Optical Spectrometers

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

Experimental Methods in Physics
[2011-2012]

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Optical spectroscopy

General properties of dispersive apparatus
- Resolvance / Luminosity

Classification of dispersive apparatus
- Prism / Grating / Interferential / Fourier / Hyperspectral

Light source → Sample → Light analyzer → Light detector
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 $L(\nu)$.

The absorption spectrum is characterized by the absorption factor $A(\nu)$.

The role of dispersive devices (prism, grating, interferential) is to determine the functions $A(\nu)$ and $L(\nu)$ with the greatest precision.
Optical spectroscopy

Keep in mind that the important physical parameter is .... the frequency, \( \nu \), ... even if we measure the wavelength!

- in the vacuum:
  \[
  \lambda_v = \frac{c}{\nu}
  \]

- in a medium of index \( n \):  
  \[
  \lambda_n = \frac{c}{n \cdot \nu}
  \]
Often in the air, it makes no difference between $\lambda_n$ and $\lambda_v$.

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, …)
Dispersive apparatus

Figures of merit

• Resolving power or resolvance

\[ \Re = \frac{\lambda}{\Delta \lambda} \]

• Luminosity

\[ L = \frac{E_M}{L_s} \]
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

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

\[
d_o = f \cdot \frac{\lambda}{w_g''}
\]
Rayleigh criterium:

Ideal case:

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

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

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vendredi, 9 décembre 2011
The intrinsic resolvance of the system is limited by the size of the dispersive element (or rather by its projection....), i.e. by the diffraction.
Influence of the width of the entrance slit
Resolvance

Influence of the width of the entrance slit

\[ E(x) = \int F(\xi) \cdot D(x - \xi) d\xi \]

\[ E = F \otimes D \]

where \( F \) is the function "slit", and \( D(x) \) the diffracted intensity in the image plane, of an infinitely thin slit.
Influence of the entrance slit width
Luminosity versus resolvance - a compromise

\[ \frac{L}{L_0} = \frac{E}{E_0} \]

\[ \frac{R}{R_0} \]

\[ \frac{L}{L_0} \times \frac{R}{R_0} \]

\[ \text{largeur d'image réduite } \frac{d}{d_0} \]

\[ \text{luminosité réduite} \]

\[ \text{résolvance réduite} \]

\[ \text{produit} \]
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

\[ n = \frac{\sin(\theta_i)}{\sin(\theta_i)} = \frac{\sin(\theta_t)}{\sin(\theta_t)} \]

If the angle of deviation, \( \delta \), is minimum

\[ n = \frac{\sin(\alpha + \delta)}{\sin(\alpha)} \]
The prism spectrometer

the resolving power is given by:

\[ R = \frac{\lambda}{\Delta \lambda} = a \frac{d\beta}{d\lambda} = e \frac{dn}{d\lambda} \]
The prism spectrometer

Example:

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

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

\[ e = 25 \text{ mm} \]

\[ R \approx \frac{1100}{3400} \text{ Crown} \]
\[ 0.17 \text{ nm} \leq \Delta \lambda \leq 0.5 \text{ nm} \]
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

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

The prism spectrometer

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

Pellin-Broca’s prism
### 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

Symmetric Stretch
Asymmetric Stretch
Scissor bending
Rocking bending

Molecular vibration modes induced by IR beam

Optical spectroscopy
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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\textsuperscript{th} order

\[ \Delta \phi = 2\pi \]

1\textsuperscript{st} order

\[ \Delta \phi = 4\pi \]

2\textsuperscript{nd} order

Optical spectroscopy
General properties of dispersive apparatus
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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**

\[ \alpha = \text{incident angle} \]

\[ \beta = \text{diffraction angle} \]

\[ k = \text{diffraction order} \]

\[ N = \text{total number of grooves} \]

\[ n = \text{grooves density [grooves/mm]} \]

\[ \lambda = \text{wavelength [nm]} \]

\[ b = \text{grating step} \]

\[ D_V = \alpha + \beta = \text{total deviation angle} \]
Grating spectrometer—basic equations

\[ D_v = \beta - \alpha \]

\[ D_v \text{ is fixed by the geometry} \]

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

- k = diffraction order
- n = grooves density
Grating spectrometer—basic equations

example of configuration

Table 1

<table>
<thead>
<tr>
<th>DV</th>
<th>α</th>
<th>β</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>17.458</td>
<td>17.458</td>
</tr>
<tr>
<td>10</td>
<td>12.526</td>
<td>22.526</td>
</tr>
<tr>
<td>20</td>
<td>7.736</td>
<td>27.736</td>
</tr>
<tr>
<td>24</td>
<td>5.861</td>
<td>29.861</td>
</tr>
<tr>
<td>30</td>
<td>3.094</td>
<td>33.094</td>
</tr>
<tr>
<td>40</td>
<td>-1.382</td>
<td>38.618</td>
</tr>
<tr>
<td>50</td>
<td>-5.670</td>
<td>44.330</td>
</tr>
</tbody>
</table>

variation de l’angle d’incidence, α, et de l’angle de diffraction, β, en fonction de l’angle de déviation DV
(réseau de 1200 l/mm, k = 0 et λ = 500 nm)
**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 influence of the aberrations).
Grating spectrometer

Superposition of the different orders of diffraction

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

\[ k \cdot \lambda = \text{cste} \]
Grating spectrometer

angular dispersion and intrinsic resolvance

\[ R_0 = \frac{\lambda}{\Delta\lambda} = w_g'' \frac{d\beta}{d\lambda} \]

\[ R_0 = \frac{\lambda}{\Delta\lambda} = w_g'' \frac{k \cdot n \cdot 10^{-6}}{\cos \beta} = w_g \cdot k \cdot n = k \cdot N \]

\[ R_0 = \frac{\lambda}{\Delta\lambda} = w_g \cdot \frac{\sin (\alpha) + \sin (\beta)}{10^{-6} \cdot \lambda} \]
Grating spectrometer

blazed gratings

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 ($D\nu$ is imposed by the geometry of the monochromator)
Grating spectrometer

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

![Diagram of a Czerny-Turner grating spectrometer]
Grating spectrometer

Aberration in PGS systems

The effect of the Coma

The effect of Spherical Aberration
Aberration in PGS spectrometer

Aberration in PGS systems
Grating spectrometer

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
**Grating spectrometer**

\[
\text{F - value}
\]

\[
N.A. = \sin \Omega
\]

\[
f/\text{value} = \frac{1}{2 NA}
\]
Radiometry and spectrometry ... geometry extent

Grating spectrometer
Grating spectrometer

One example: Jobin-Yvon HR 250
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)

**Keywords:**
- Toroidal mirror
- Entrance ports
- On-Axis Turret
- Exit Ports
- Large focusing mirror
- Asymmetric design
- TRIAX 550
PF spectrometer [Fabry-Perot]
Interferential spectrometer

\[ \nu = \frac{c}{2L} \]
\[ \nu = \frac{c}{L} \]
\[ \nu = \frac{3c}{2L} \]
\[ \nu = \frac{2c}{L} \]

Classification of dispersive apparatus
- Prism
- Grating
- Interferential
- Fourier
- Hyperspectral
Iterferential spectrometer
Interferential spectrometer

\[ S = 2nd \cos \theta \]

\[ E_{\text{trans}} = E_{\text{inc}} \left[ tt + trrte^{-jk_0S} + trrrrte^{-jk_02S} + \ldots \right] \]
Interferential spectrometer

avec \( R = |r|^2 \) et \( T = |t|^2 \)

\[
F = \frac{4R}{(1 - R)^2} \quad \quad \quad \quad \nu_0 = \frac{c}{S} = \frac{c}{2 \pi d \cos \theta}
\]

\[
\frac{I_{\text{trans}}}{I_{\text{inc}}} = \frac{1}{1 + F \sin^2 \left( \frac{\pi \nu}{\nu_0} \right)}
\]
Interferential spectrometer

Home-Built Scanning Fabry-Perot Interferometer 1
Interferential spectrometer

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

\[ R = \frac{\nu}{\Delta \nu} = \frac{\nu}{\nu_0} \cdot \frac{1}{FWHM} = \frac{\nu}{\nu_0} \cdot \xi = m \cdot \xi \]

F = 380, \quad \xi = 30.6, \quad \nu_0 = 15 \text{ GHz}, \quad m = 40000 \quad \Rightarrow \quad R = 1.2 \times 10^6
Interferential spectrometer

Raie de transition laser

"Q résultant" de la cavité

Emission laser monomode

Q de la cavité laser

Q de la cavité étalon

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J-D Ganiere

vendredi, 9 décembre 2011
Liquid Crystal \quad \text{Quartz}

Glass Substrates Coated With ITO

\begin{align*}
\Delta n &= n_e - n_o & \text{Birefringence} \\
\Gamma &= d\Delta n & \text{Retardance} \\
\Gamma_{\text{Total}} &= \Gamma_{\text{LC}} + \Gamma_{\text{Quartz}} \\
\delta &= 2\pi \Gamma_{\text{Total}} / \lambda & \text{Phase delay} \\
T(\lambda) &= \cos^2 \delta \\
T(\lambda) &= \cos^2 \left( 2\pi d\Delta n / \lambda \right) \\
T &= 1; \ \ m\lambda = d\Delta n & \text{for integer } m
\end{align*}
Interferential spectrometer  LCPF

\[ \Gamma_{n+1} = 2 \times \Gamma_n \]

\[ T_{\text{Total}} = T_1 \times T_2 \times T_3 \times T_4 \times T_5 \times T_6 \]
Interferential spectrometer LCPF

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vendredi, 9 décembre 2011

J-D Ganiere
Spectral imaging filter

MULTISPECTRAL IMAGING ENABLED BY VariSpec™ tunable imaging filters

- High resolution remote sensing
- Non-destructive QA / QC
- Imaging spectroscopy

- Flexibly
- Quickly
- Reliably
- Efficiently

Wavenumber (cm⁻¹): 20613

Wavelength (nm): 488
**Spectral imaging filter**

**SPECIFICATIONS**

<table>
<thead>
<tr>
<th>Specification</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>LC filter aperture</td>
<td>20 mm (VIS and NIR)</td>
</tr>
<tr>
<td></td>
<td>35 mm (VIS only)</td>
</tr>
<tr>
<td>Computer interface</td>
<td>USB 1.1 control and power (Serial with virtual COM ports)</td>
</tr>
<tr>
<td>Bandwidth (FWHM)</td>
<td>0.25 nm to 20 nm available</td>
</tr>
<tr>
<td>Wavelength range</td>
<td>VIS: 400 nm to 720 nm</td>
</tr>
<tr>
<td></td>
<td>SNIR: 650 nm to 1100 nm</td>
</tr>
<tr>
<td></td>
<td>LNIR: 850 nm to 1800 nm</td>
</tr>
<tr>
<td></td>
<td>XNIR: 1200 nm to 2450 nm</td>
</tr>
<tr>
<td>Wavelength accuracy</td>
<td>Bandwidth/8</td>
</tr>
<tr>
<td>Maximum optical throughput</td>
<td>500 mW/cm²</td>
</tr>
<tr>
<td>Power for electronics box</td>
<td>110/220 VAC, 50/60 Hz</td>
</tr>
<tr>
<td>Operating temperature</td>
<td>10° to 40° C</td>
</tr>
<tr>
<td>Storage temperature</td>
<td>-15° to 55° C</td>
</tr>
</tbody>
</table>

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.
Acousto-optic spectrometer .. AOTF
**Acousto-optic spectrometer .. AOTF**

![Diagram of an Acousto-optic spectrometer system]

**Fig. 3.** Schematic diagram of the AOTF-ICP-AES system.
Acousto-optic spectrometer AU AOTF

275.574 nm - Fe
279.553 nm - Mg
279.827 nm - Mn
283.306 nm - Pb

Frequency (MHz)

Signal (V)

Wavelength (nm)
Acousto-optic spectrometer .. AOTF

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

FT-IR System

Optical Bench

Optical spectroscopy
General properties of dispersive apparatus
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vendredi, 9 décembre 2011
**FTIR spectrometer**

**Typical Fourier Transform Spectrometer**

- **Moving Mirror**
- **Stationary Mirror**
- **Optical Source**
- **Beamsplitter**
- **Sample**
- **Detector**

**Typical Response for a Monochromatic Source**

![Diagram of a FTIR spectrometer](image)
FTIR spectrometer

\[ I_{\nu_1}(x) = B(\nu_1) \cdot \cos 2\pi \nu_1 x \]

\[ I_{\nu_2}(x) = B(\nu_2) \cdot \cos 2\pi \nu_2 x \]

\[ I(x) = I_1(x) + I_2(x) \]
The measured intensity (interferogram) in function 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 \( B(\nu) \) is nothing else than the Fourier transform of the measured intensity:

\[
B(\nu) = \int_{-\infty}^{\infty} I(x) \cdot \cos(2\pi\nu x) \, dx
\]
**Fast Fourier Transformation**

2 waves:

![Graph showing 2 waves and their FFT](image1)

3601 waves:

![Graph showing 3601 waves and their FFT](image2)

**Interferogram**

**FFT= Fast Fourier Transform**
FTIR spectrometer

Getting the Transmission Spectrum

Sample: Fourier Transform

Interferogram

Data Points

Sample

Emissivity

Wavenumbers

Spectrum

Transmittance

Ratio

Background: Fourier Transform

Interferogram

Data Points

Background

Emissivity

Wavenumbers
Visual perception of colors
Hyperspectral Imaging

Images from Two Single Spectral Samples (Left) And Spectra from Two Different Spatial Samples (Below) Observed With a 128 x 128 Imaging FTS

2129 cm⁻¹ (4.7 μm)

2314 cm⁻¹ (4.3 μm)

2314 cm⁻¹ (high gain)

Spectrum for Pixel (37,64) on face

4.3 μm (2314 cm⁻¹) CO₂ Absorption Band

Spectrum for Pixel (90,63) in breath
Schematic diagram of the basic elements of an imaging spectrometer. Some sensors use multiple detector arrays to measure hundreds of narrow wavelength (λ) bands.
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.
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.
Airborne, LEO, & GEO Hyperspectral Activities
5th Workshop on Hyperspectral Science (University of Wisconsin, Madison WI)

1st Hyperspectral Soundings

High Resolution Interferometer Sounder (HIS) (1985- )

NAST-I / SHIS (1995 - )

Hyperspectral Resolution Imagery

Aqua AIRS (2002- )

METOP-IASI (2006- )

NPP/NPOESS/CrIS (2008- )

GIFTS, HES, IRS (??, 2012, 2016)

Satellite

Grating

EOS Hyperspectral Spectrometer

European Hyperspectral Sounder

US Hyperspectral Resolution Sounder

Geostationary Imaging 4-d T,q,“V” Sounder

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"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/CRI/GIFTS Hyperspectral Sounders

FTS (Michelson Interferometer)

AIRS Dispersion (Grating)

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NAST and AIRS Characteristics

- 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 Optical spectroscopy
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Water Vapor Flux (3 x 3 GIFTS Cubes)
Minimum Deviation by a Prism

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

\[ \alpha = \theta_{t1} + \theta_{i2} \]

\[ \delta = \theta_{i1} + \theta_{t2} - \alpha \]

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

![Diagram showing minimum deviation angle with angles labeled as $i$, $t_1$, $t_2$, and $\alpha$]

$n = 1.5$

\[ \delta \]

\[ \theta_{i1} \]

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