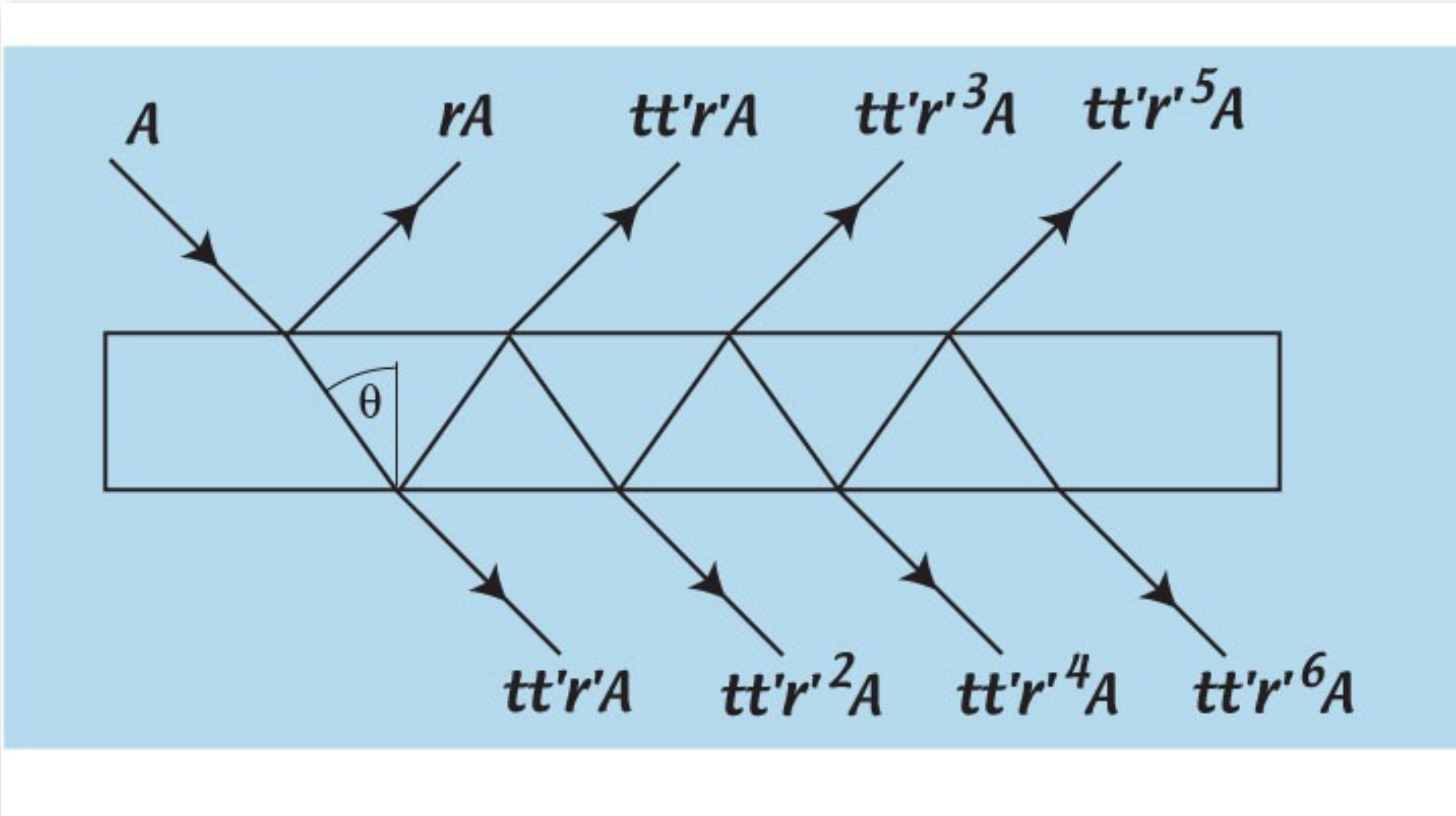
Resolution: 0.06 nm (microstep option)



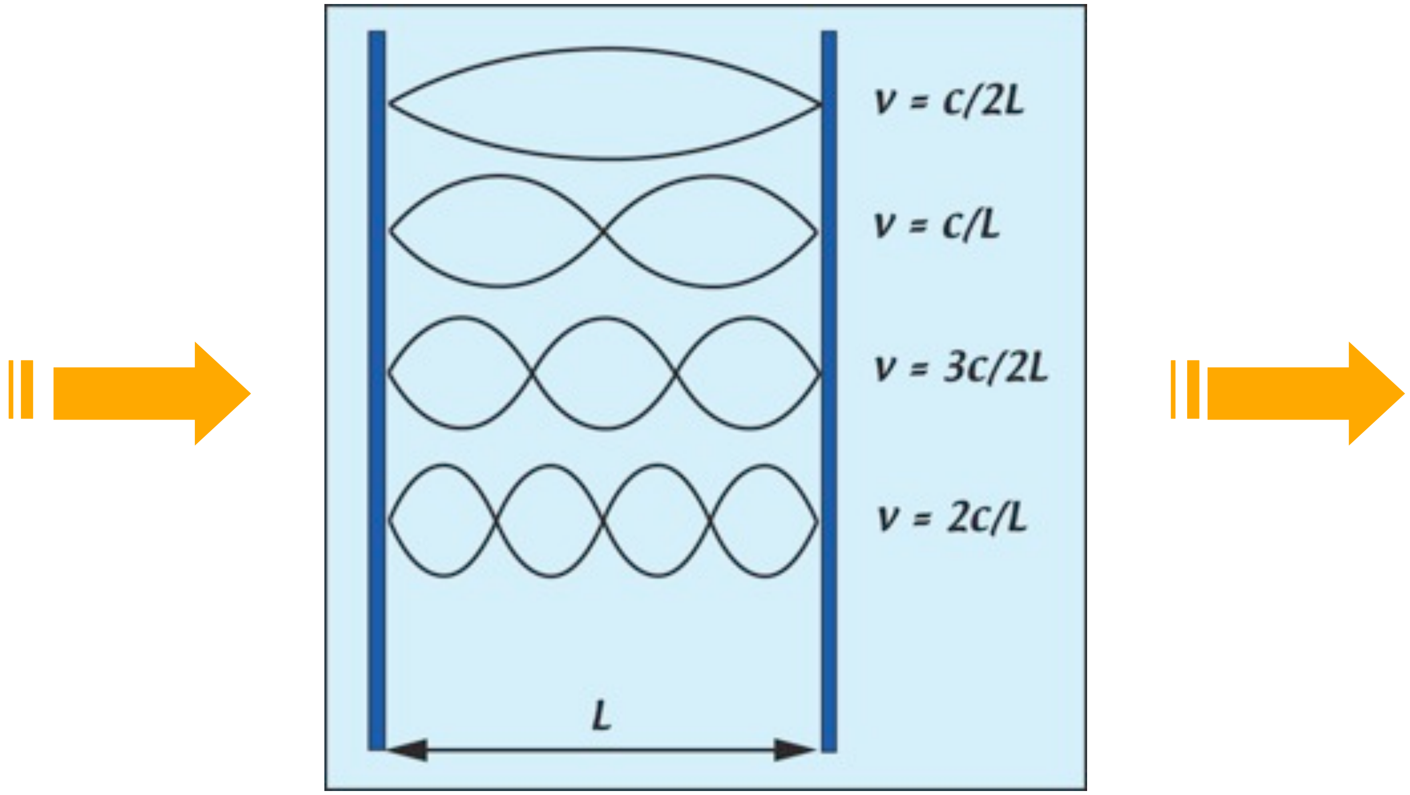
TRIAX 550

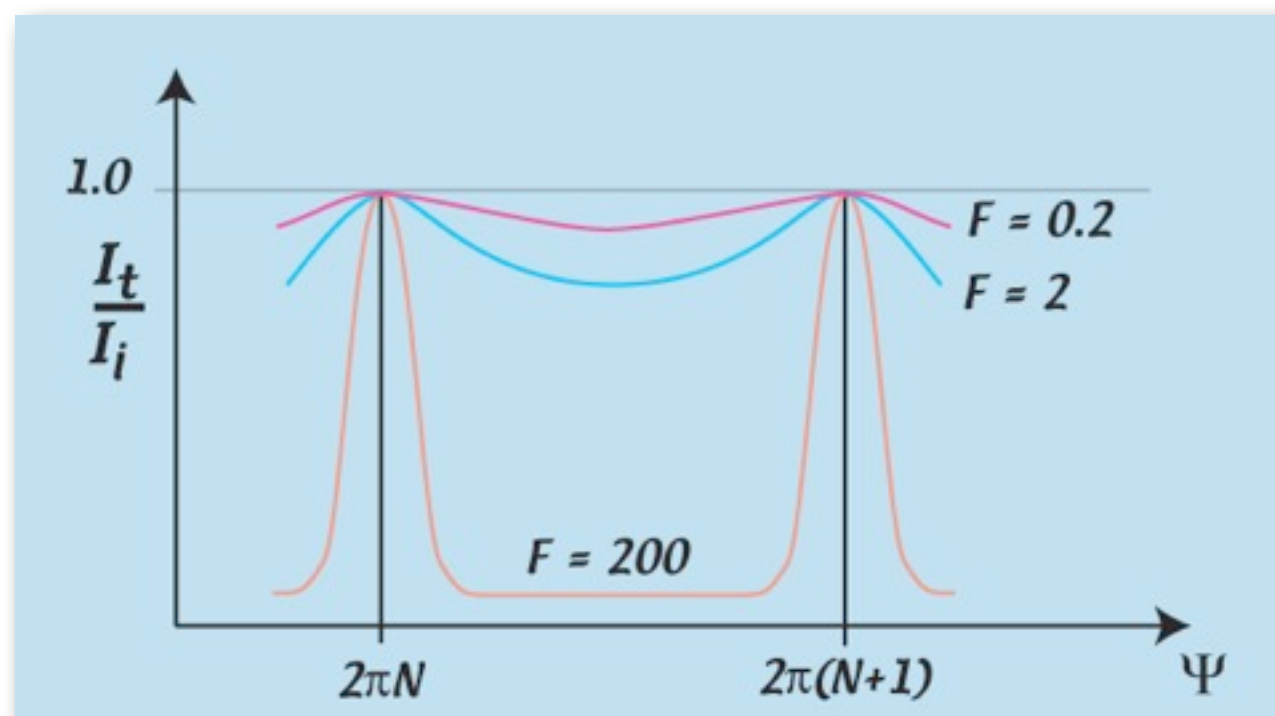
Keywords:

PF spectrometer [Fabry-Perot]

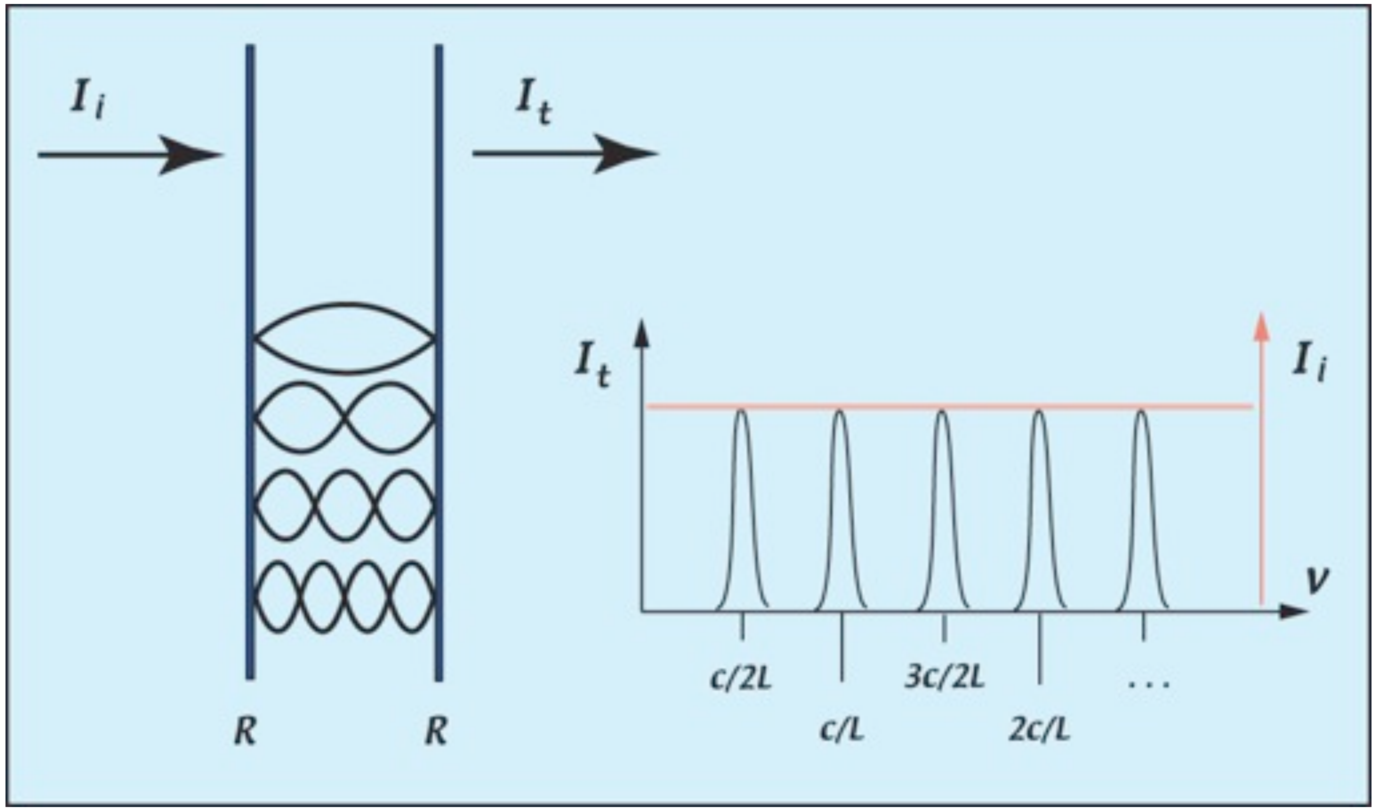


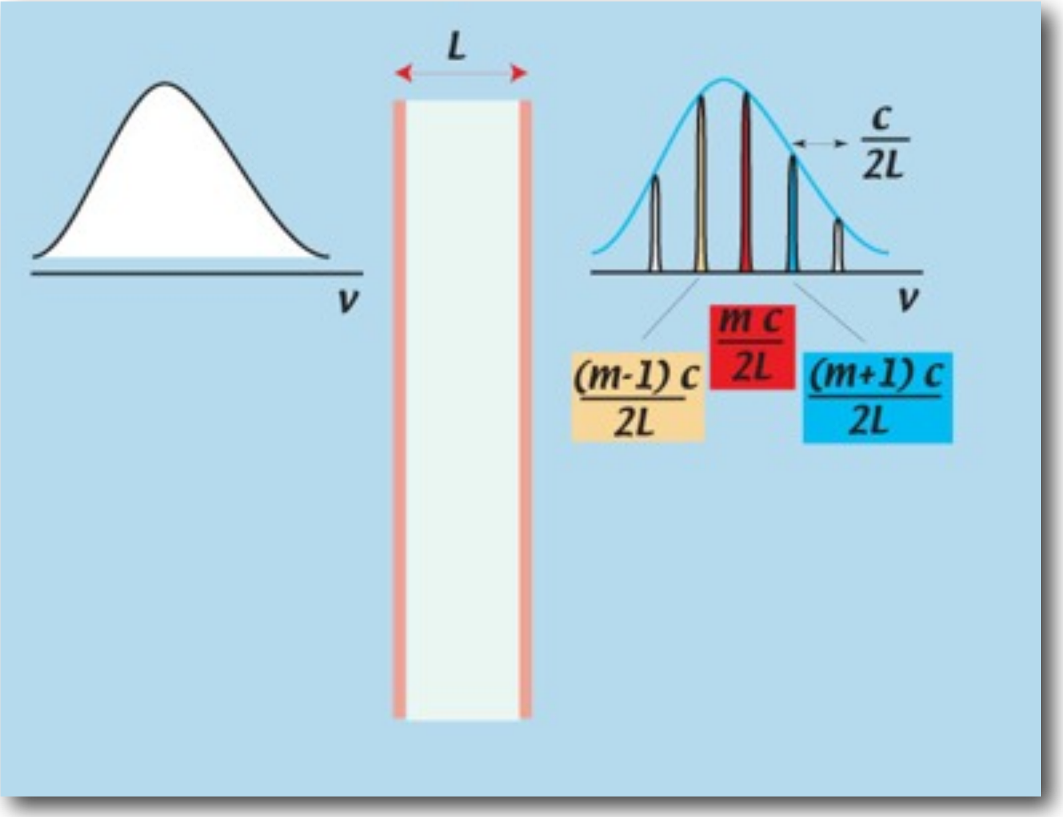
Interferential spectrometer



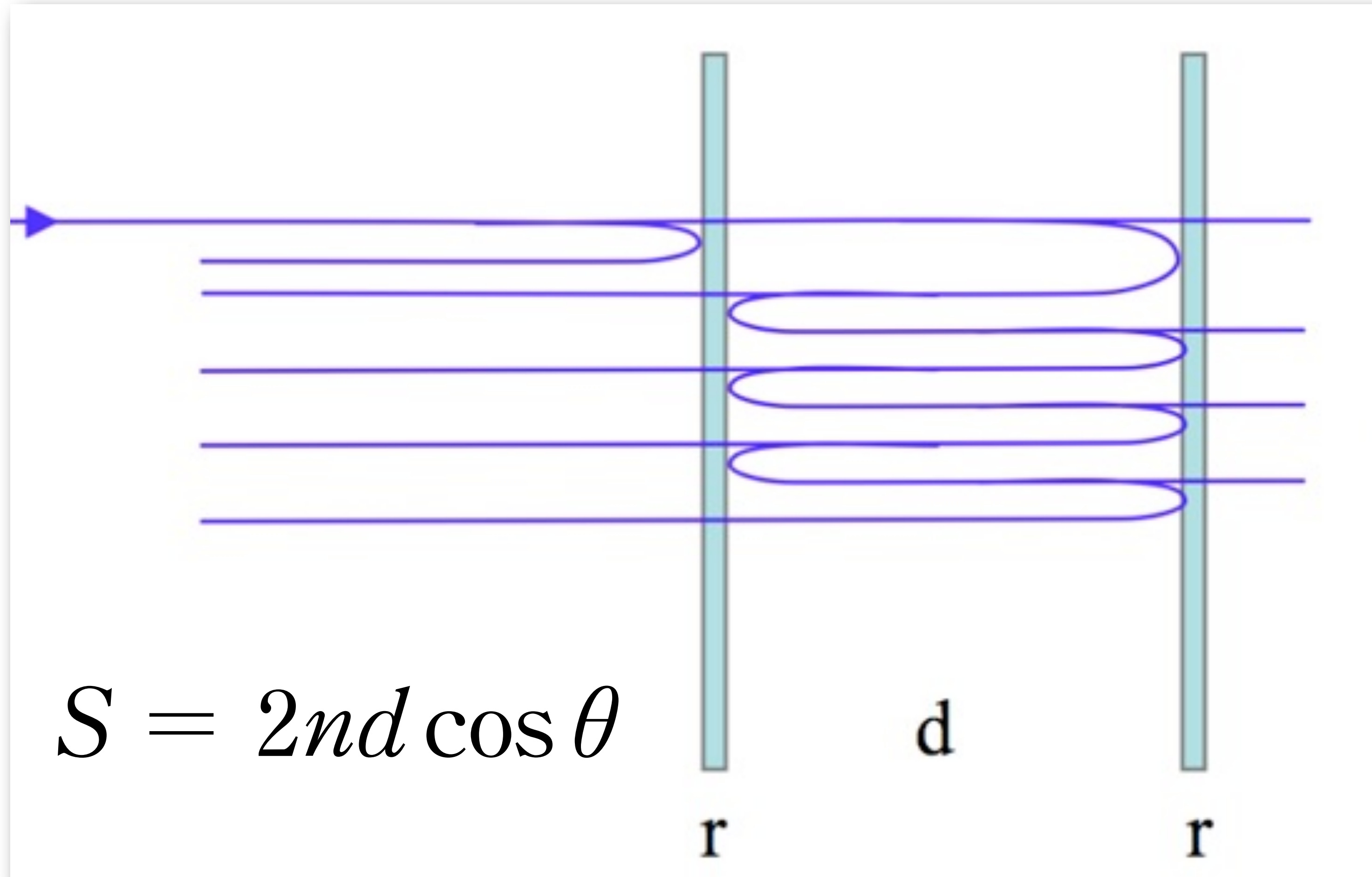


Iterferential spectrometer





Interferential spectrometer



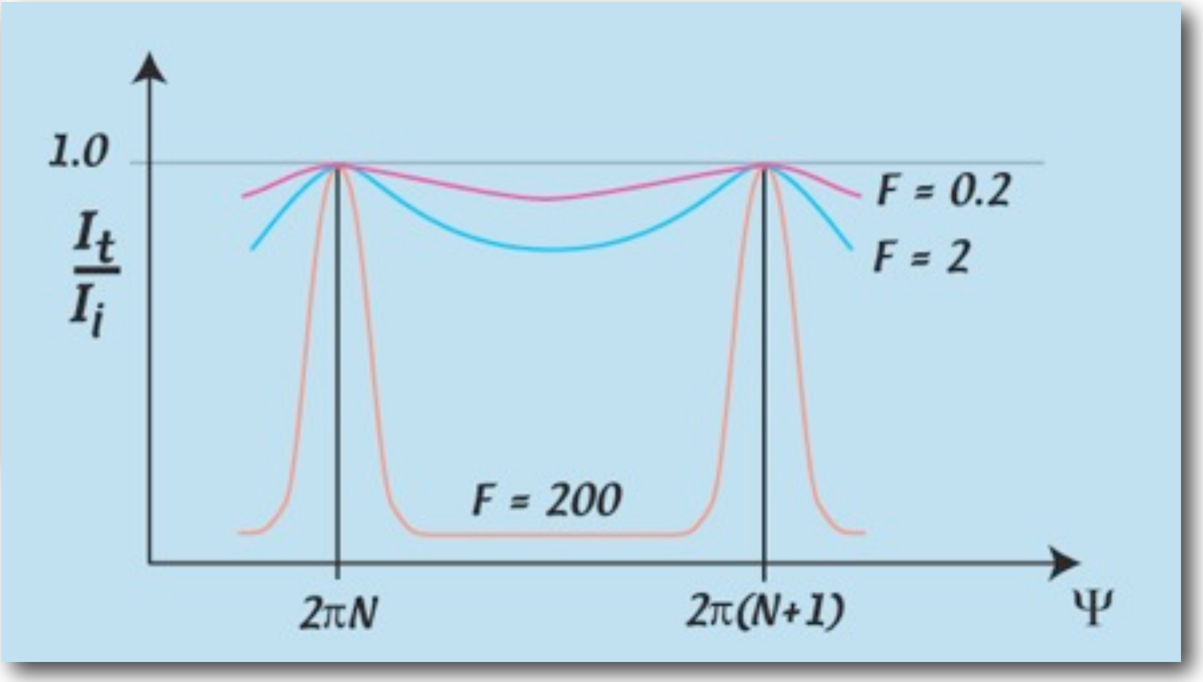
$$E_{trans} = E_{inc}\left[tt + trrte^{-jk_0S} + trrrrte^{-jk_0 2S} + \ldots\right]$$

Interferential spectrometer

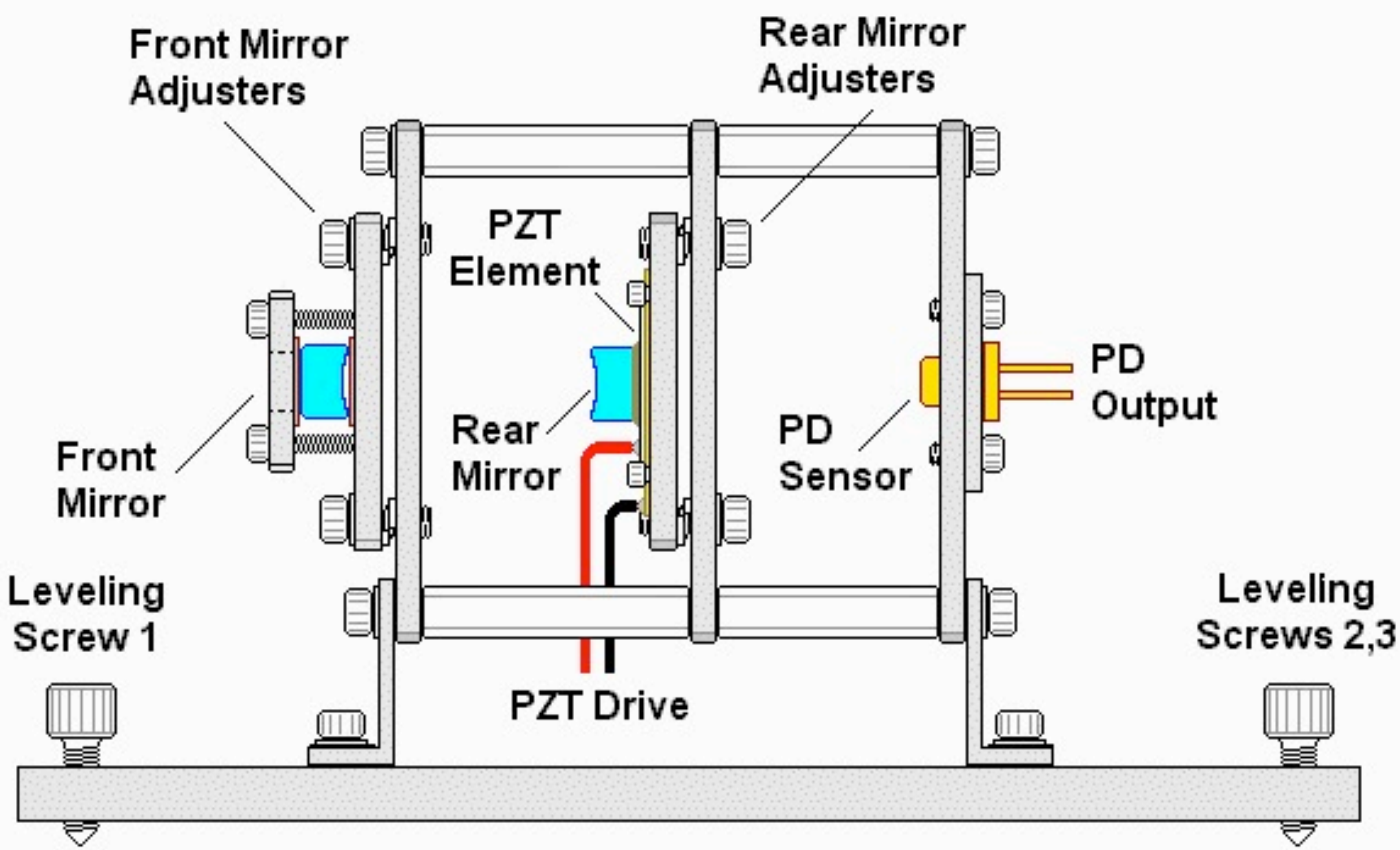
$$avec\ R = |r|^2\ et\ T = |t|^2$$

$$F = \frac{4R}{(1-R)^2} \qquad \nu_0 = \frac{c}{S} = \frac{c}{2nd\cos\theta}$$

$$\frac{I_{trans}}{I_{inc}} = \frac{1}{1 + F\sin^2\left(\frac{\pi\nu}{\nu_0}\right)}$$



Interferential spectrometer



Home-Built Scanning Fabry-Perot Interferometer 1

Interferential spectrometer

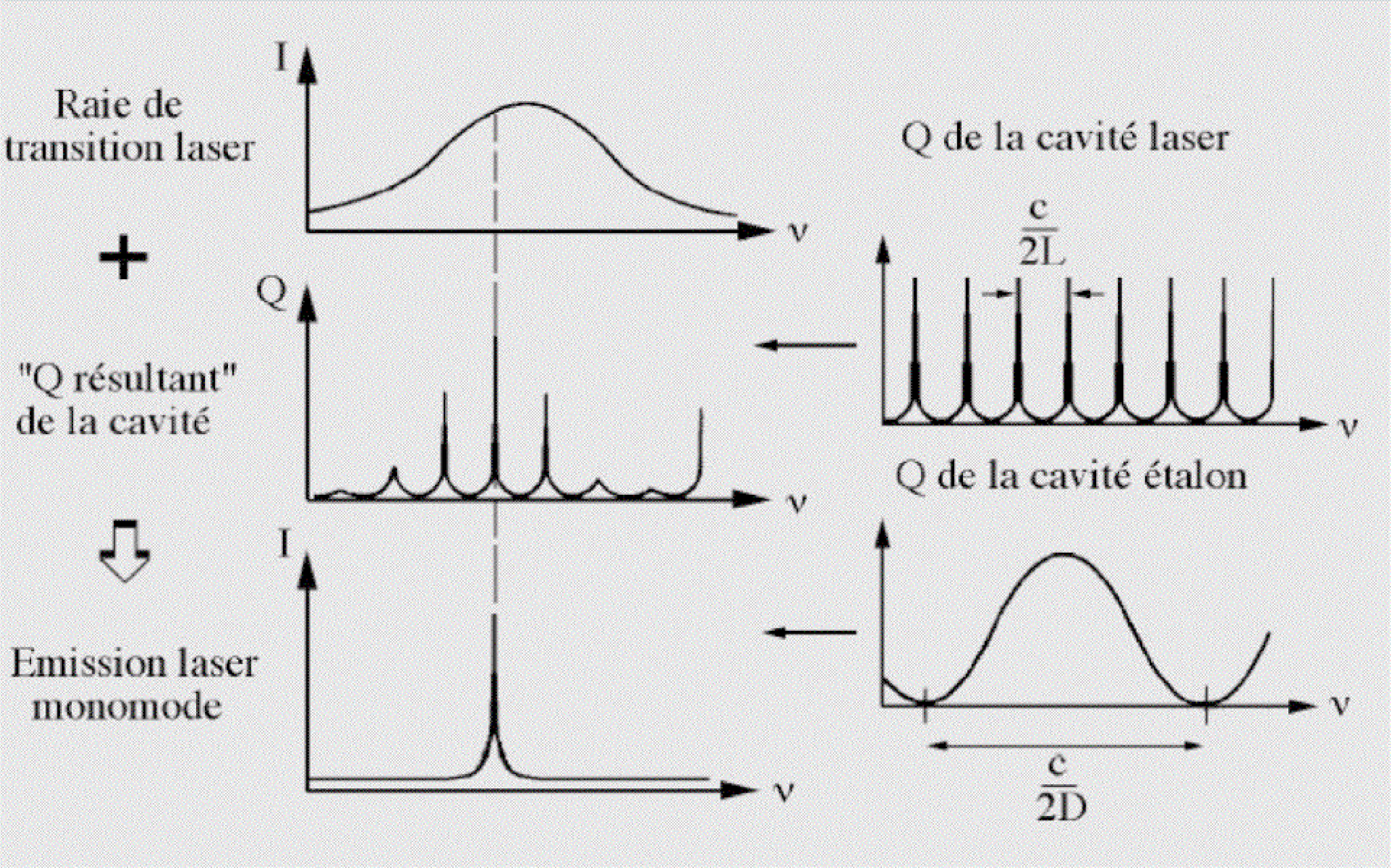
$$FWHM = \frac{2}{\pi}\sin^{-1}\left(\frac{1}{\sqrt{F}}\right) \approx \frac{2}{\pi\sqrt{F}} = \frac{1}{\xi}$$

finesse

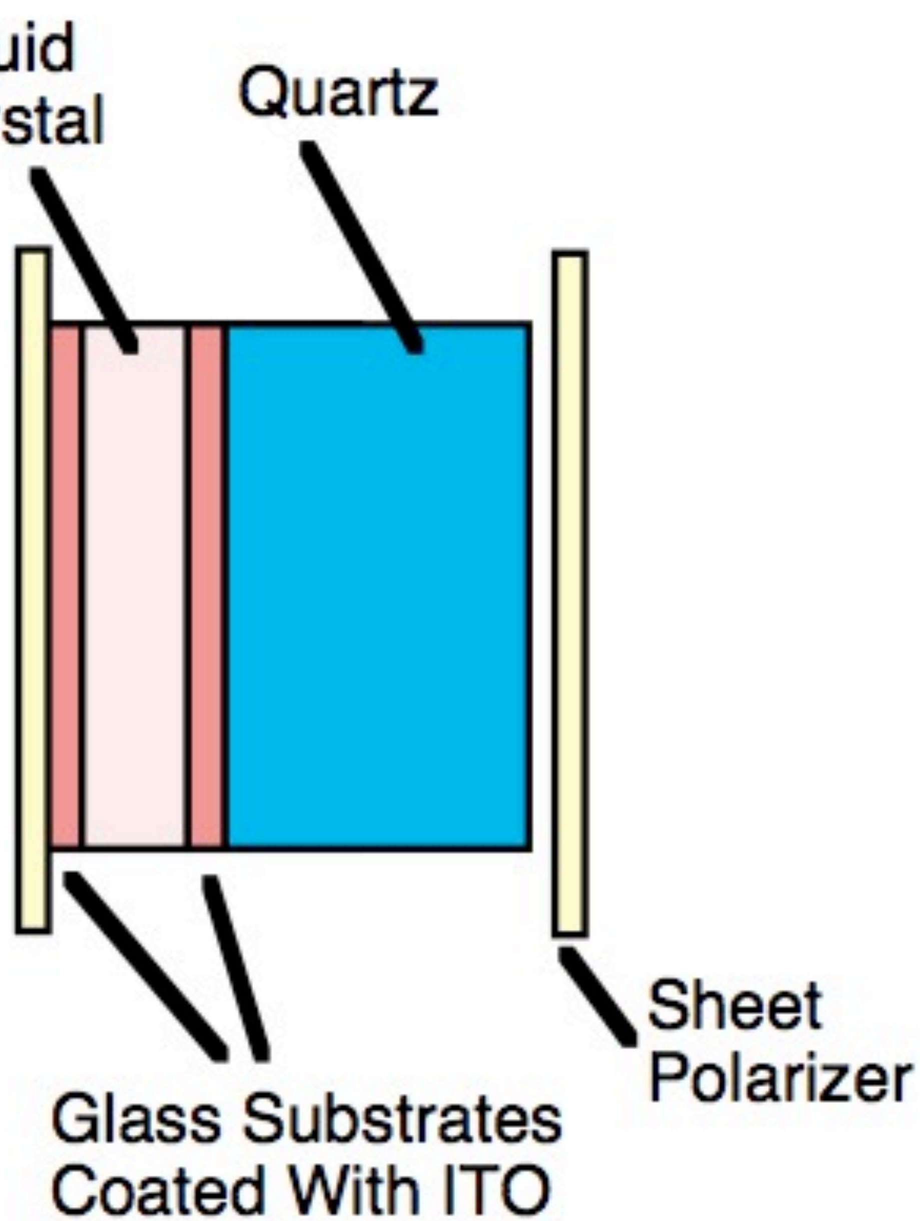
$$\Re = \frac{\nu}{\Delta\nu} = \frac{\nu}{\nu_0}\cdot\frac{1}{FWHM} = \frac{\nu}{\nu_0}\cdot\xi = m\cdot\xi$$

F=380, ξ = 30.6, ν_0= 15 GHz, m = 40000 → $\Re$ = 1.2 10^6

Interferential spectrometer



Hyperspectral spectrometer LCPF



$\Delta n = n_e - n_o$ Birefringence

$\Gamma = d\Delta n$ Retardance

$\Gamma_{Total} = \Gamma_{LC} + \Gamma_{Quartz}$

$\delta = 2\pi\Gamma_{Total} / \lambda$ Phase delay

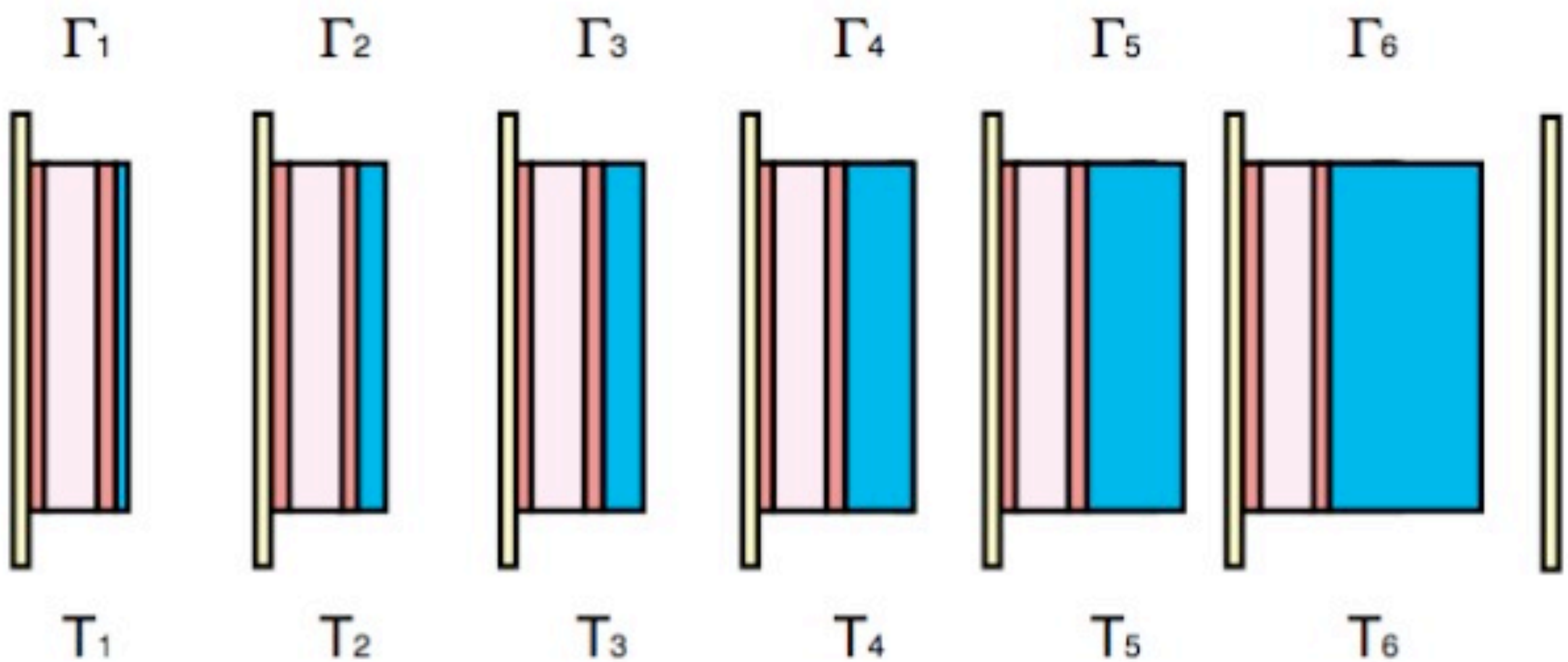
$T(\lambda) = \cos^2 \delta$

$T(\lambda) = \cos^2 (2\pi d\Delta n/\lambda)$

$T = 1;\ m\lambda = d\Delta n$
for integer m

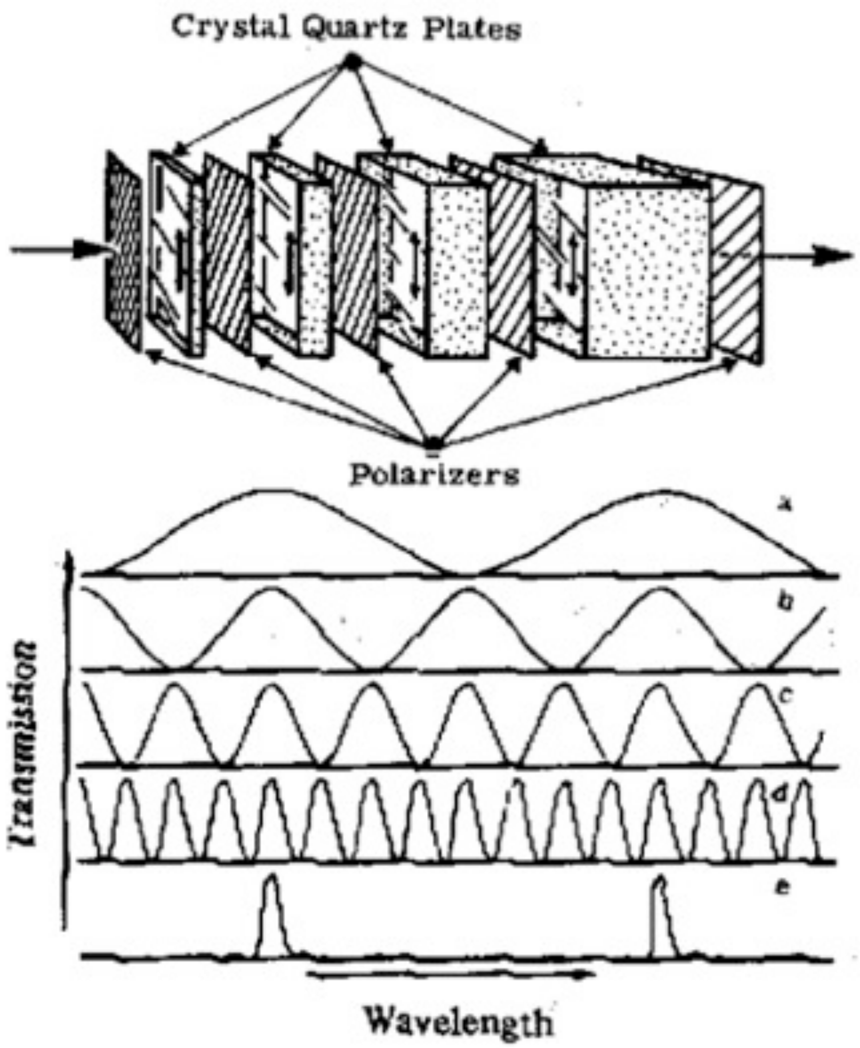
Interferential spectrometer LCPF

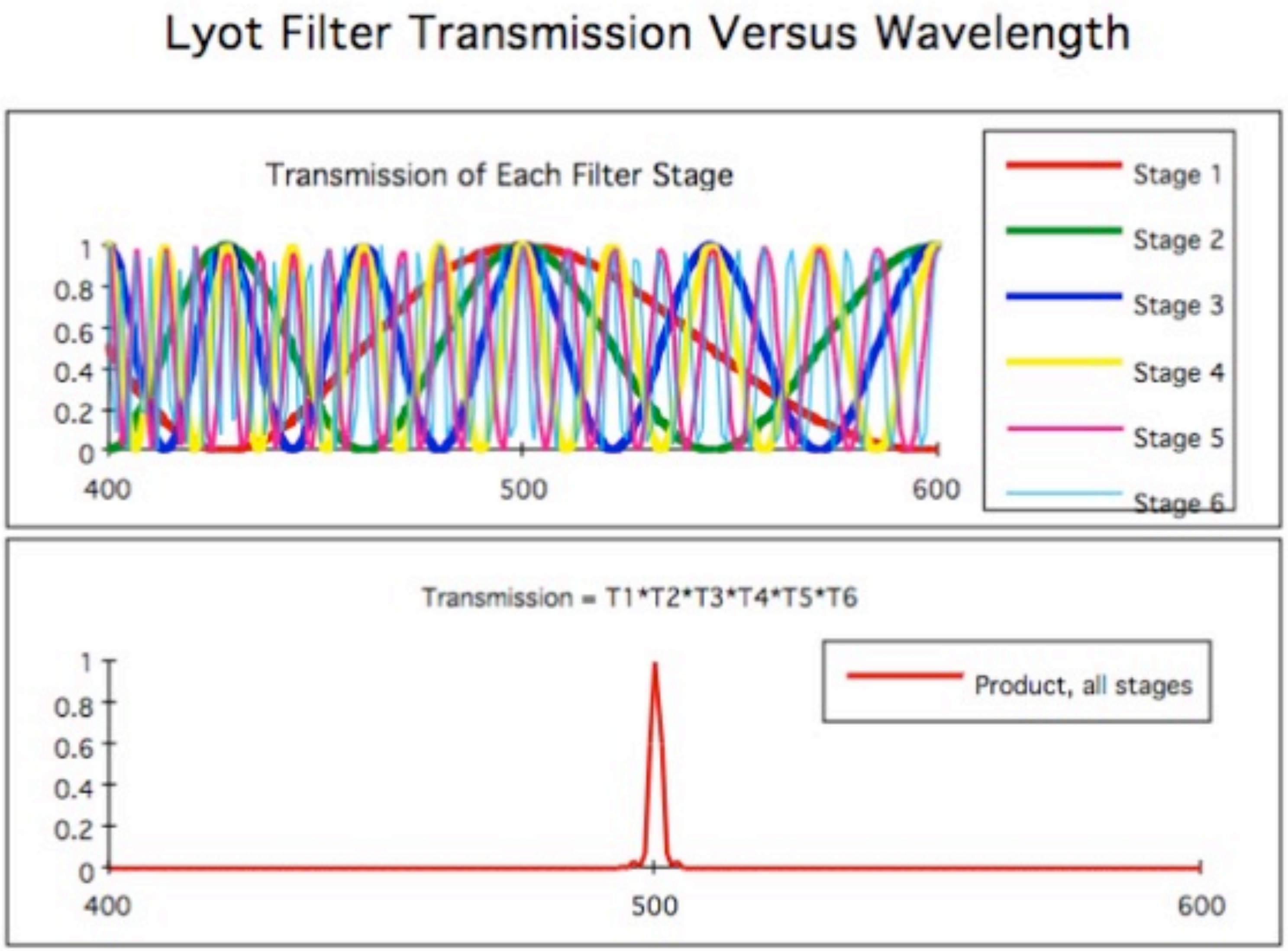
$$\Gamma_{n+1} = 2 * \Gamma_n$$



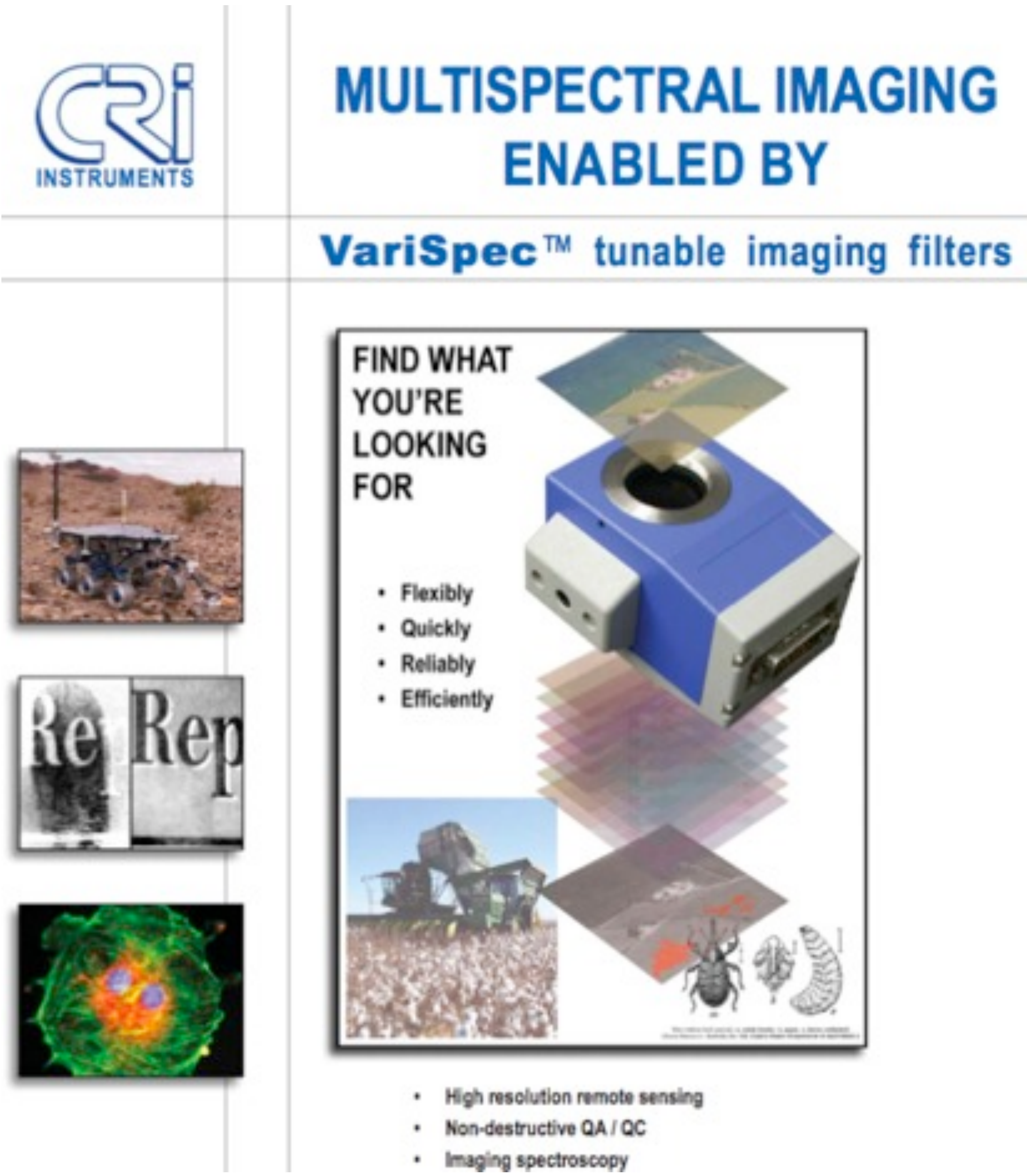
$$T_{Total} = T_1 * T_2 * T_3 * T_4 * T_5 * T_6$$

Interferential spectrometer LCPF





Spectral imaging filter



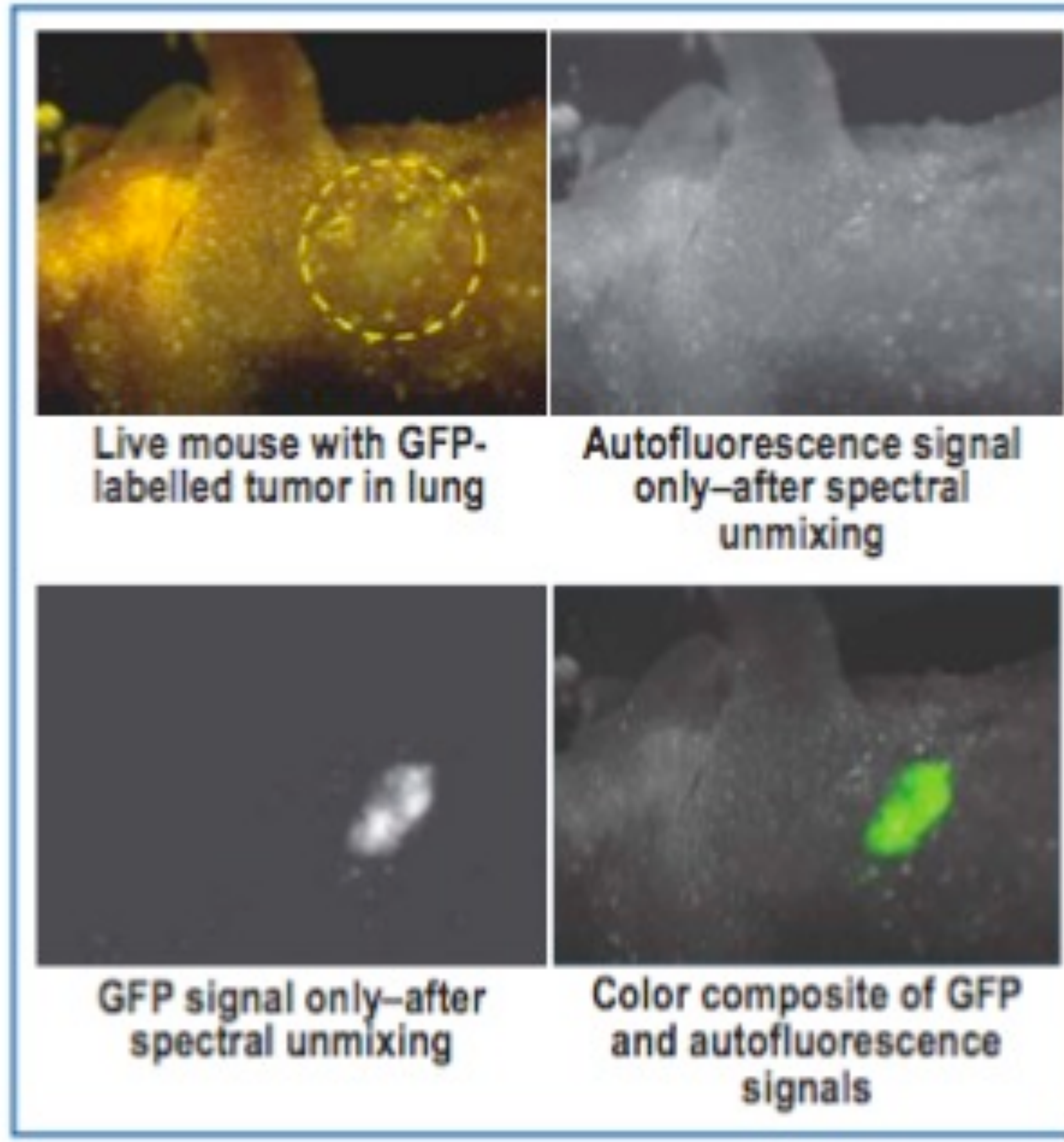
Spectral imaging filter

SPECIFICATIONS

LC filter aperture	20 mm (VIS and NIR) 35 mm (VIS only)
Computer interface[1]	USB 1.1 control and power (Serial with virtual COM ports)
Bandwidth (FWHM)	0.25 nm to 20 nm available
Wavelength range	VIS: 400 nm to 720 nm SNIR: 650 nm to 1100 nm LNIR: 850 nm to 1800 nm XNIR: 1200 nm to 2450 nm
Wavelength accuracy	Bandwidth/8
Maximum optical throughput	500 mW/cm^2
Power for electronics box	110/220 VAC, 50/60 Hz
Operating temperature	10° to 40° C
Storage temperature	-15° to 55° C

[1] USB Type-A to Type-B cable included.

Third-party software packages are available with CRI-compatible drivers for image capture, display, and analysis. See your authorized CRI distributor, or visit www.cri-inc.com for more information.



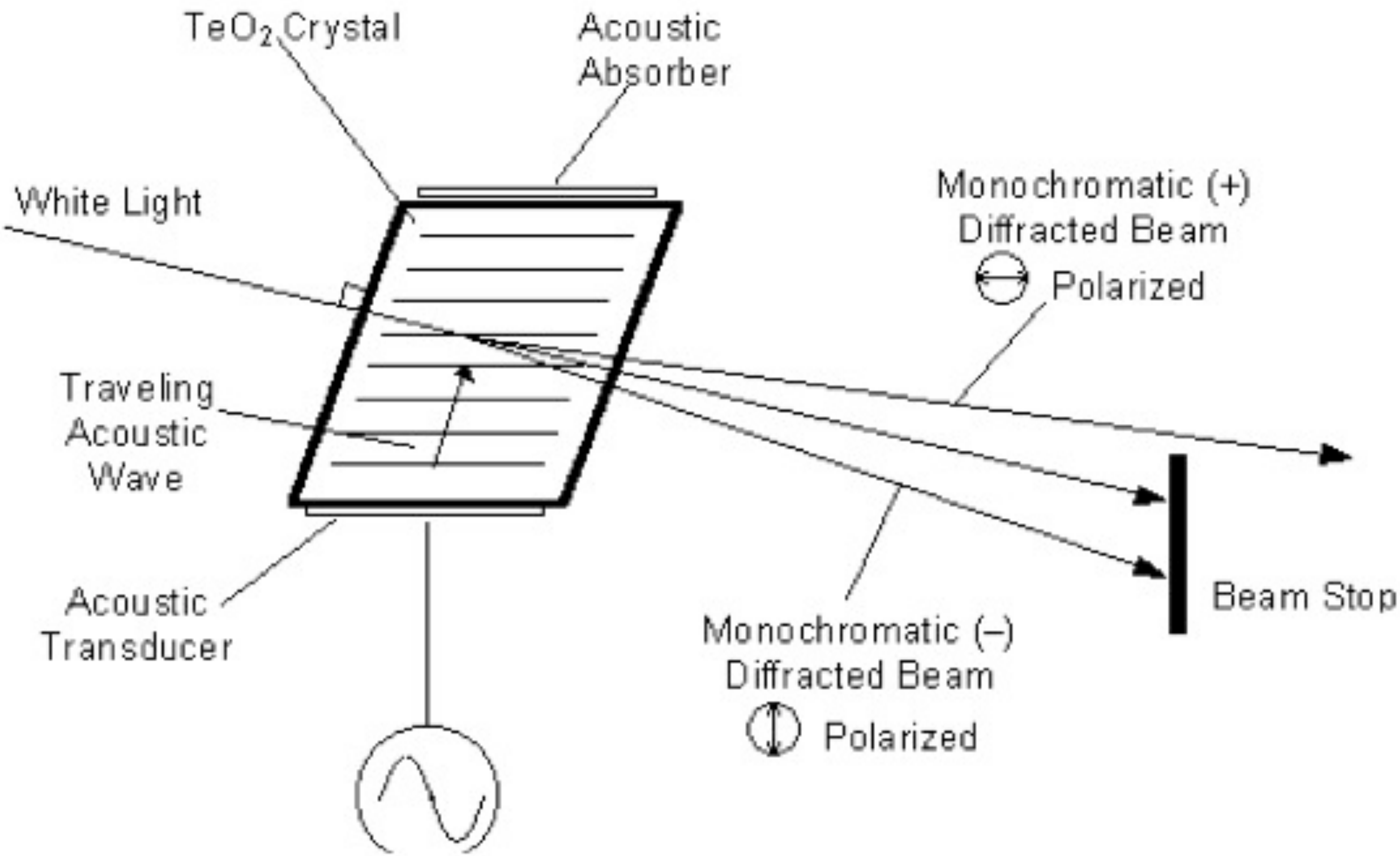
Live mouse with GFP-labelled tumor in lung

Autofluorescence signal only–after spectral unmixing

GFP signal only–after spectral unmixing

Color composite of GFP and autofluorescence signals

Acousto-optic spectrometer .. AOTF



Acousto-optic spectrometer .. AOTF

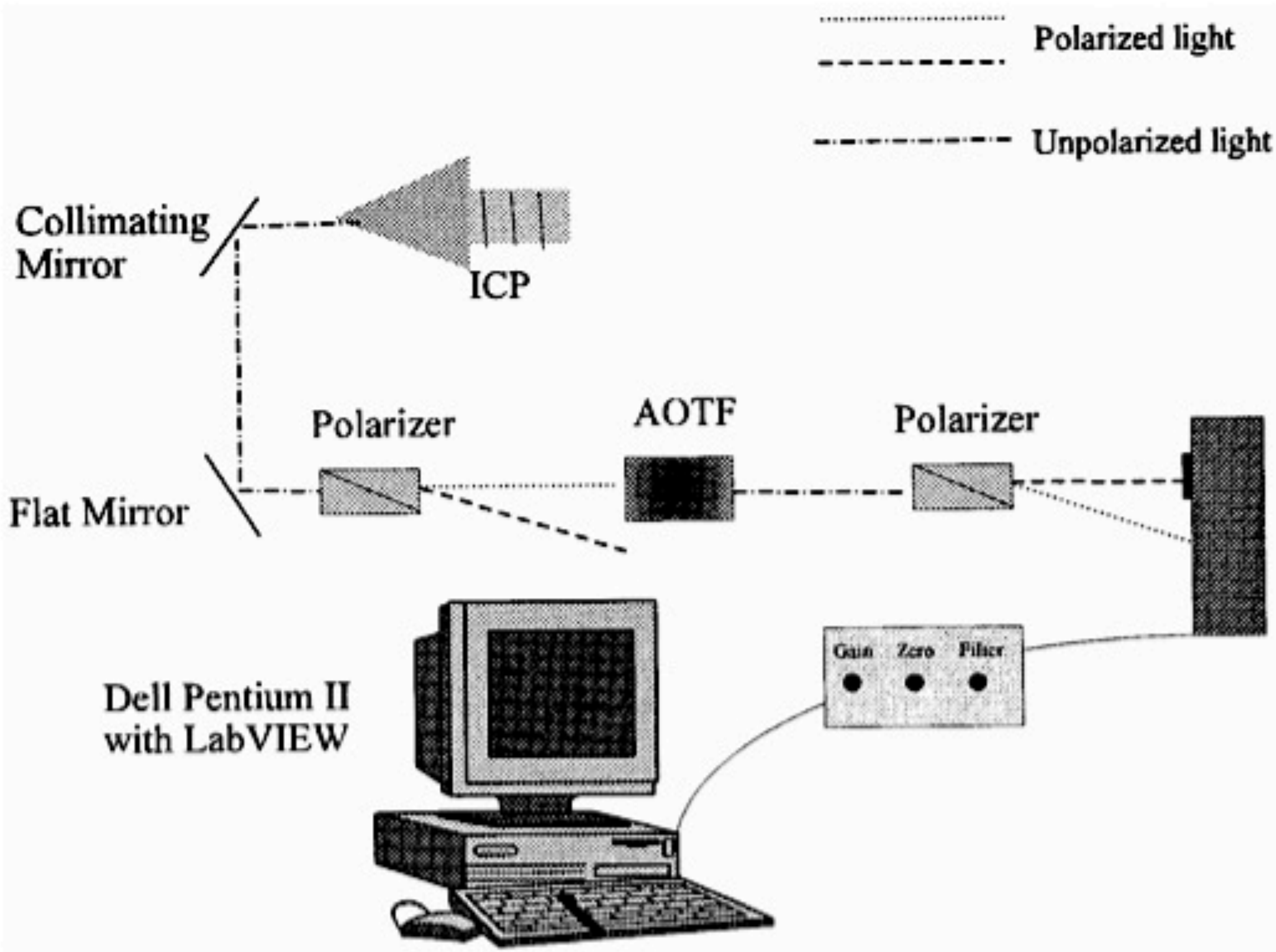
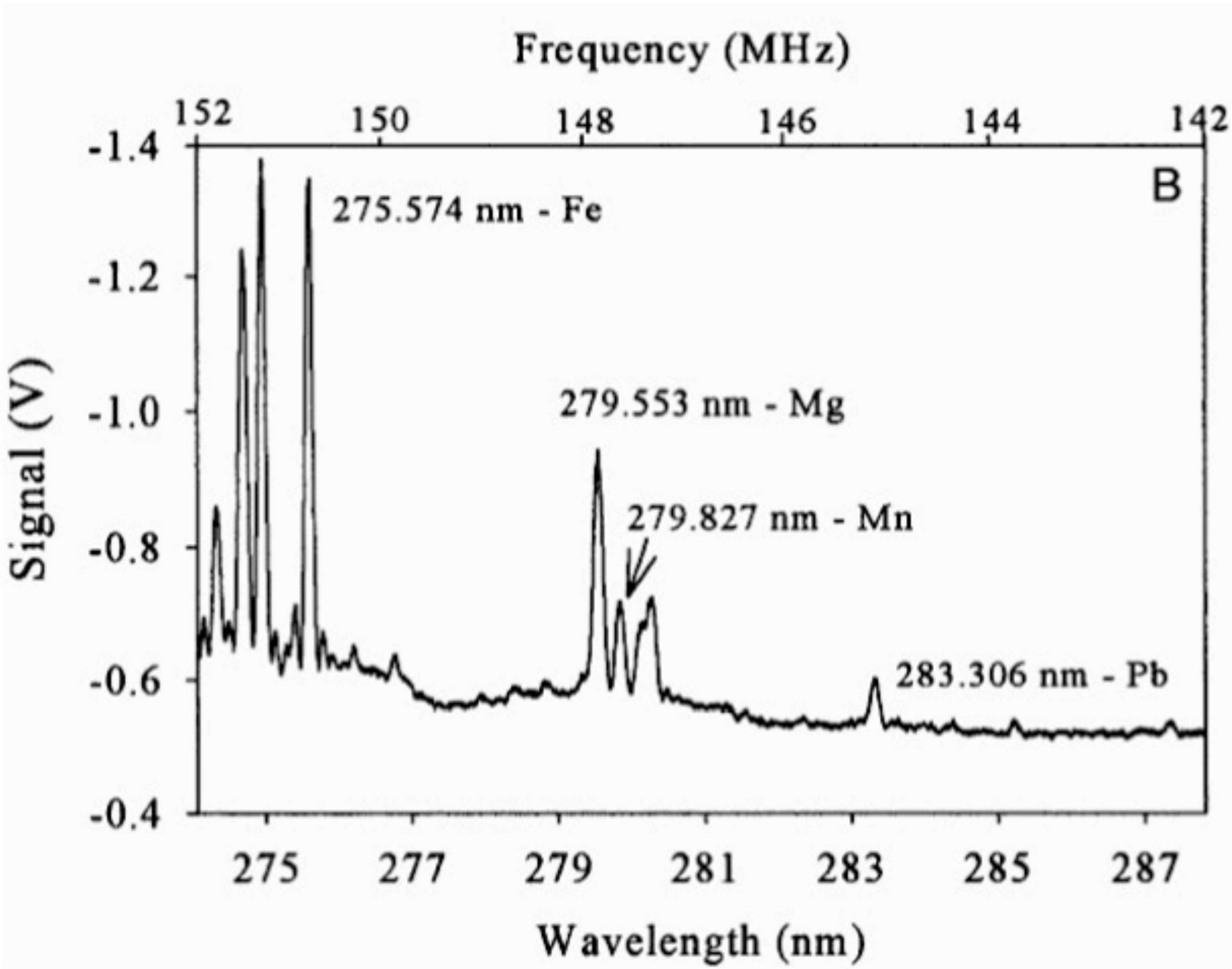
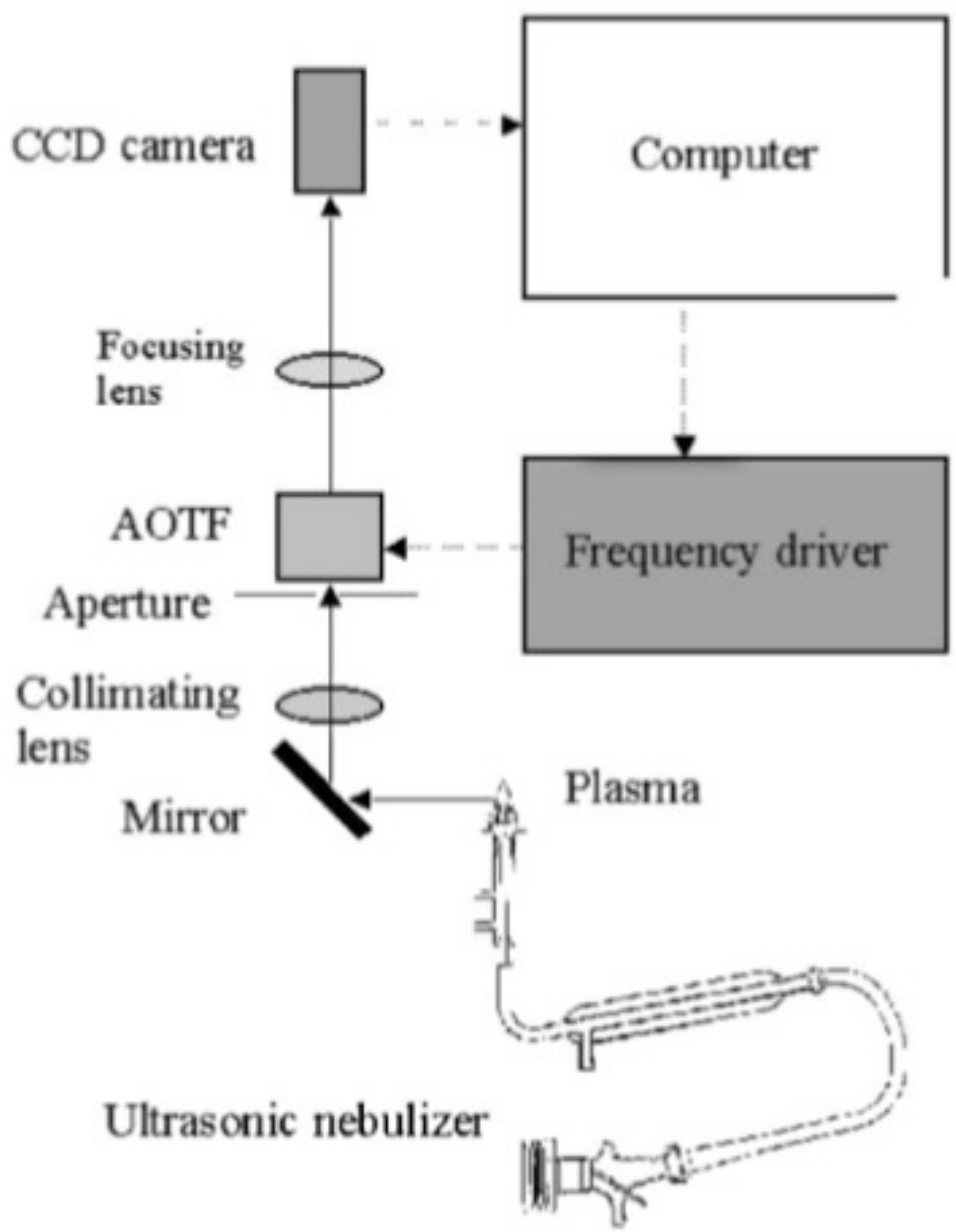


FIG. 3. Schematic diagram of the AOTF-ICP-AES system.

Acousto-optic spectrometer .. AOTF



Acousto-optic spectrometer .. AOTF



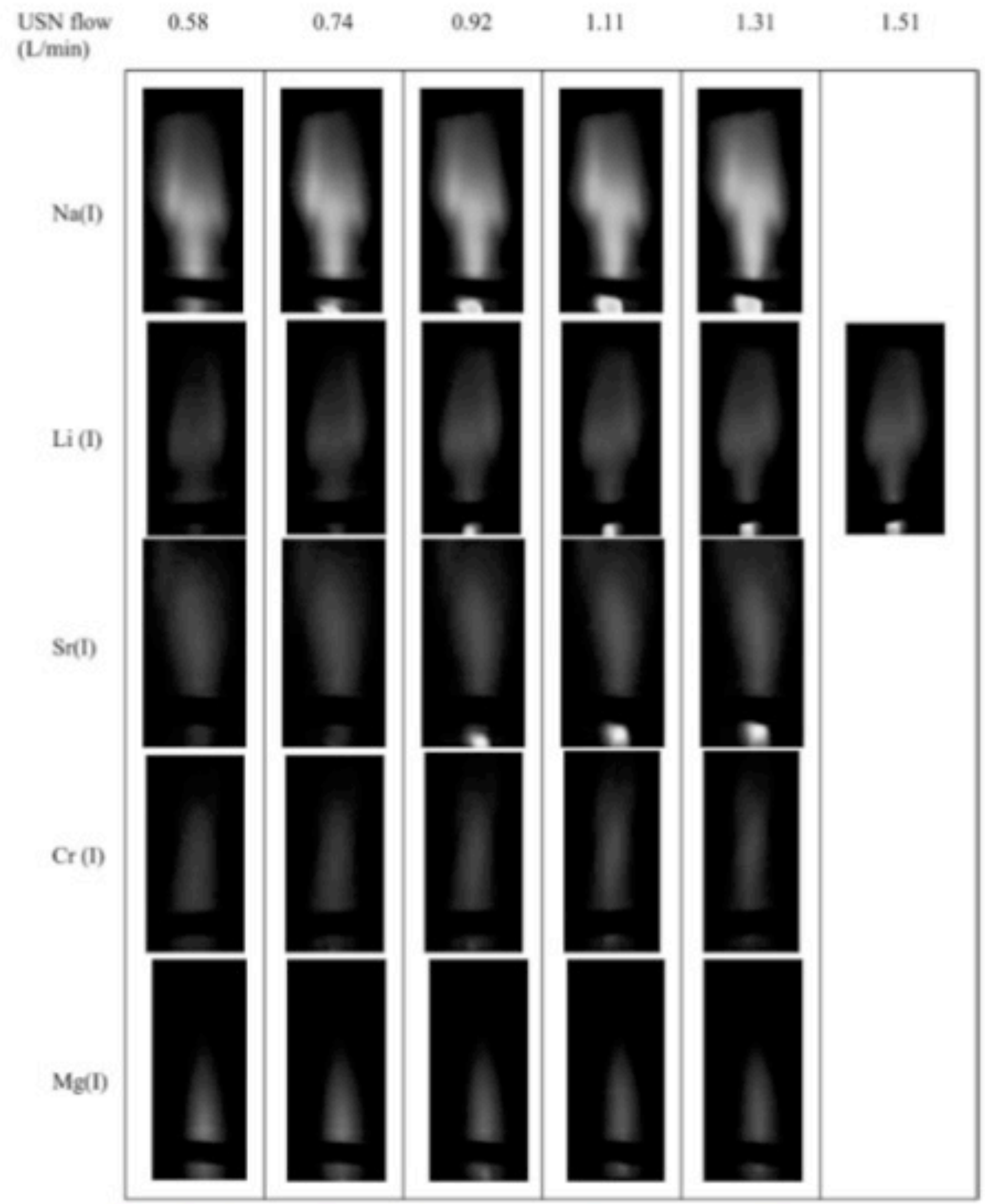


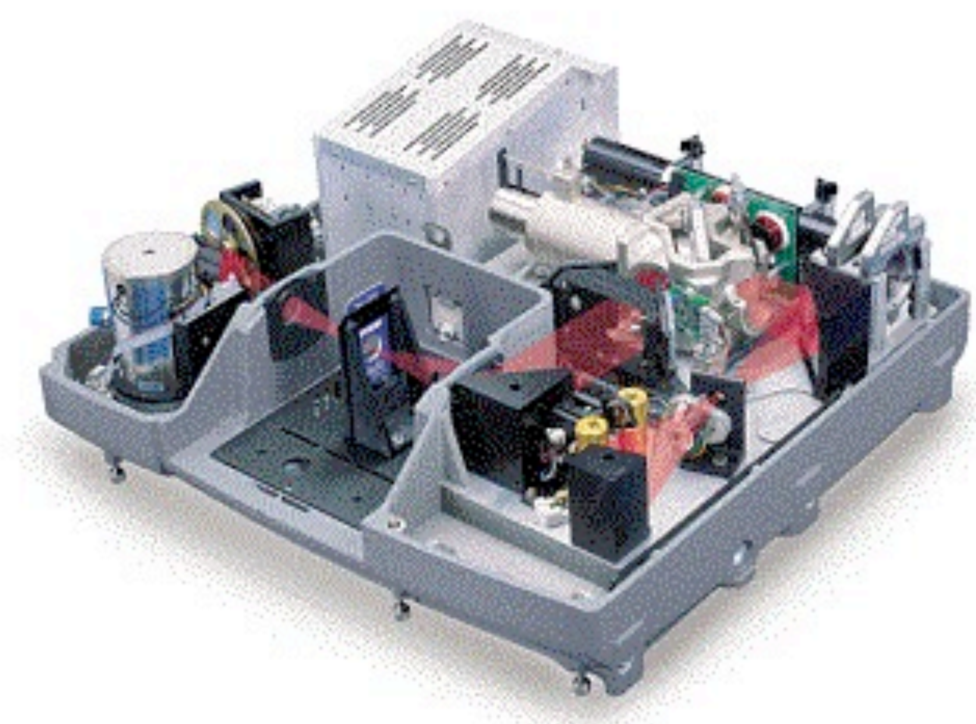
Fig. 4 Effects of USN sample carrier gas flow rate on selected elements.

FTIR spectrometer

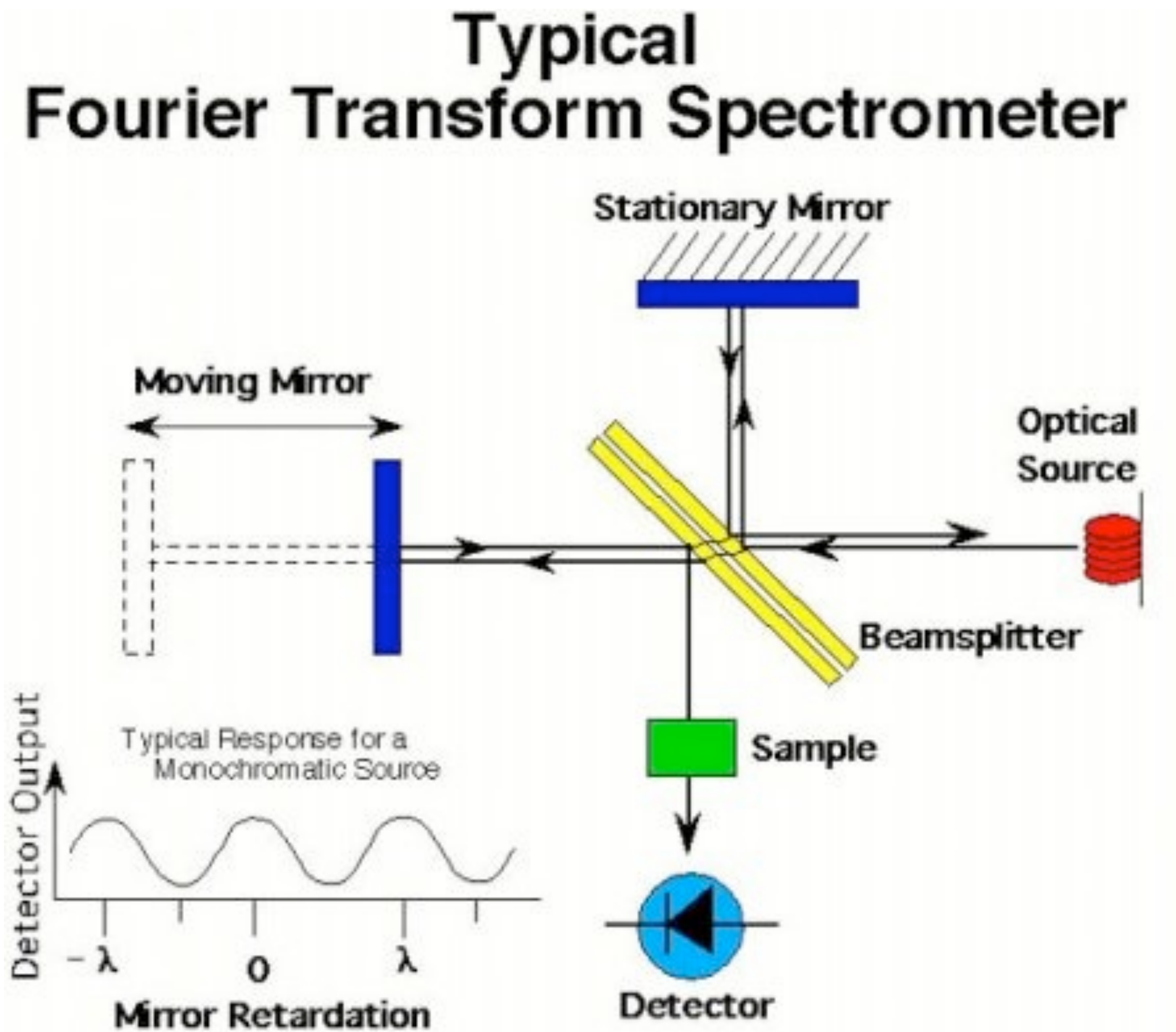
Thermo Nicolet

FT-IR System

Optical Bench

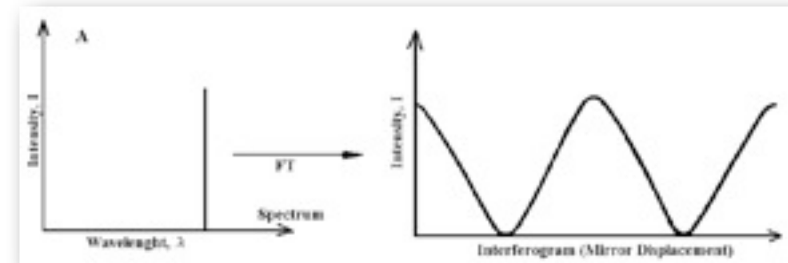


FTIR spectrometer

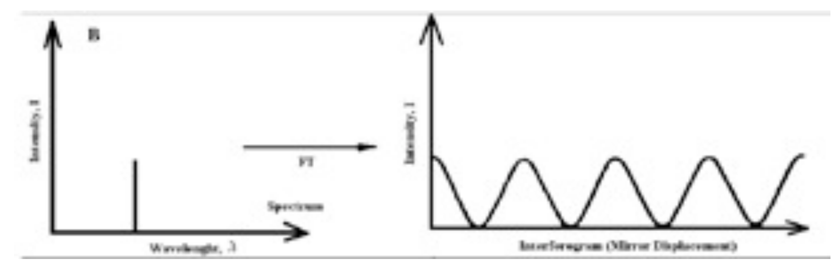


FTIR spectrometer

$$I_{\nu 1}(x) = B(\nu_1) \cdot \cos 2\pi\nu_1 x$$



$$I_{\nu 2}(x) = B(\nu_2) \cdot \cos 2\pi\nu_2 x$$



$$I(x) = I_1(x) + I_2(x)$$

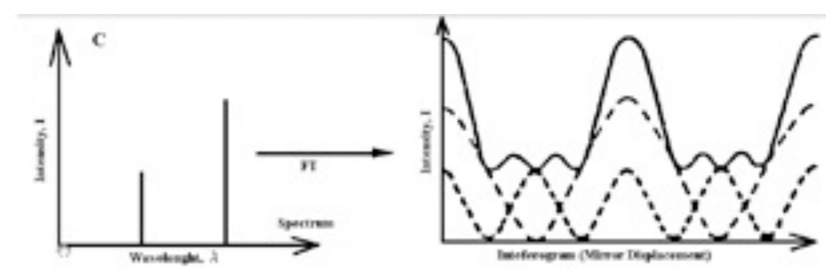


Fig. 3 A He-Ne laser line passed through interferometer.
B Laser line 0.5 intensity and 0.5 λ of He-Ne passed through interferometer.
C Both line sources passed through interferometer.

FTIR spectrometer

The mesured intensity (interferogram) in fonction of the displacement, x, is given by:

$$I(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} B(\nu) \cdot \cos(2\pi\nu x)\, d\nu$$

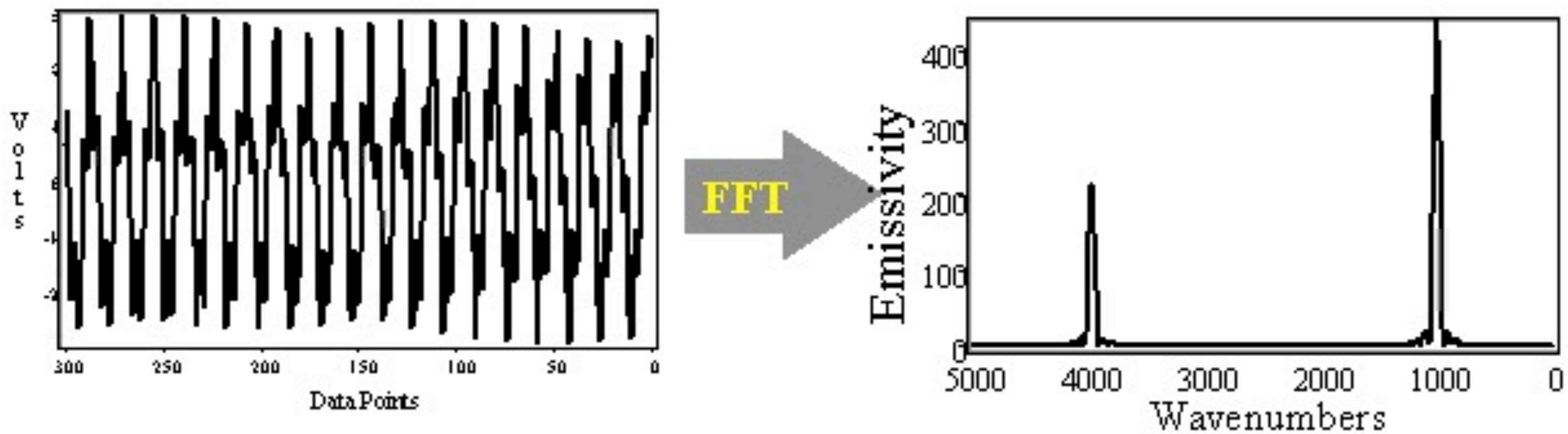
we observe immediately that the spectral information B(V) is nothing else than the Fourier transform of the measured intensity:

$$B(\nu) = \int_{-\infty}^{\infty} I(x) \cdot \cos(2\pi\nu x)\, dx$$

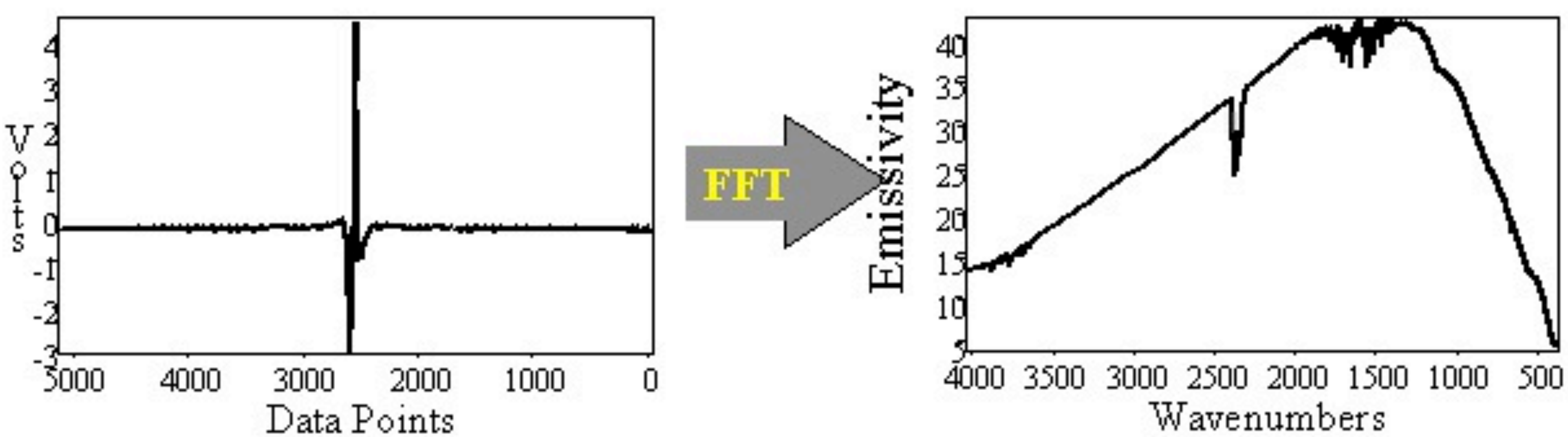
FTIR spectrometer

Fast Fourier Transformation

2 waves:



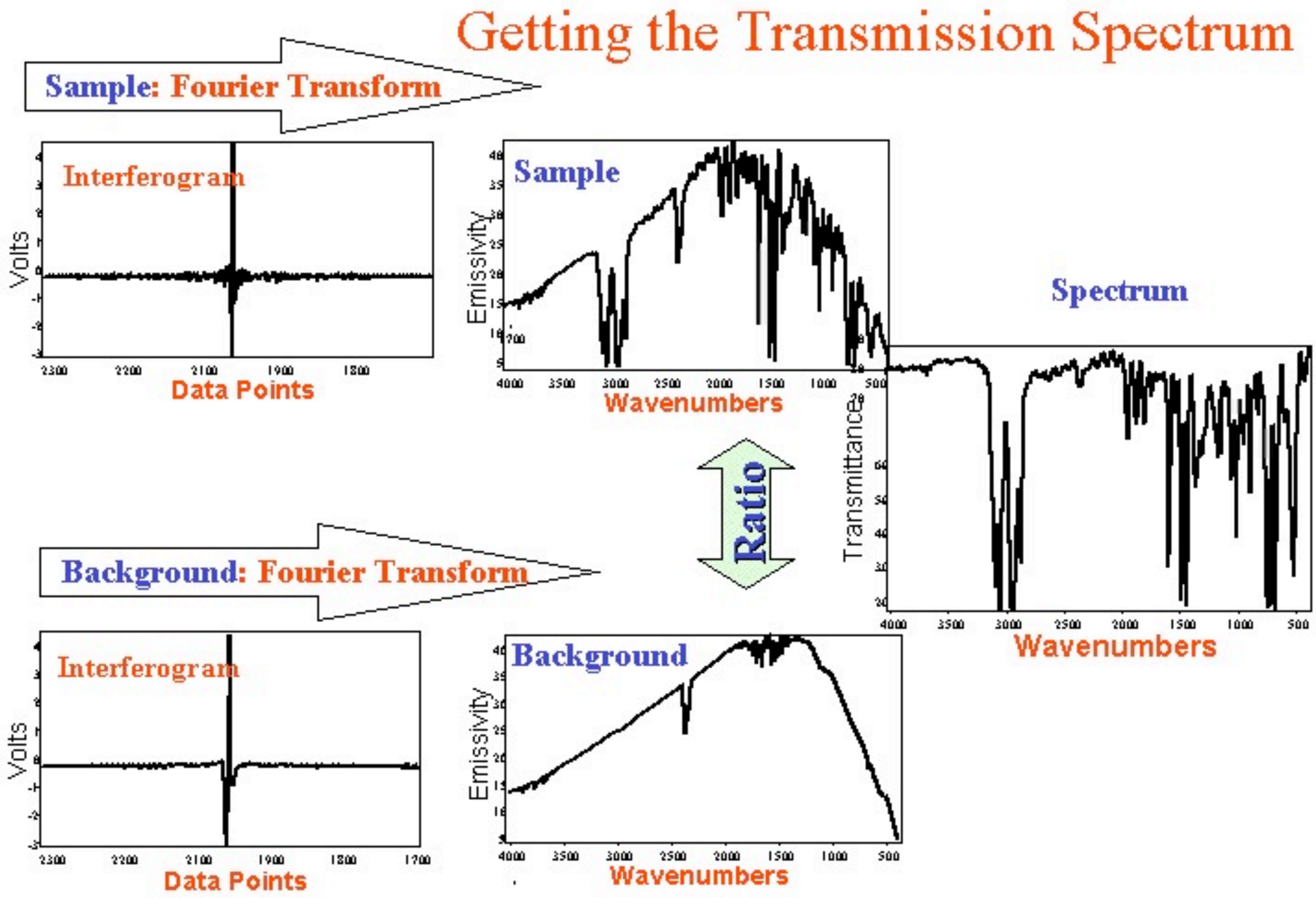
3601 waves:



Interferogram

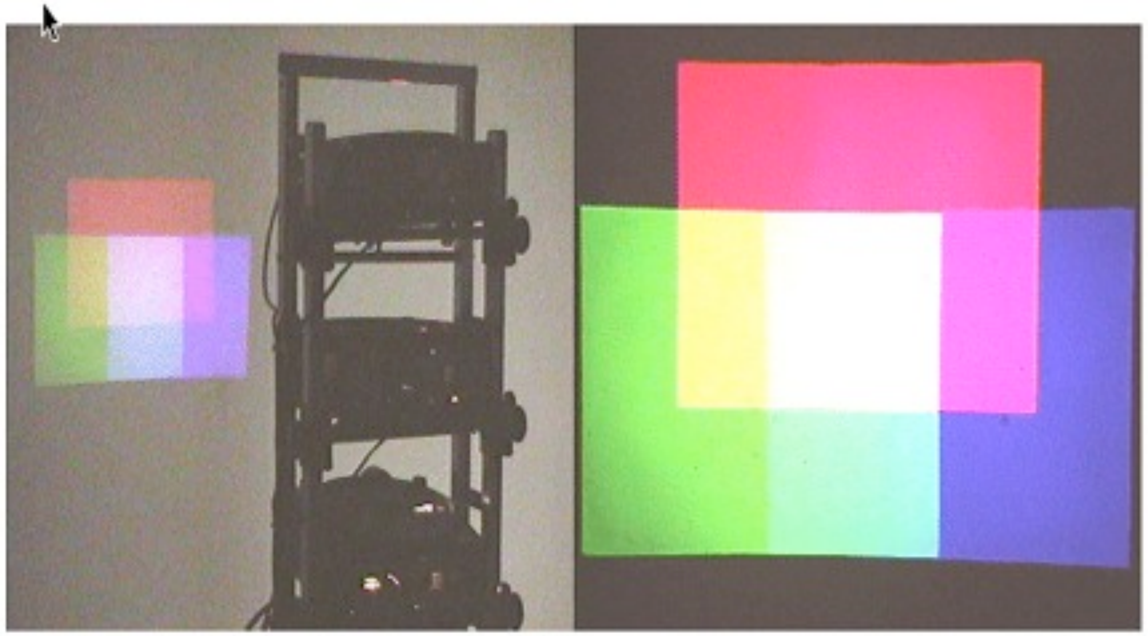
FFT= Fast Fourier Transform

FTIR spectrometer

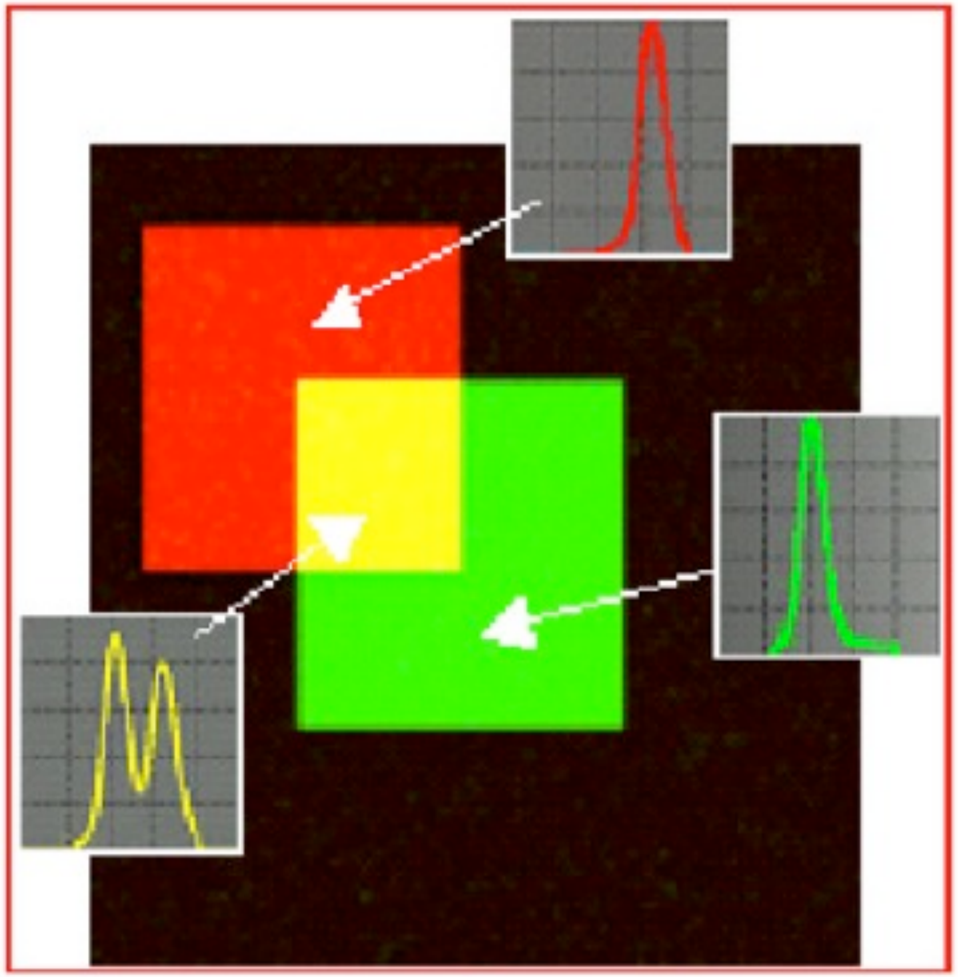


Hyperspectral

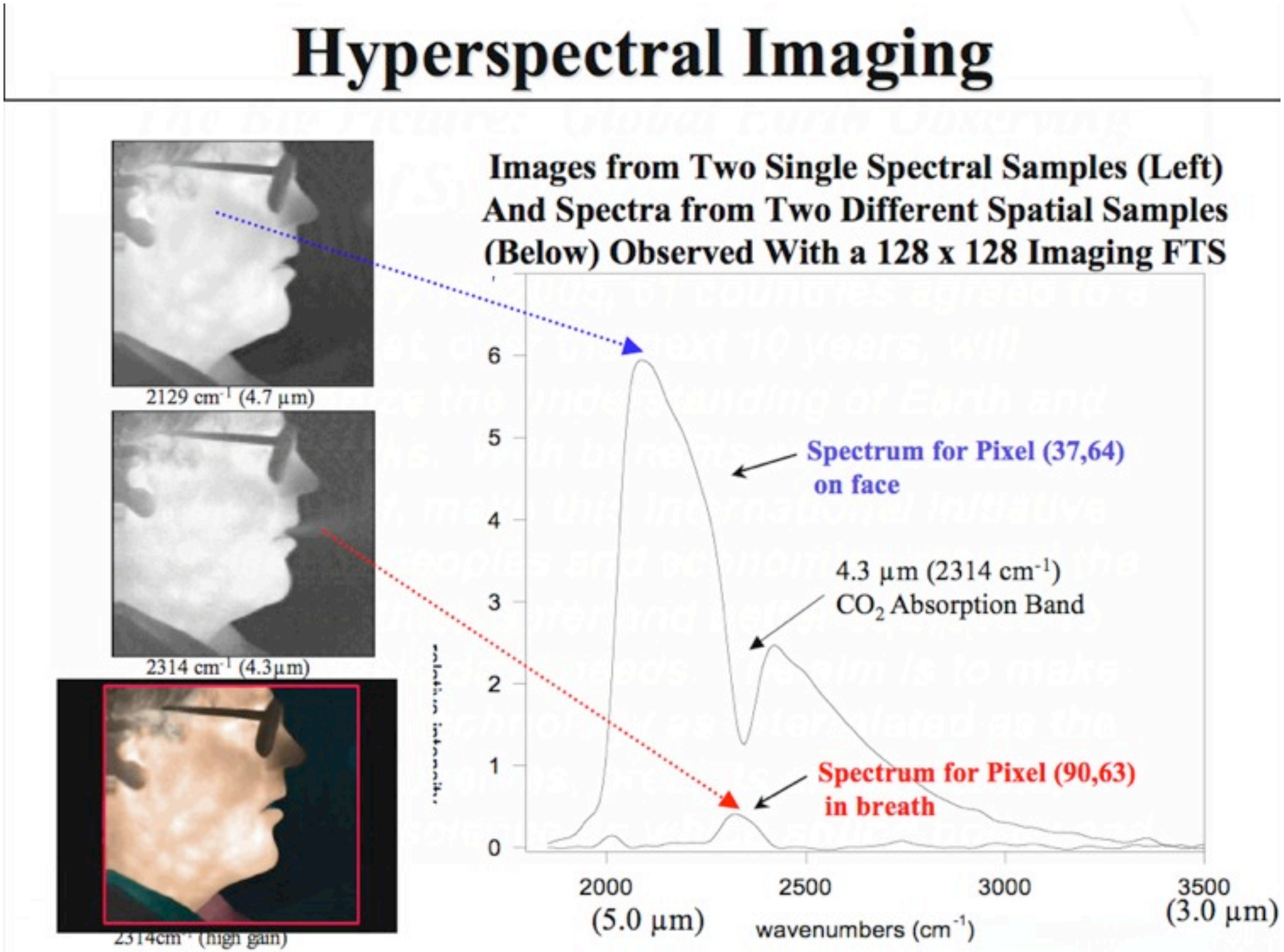
Visual perception of colors



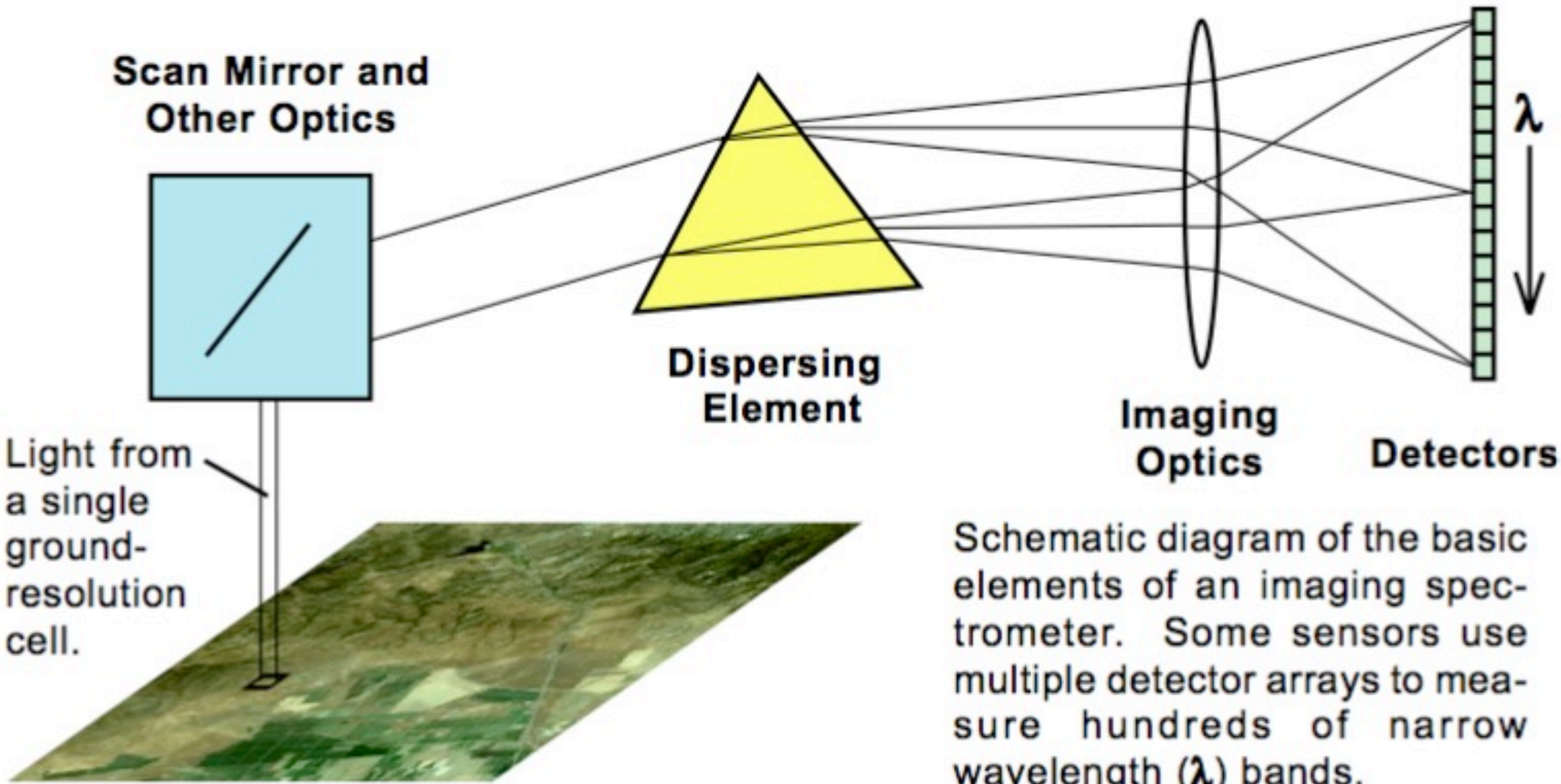
N3-02: ADDITIVE COLOR MIXING - PROJECTORS



Hyperspectral



Hyperspectral



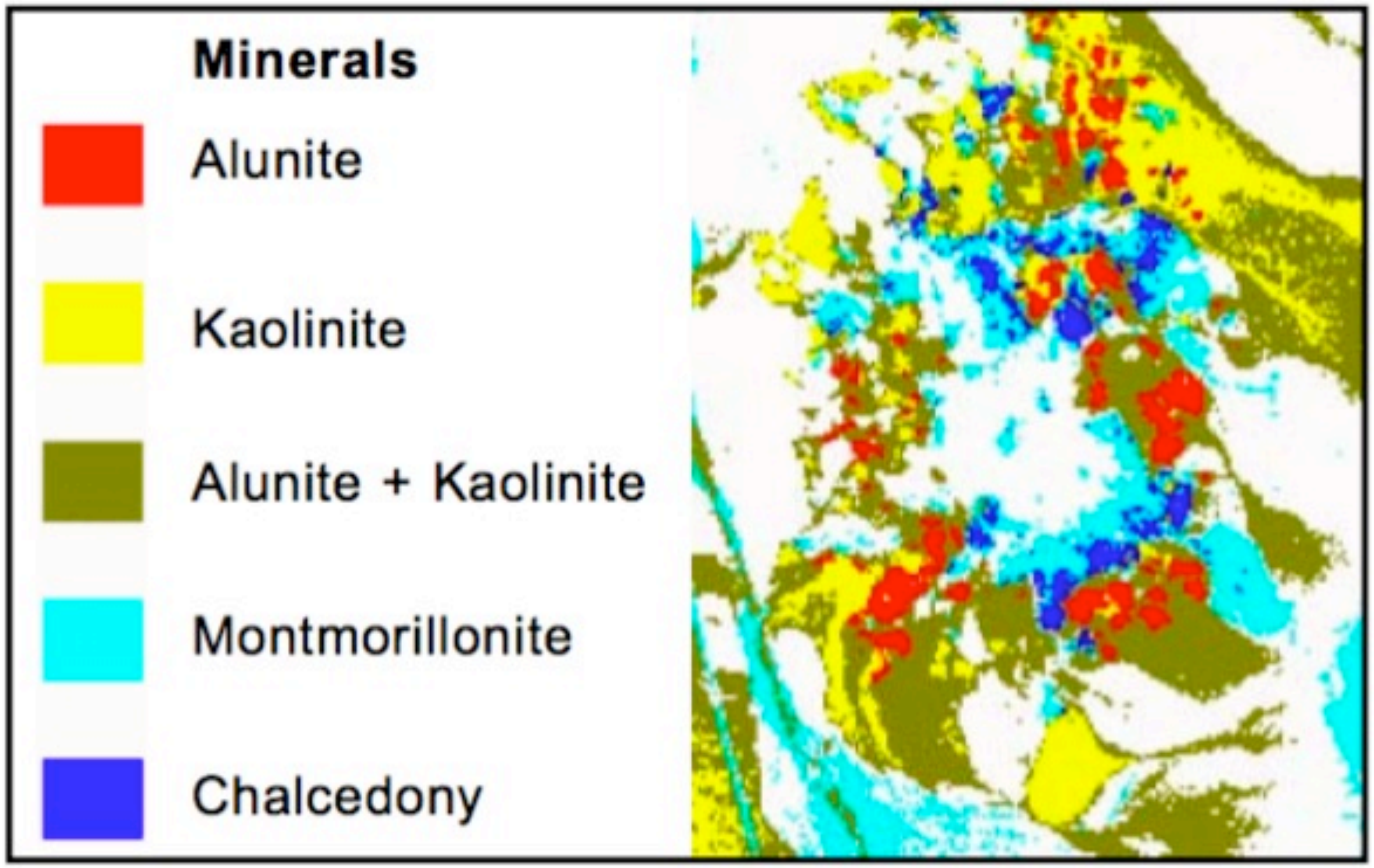
Schematic diagram of the basic elements of an imaging spectrometer. Some sensors use multiple detector arrays to measure hundreds of narrow wavelength (λ) bands.

Hyperspectral

(a) (b)

Figure 14. (a) OKSI's LCTF system in precision agriculture ground truth validation produces images such as in (b) showing spectral details of plant canopy and soil that allow measuring spatial variability in properties in support of canopy models and remote sensing observations.

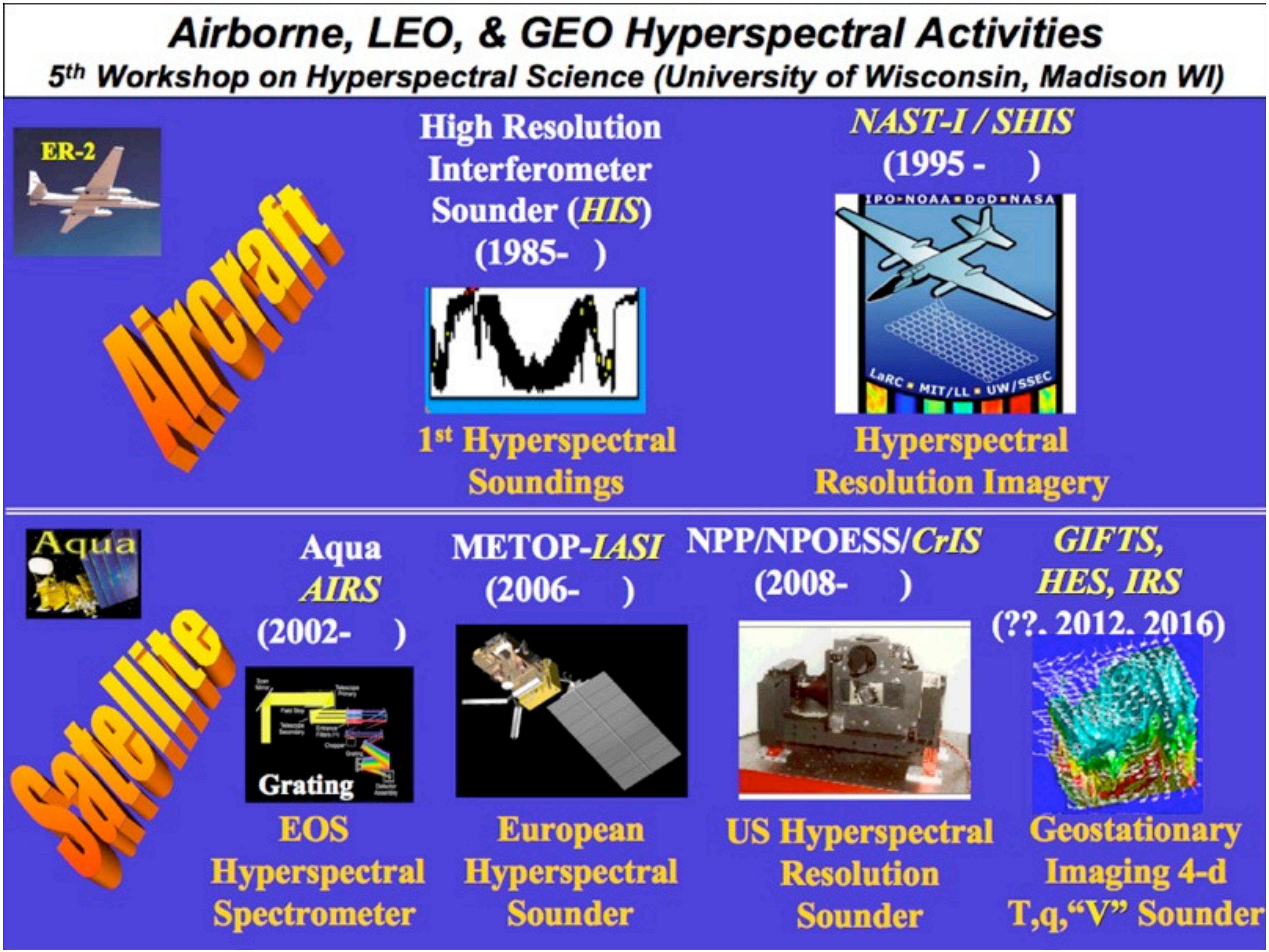
Hyperspectral



erence library.

Mineral map for part of the Cuprite AVIRIS scene, created by matching image spectra to mineral spectra in the USGS Spectral Library. White areas did not produce a sufficient match to any of the selected reflectance spectra, and so are left unassigned.

Hyperspectral



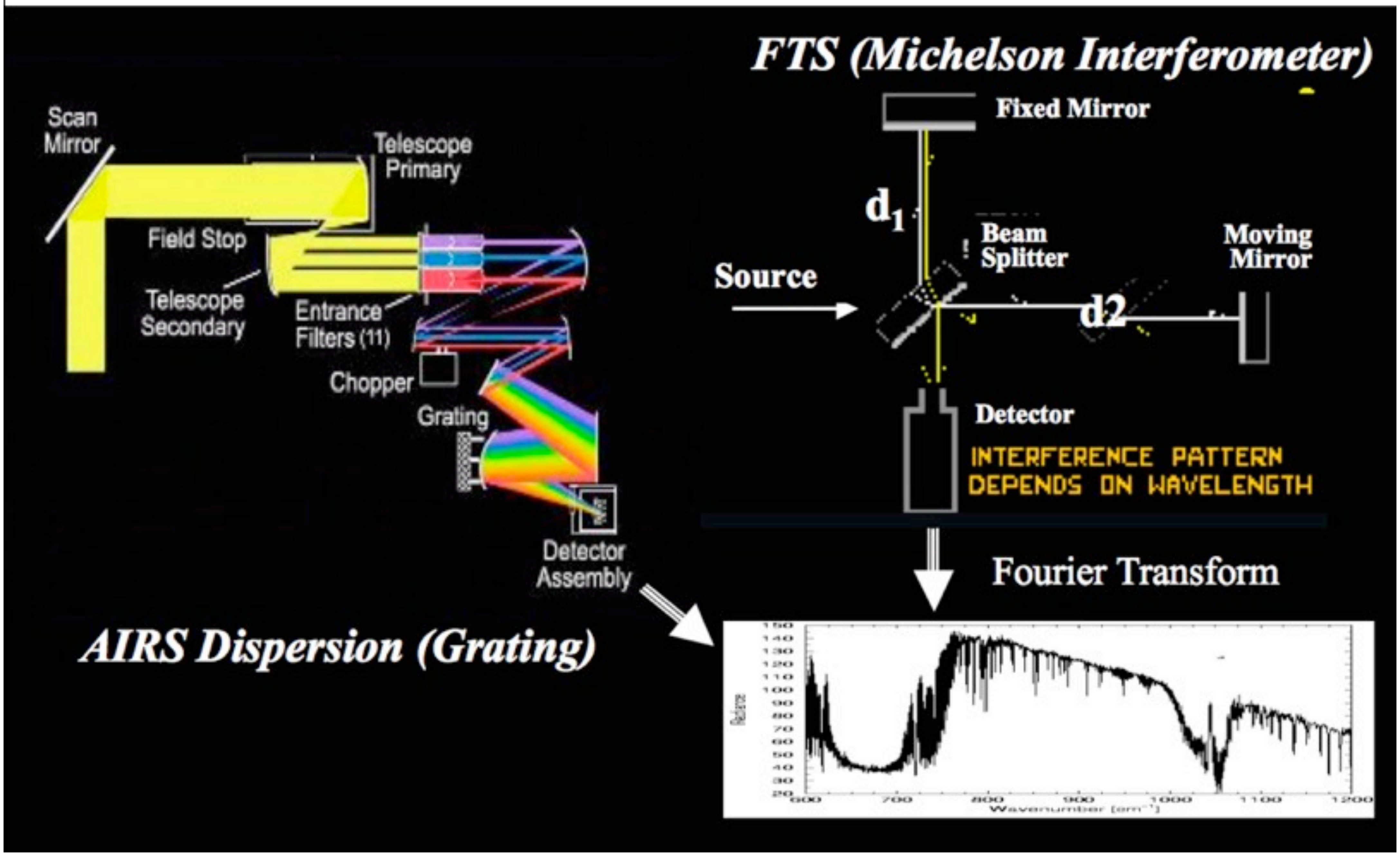
Hyperspectral

The Big Picture: Global Earth Observing System of Systems (GEOSS) Objective

"On February 16, 2005, 61 countries agreed to a plan that, over the next 10 years, will revolutionize the understanding of Earth and how it works. With benefits as broad as the planet itself, make this international initiative promises to peoples and economies around the globe healthier, safer and better equipped to manage basic daily needs. The aim is to make 21st century technology as interrelated as the planet it observes, predicts and protects, providing the science on which sound policy and decision-making must be built." - EPA

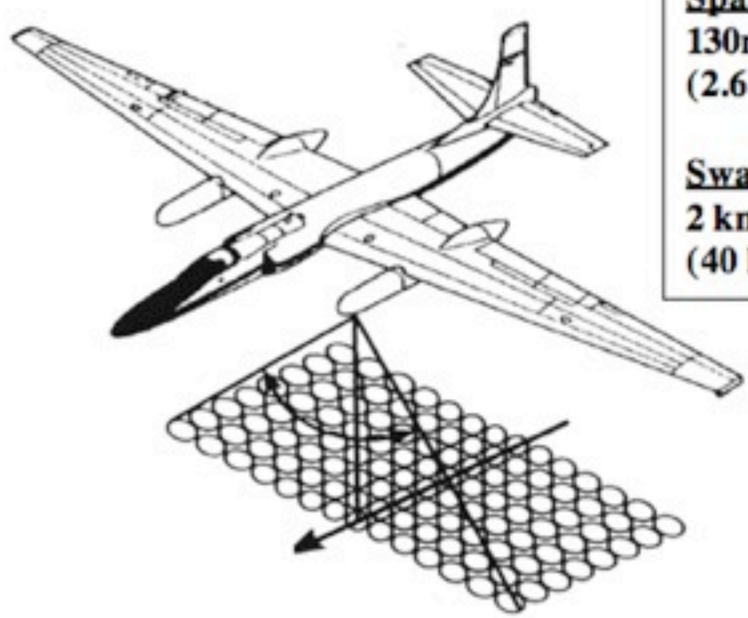
Hyperspectral

Grating (Dispersive) Spectrometer and Fourier Transform (Interferometer) Spectrometer – Basis for AIRS/IASI/CrIS/GIFTS Hyperspectral Sounders



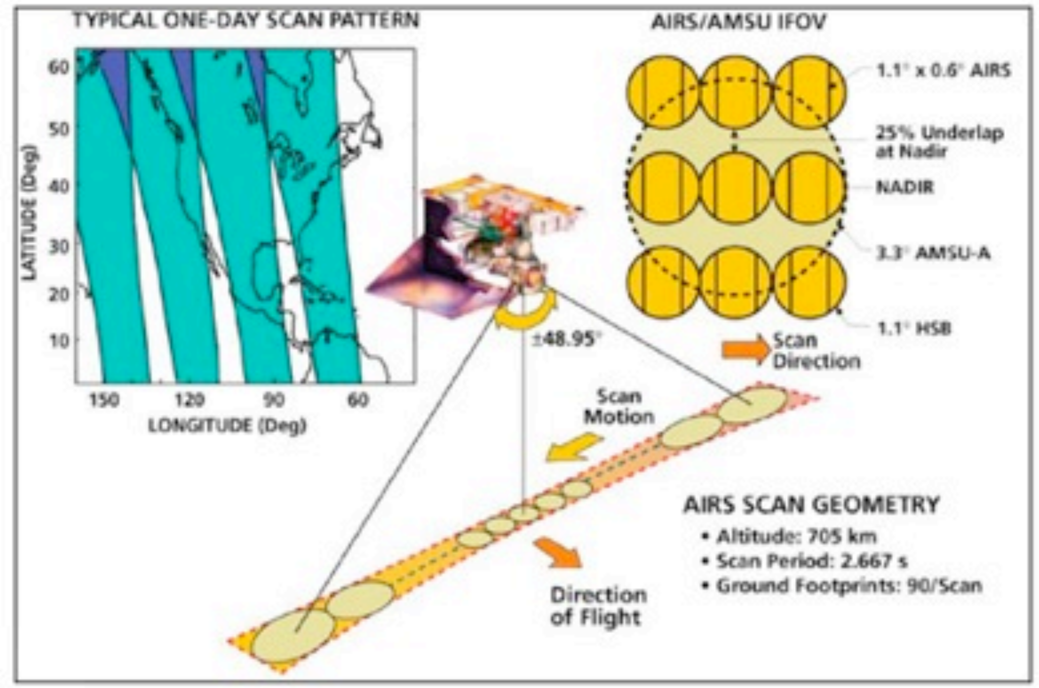
Hyperspectral

NAST and AIRS Characteristics



Spatial Resolution
130m/km flight alt.
(2.6 km from 20km)

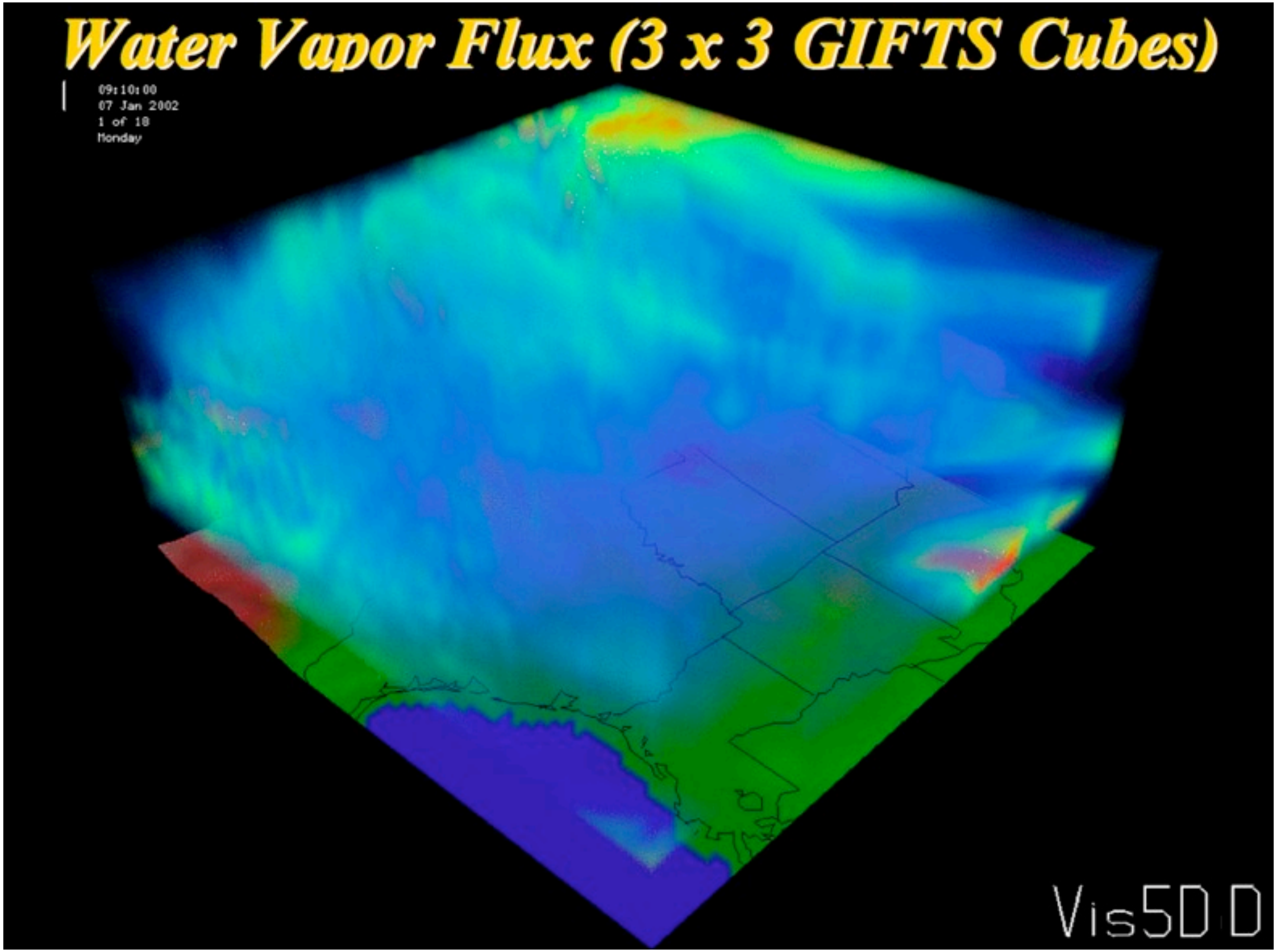
Swath Width
2 km /km flight alt.
(40 km from 20 km)



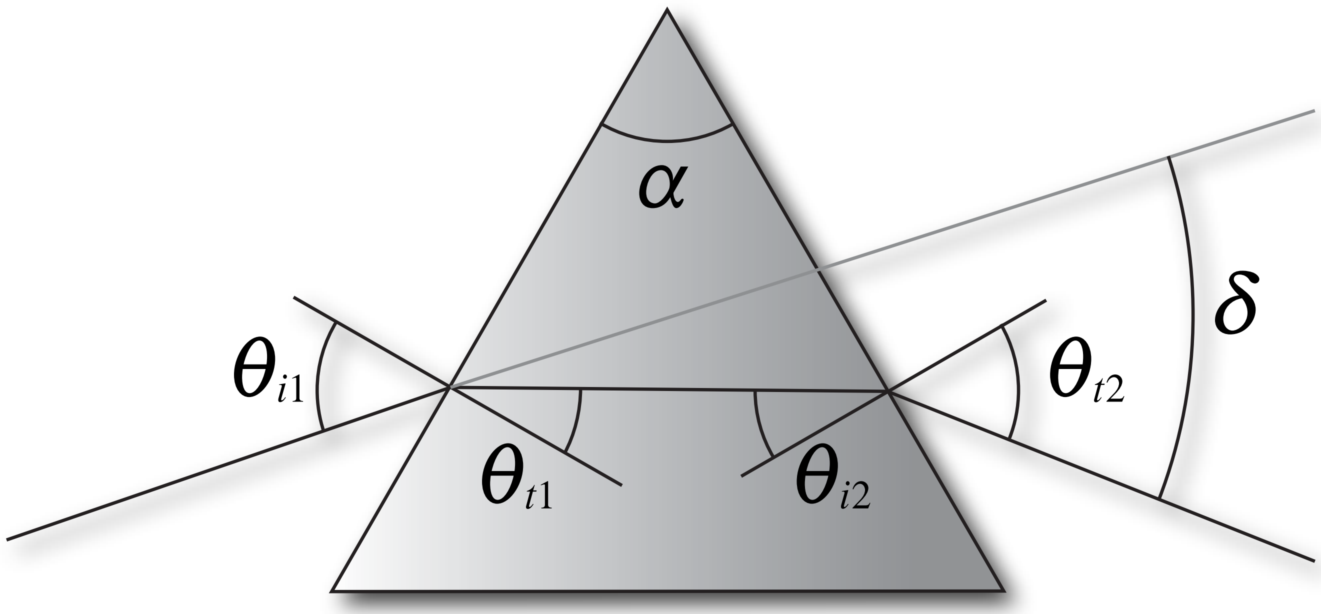
- The *NPOESS-I Aircraft Sounder Testbed – Interferometer* (NAST-I) consists of a 9000 spectral channel infrared interferometer (600-2850 cm^{-1}) with a spectral resolution of 0.25 cm^{-1}. NAST-I spatially scan and provide a ground resolution of about 2.6 km and a swath width of approximately 40 km, from an aircraft altitude of 20 km.

- The *Aqua AIRS* instrument is a ~2500 spectral channel cooled grating spectrometer with a spectral resolving power of ~ 1200 (0.5 – 2 cm^{-1} spectral resolution) operating within the spectral range 650 – 2700 cm^{-1}. The spatial resolution of the AIRS is about 15 km, at nadir, and its cross track scan providing a swath width of ~ 1400 km.

Hyperspectral



Minimum Deviation by a Prism



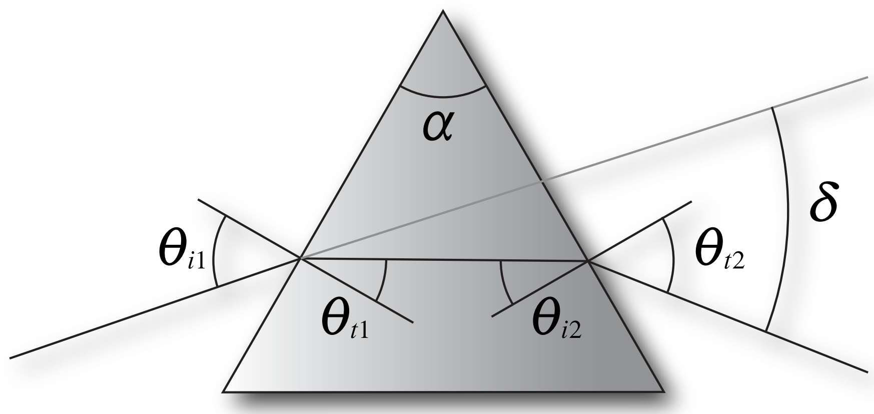
$$n = \frac{\sin(\theta_{i1})}{\sin(\theta_{t1})} = \frac{\sin(\theta_{t2})}{\sin(\theta_{i2})}$$

$$\alpha = \theta_{t1} + \theta_{i2}$$

$$\delta = \theta_{i1} + \theta_{t2} - \alpha$$

$$\delta = \theta_{i1} + \arcsin\left[n \cdot \sin\left(\alpha - \arcsin\left\{\frac{\sin\theta_{i1}}{n}\right\}\right)\right] - \alpha$$

Minimum deviation angle



n=1.5