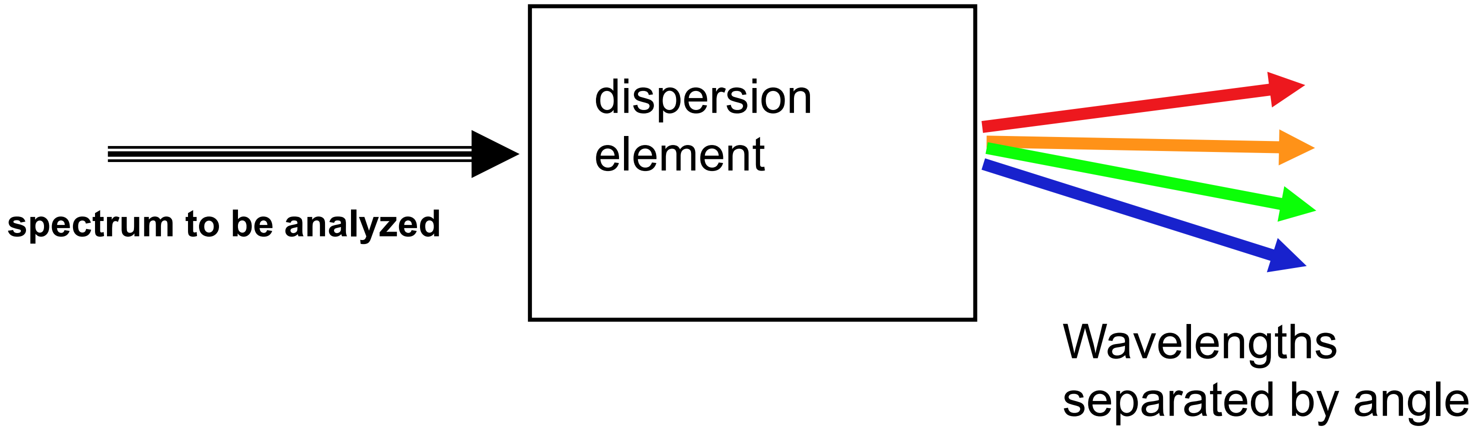
Reflectance and Diffuse Spectroscopy

Spectroscopy

- **What is it ? from the Greek:**
  - spectro = color + scope = look at or observe
    = measuring/recording the colors of light
- **What can we learn from it?**
  - Energy levels of atoms and molecules
  - Fundamental processes
  - The molecular constituents in tissues
- **When you measure how much of each color there is, you're measuring a "spectrum."**



Newton's prism

Dispersion with a Prism

• n=n(λ)

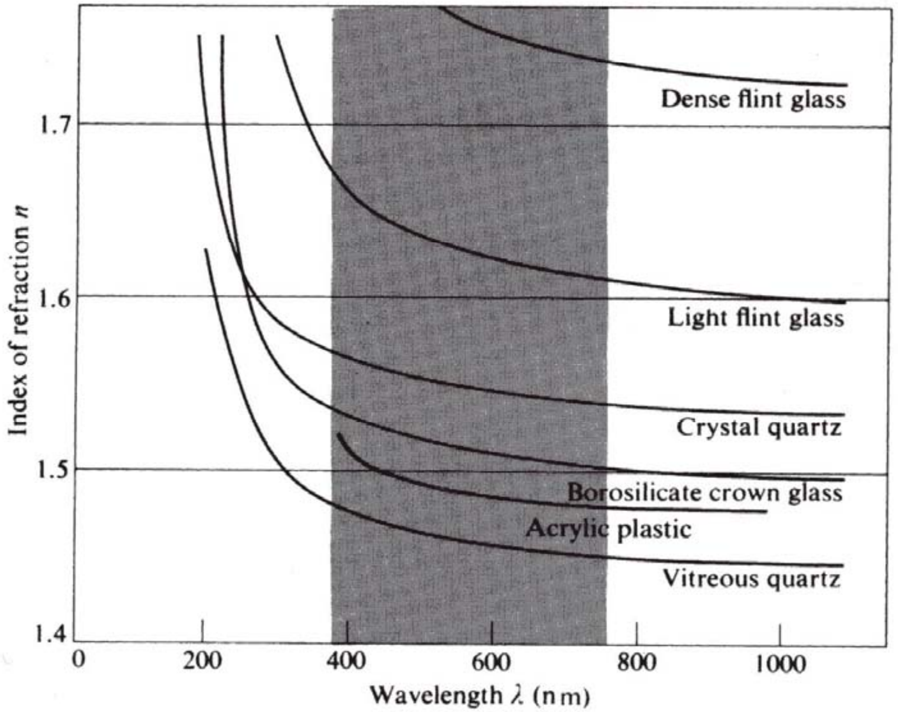
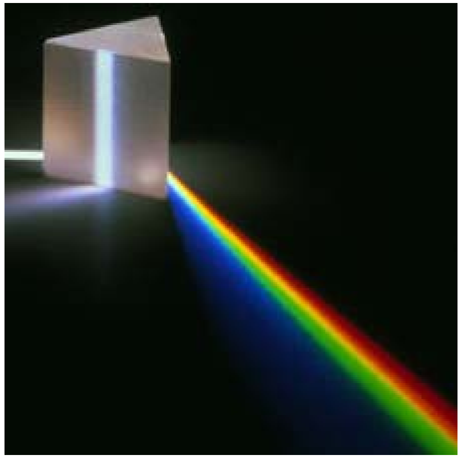
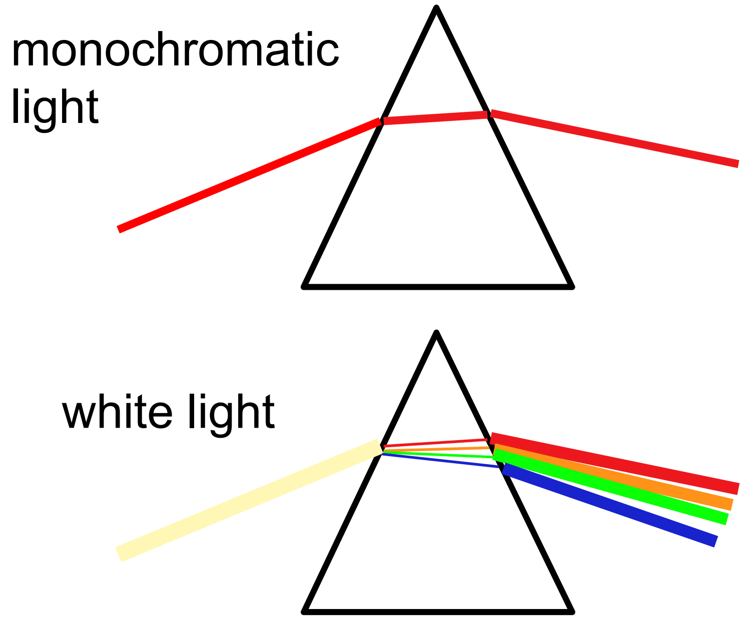


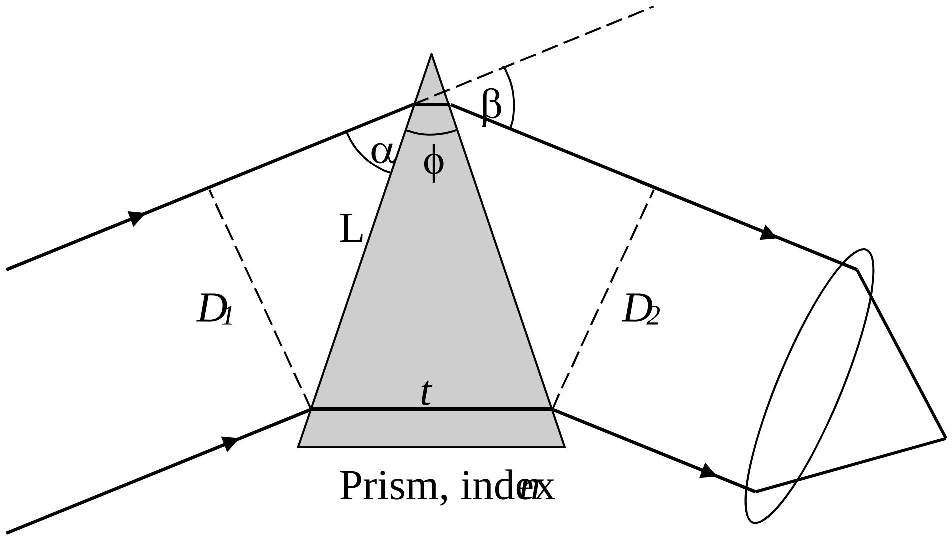
Figure 3.40 The wavelength dependence of the index of refraction for various materials.





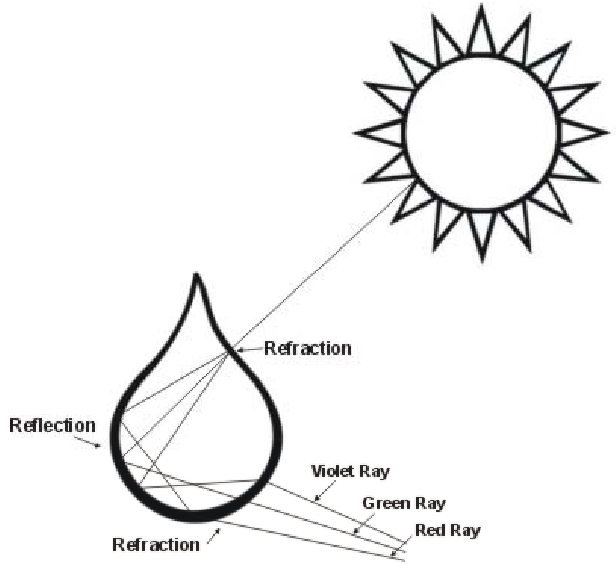
Dispersion with a Prism

- **Resolving Power** $R_{prism} = \frac{\lambda}{\delta\lambda} = t\frac{dn}{d\lambda}$
- **Spectral Resolution** $\delta\lambda = \frac{\lambda}{R}$
- **Useful where only low resolving power is required**
- **Advantages:**
  - simple (but glass must be of high quality)
  - multiple-order overlap not a problem - only one order!
- **Disadvantages:**
  - high resolving power not possible
  - resolving power/resolution can vary strongly with λ



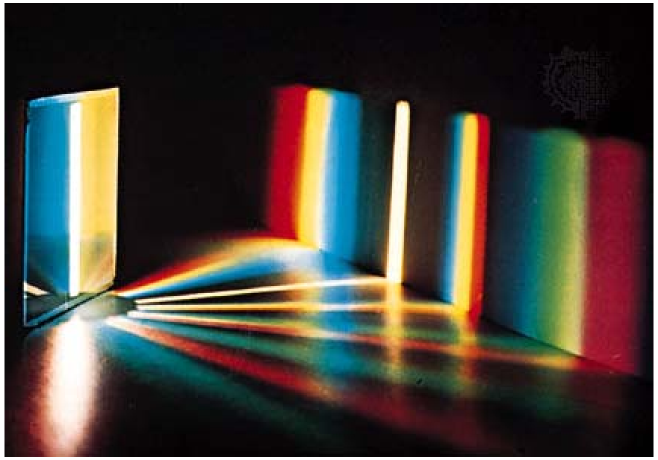
Rainbows

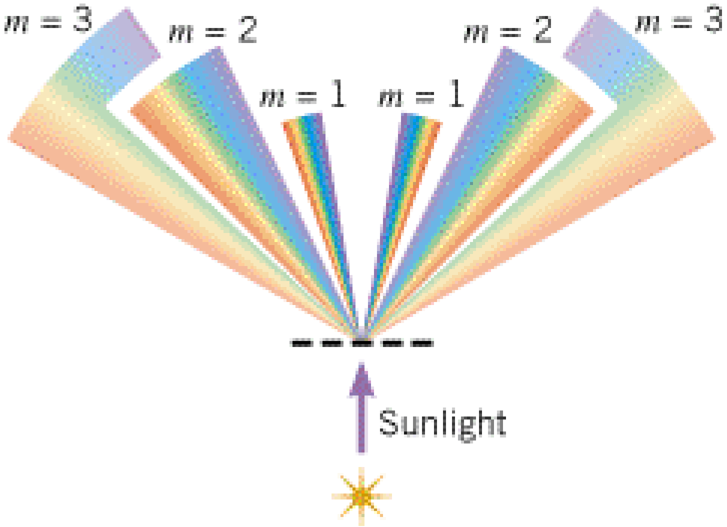
- **What causes rainbows?**
  - Diffraction by rain drops
  - Angle between incident and diffracted rays
    - 42 degrees for red
    - 40 degrees for violet.
  - Form a circular rim of color in the sky → a rainbow!
- **Secondary rainbows**
  - Double reflection of sunlight inside the raindrops
  - Appear at an angle of 50–53 degrees
  - The droplets have to be the right size to get two reflections to work
- **Higher order rainbows are possible**

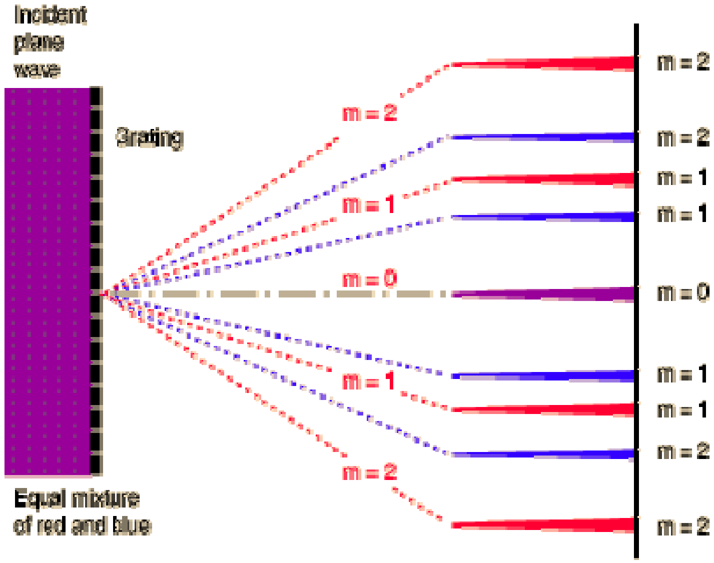


Dispersion with a Grating

- **Diffraction grating**
  - An optical unit that separates polychromatic light into constant monochromatic composition.

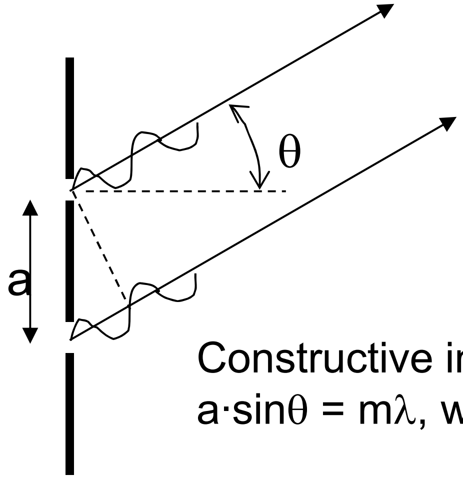




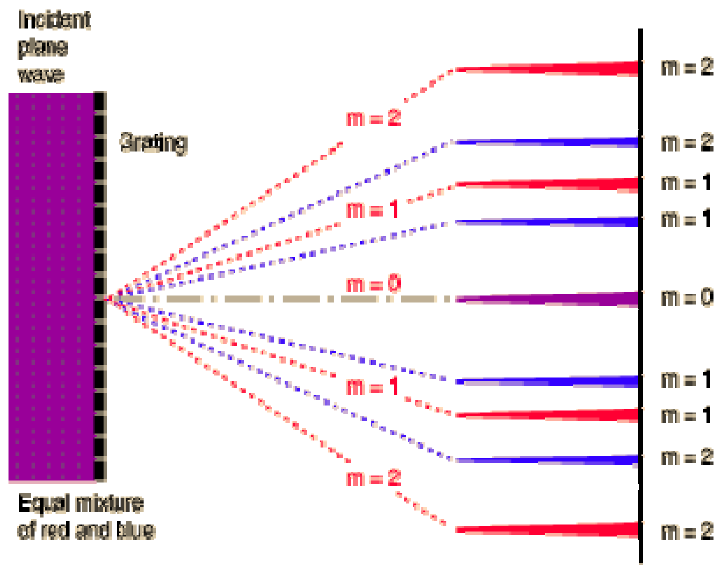


Dispersion with a Grating

- **Multi-slit arrangement**
  - Uses diffraction to separate light wavelengths with high resolution and high intensity.
  - The resolving power is achieved by interference of light.



Constructive interference when
a·sinθ = mλ, where m is an integer



Dispersion with a Grating

- **Diffraction**

$$\frac{m\lambda}{\Lambda} = \sin(a) + \sin(b)$$

- **Littrow's angle (α=β)**

$$\frac{m\lambda}{2\Lambda} = \sin(a)$$

- **Resolving Power**

$$R = \frac{\lambda_o}{\delta\lambda} = mN_{lines} = \frac{mD_a}{\Lambda}$$

- **Spectral Resolution**

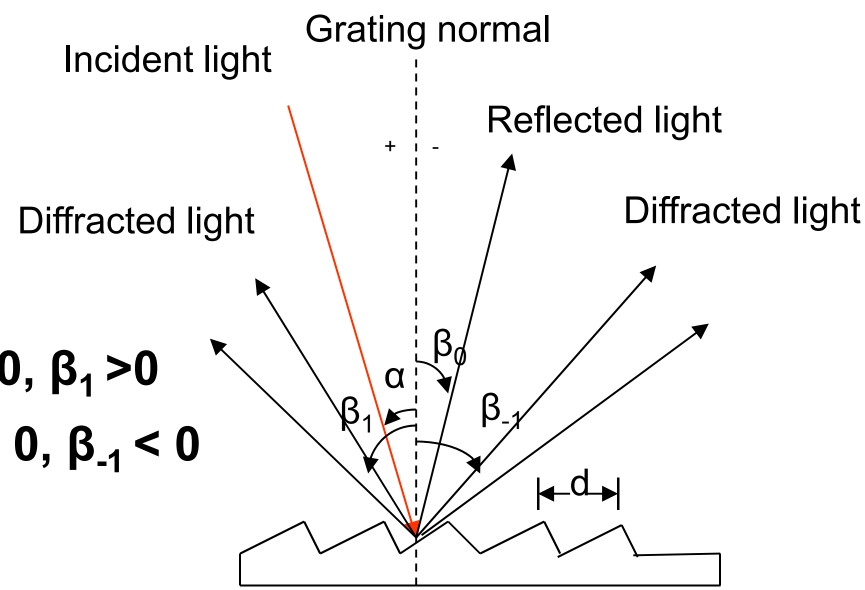
$$\delta\lambda = \frac{\lambda_o \Lambda}{mD_a}$$

- **Efficiency drops with Λ and m**

A Reflection grating

$\alpha > 0$, $\beta_1 > 0$

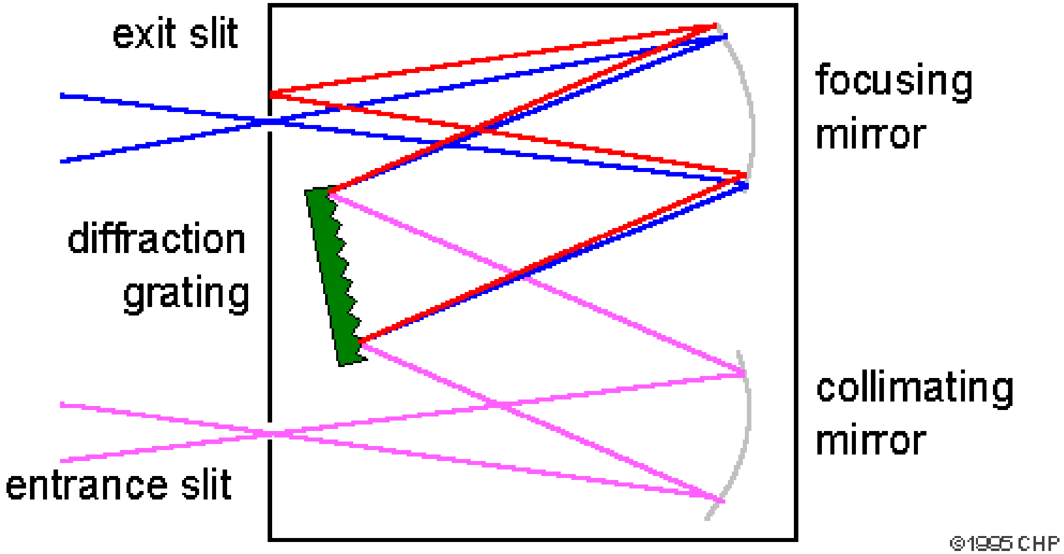
$\beta_0 < 0$, $\beta_{-1} < 0$

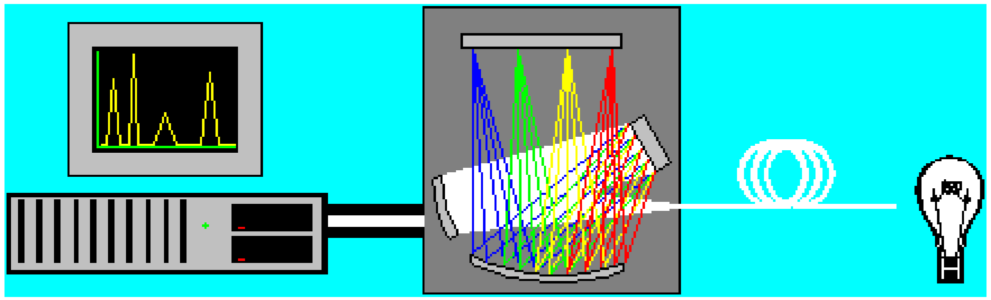


- m: the diffraction order (an integer),
- λ : the wavelength
- Λ = 1/d is the period of grooves
- α: incident angle
- β: diffracted angle
- D_a: aperture diameter (i.e. diameter of grating illuminated)

Anatomy of a grating spectrometer

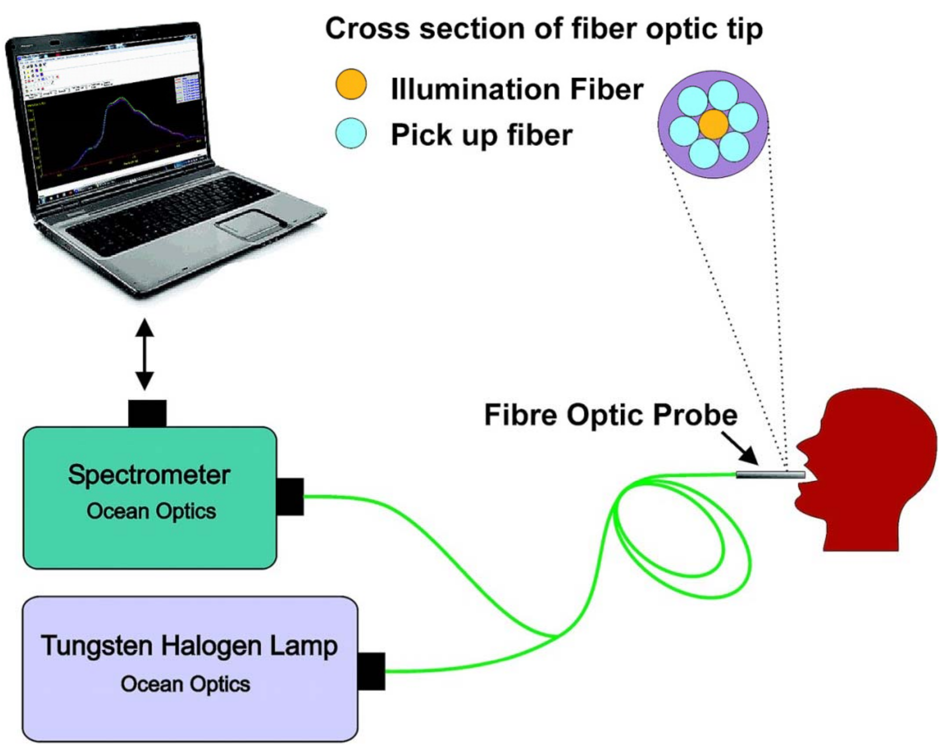
- **Spectrometer**
  - Device to obtain spectrum of light
  - Usually grating
- **Width of slit determines:**
  - Resolving power (w ↓, R↑)
  - Throughput → SNR (w ↓ , I ↓)
- **Hence there is always a tradeoff between throughput and spectral information**





Reflectance Spectroscopy

- **Measures**
  - Changes to source spectrum
- **Effects of**
  - Elastic Scattering
    - Mie and Rayleigh
  - Absorption
    - Many absorbers in tissue
- **Instrumentation**
  - Single point
  - Imaging
    - Many collection fibers → imaging spectrograph
      - Limited spatial resolution
    - Camera with variable filter
      - Limited spectral resolution
- **Applications**
  - E.g. pulse oximeter



Reflectance Spectroscopy

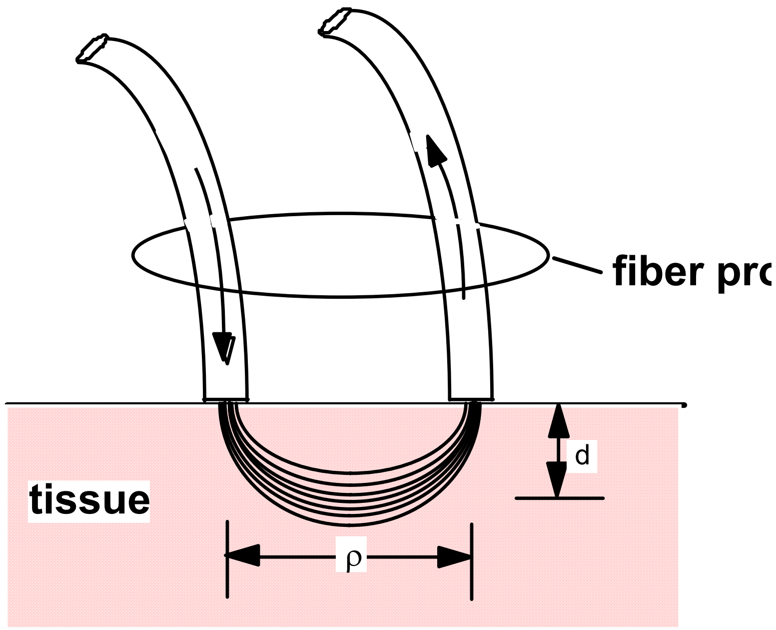
$$I(\rho) = I_0\left[\frac{1}{\mu_t'}\left(\mu_{\text{eff}} + \frac{1}{r_1}\right)\frac{\exp(-\mu_{\text{eff}} r_1)}{r_1^{\,2}} + \left(\frac{1}{\mu_t'} + 2z_b\right)\left(\mu_{\text{eff}} + \frac{1}{r_2}\right)\frac{\exp(-\mu_{\text{eff}} r_2)}{r_1^{\,2}}\right],$$

where

$$r_1 = \left[\left(\frac{1}{\mu_t'}\right)^2 + \rho^2\right]^{1/2}, \quad r_2 = \left[\left(\frac{1}{\mu_t'} + 2z_b\right)^2 2 + \rho^2\right]^{1/2}$$

$$\mu_{\text{eff}} = \sqrt{\frac{\mu_a}{D}},\ \mu_t' = \mu_a + \mu_s' \text{ and } z_b = 2AD,$$

(D=1/μt') and A relates to internal reflection.)



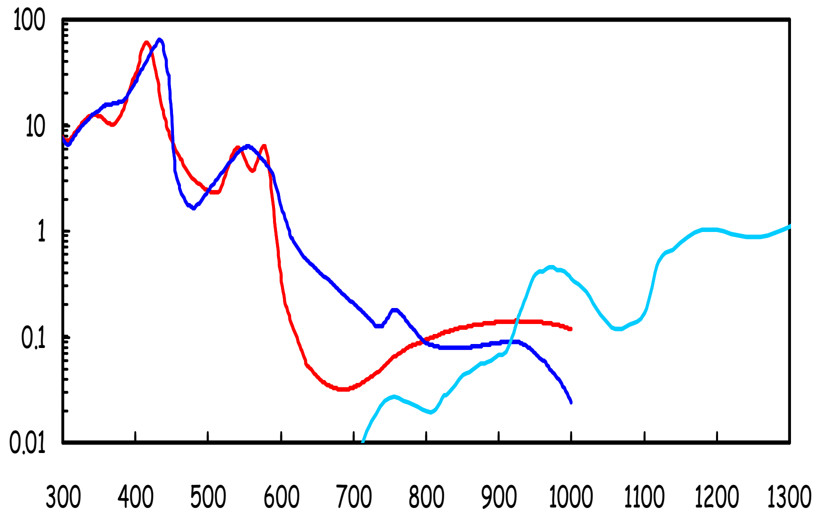
Mourant, etc., and Bigio, Appl. Optics 36, No.4, p.949 (1997)

The Pulse Oximeter

- **Function: Measure arterial blood saturation**
- **Advantages:**
  - Non-invasive
  - Highly portable
  - Continuous monitoring
  - Cheap
  - Reliable

The Pulse Oximeter

- **How:**
  - Illuminate tissue at 2 wavelengths
  - straddling isosbestic point (eg. 650
  - and 805 nm)
    - Isosbestic point: wavelength → where Hb and HbO2 spectra cross.
  - Detect signal transmitted through finger
- **Isolate varying signal due to pulsatile flow (arterial blood)**
- **Assume detected signal is proportional to absorption coefficient**
  - Get the two μ_a
  - Calculate the concentrations (Two measurements, two unknowns)
- **Calibrate instrument by correlating detected signal to arterial saturation measurements from blood samples**



$$\mu_a^{\lambda_1} = \ln 10 * \left\{ \varepsilon_{HbO_2}^{\lambda_1} [HbO_2] + \varepsilon_{Hb}^{\lambda_1} [Hb] \right\}$$

$$\mu_a^{\lambda_2} = \ln 10 * \left\{ \varepsilon_{HbO_2}^{\lambda_2} [HbO_2] + \varepsilon_{Hb}^{\lambda_2} [Hb] \right\}$$

$$\text{Arterial } O_2 \text{ saturation} = \frac{[HbO_2]}{[HbO_2 + Hb]} * 100\%$$

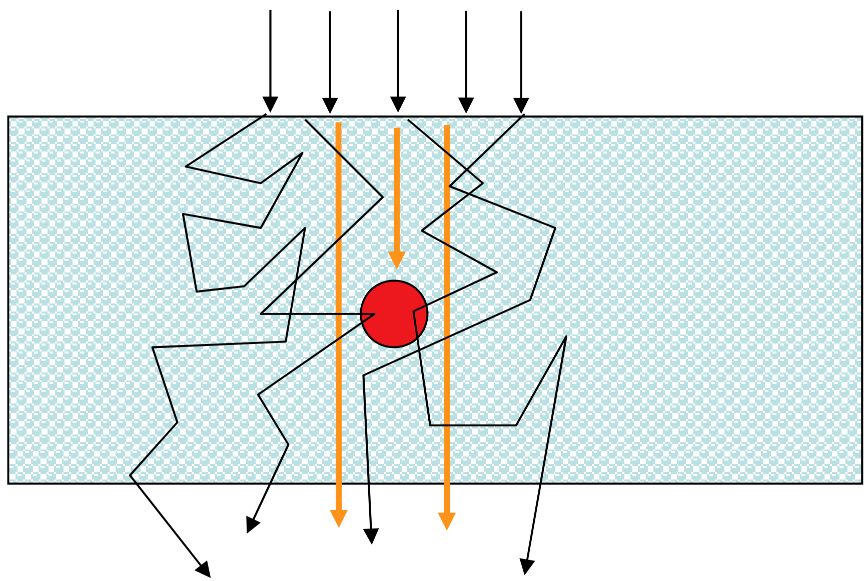
ε is the extinction coefficient

The Pulse Oximeter

- **Limitations:**
  - Reliable when O_2 saturation above 70%
  - Not very reliable when flow slows down
  - Can be affected by motion artifacts and room light variations
  - Doesn't provide tissue oxygenation levels

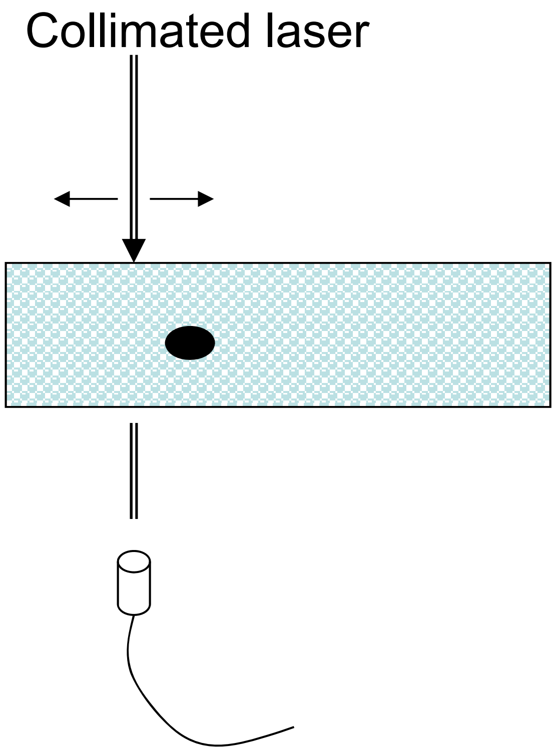
Turbid Media

- **How can we image objects embedded in turbid media?**
  - **Cheat !!**
- **Try to devise a method to detect only the photons that have not scattered**
  - Generating a direct shadow image (like an x-ray).
- **Possible methods**
  - Collimated Illumination
    - Use of polarizers
  - Detect “snake” photons

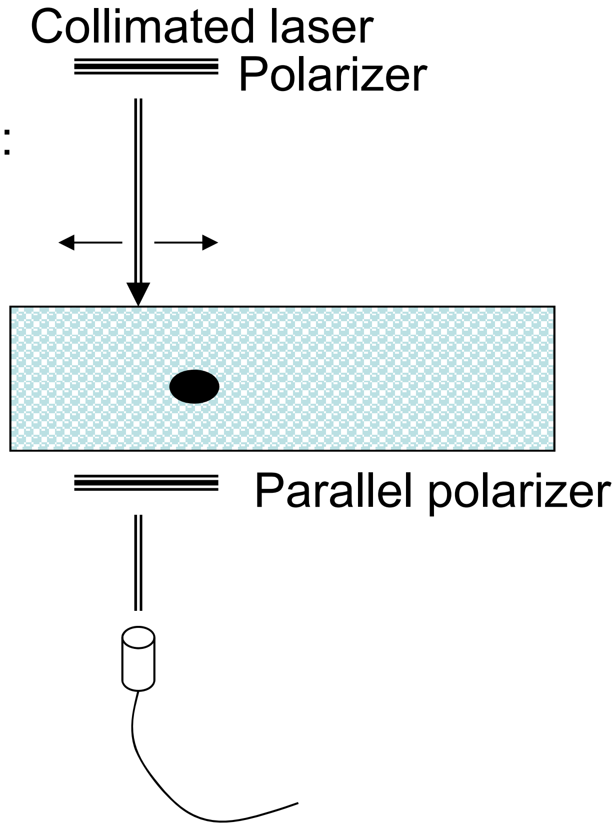


Turbid Media

- **Collimated illumination and detection**

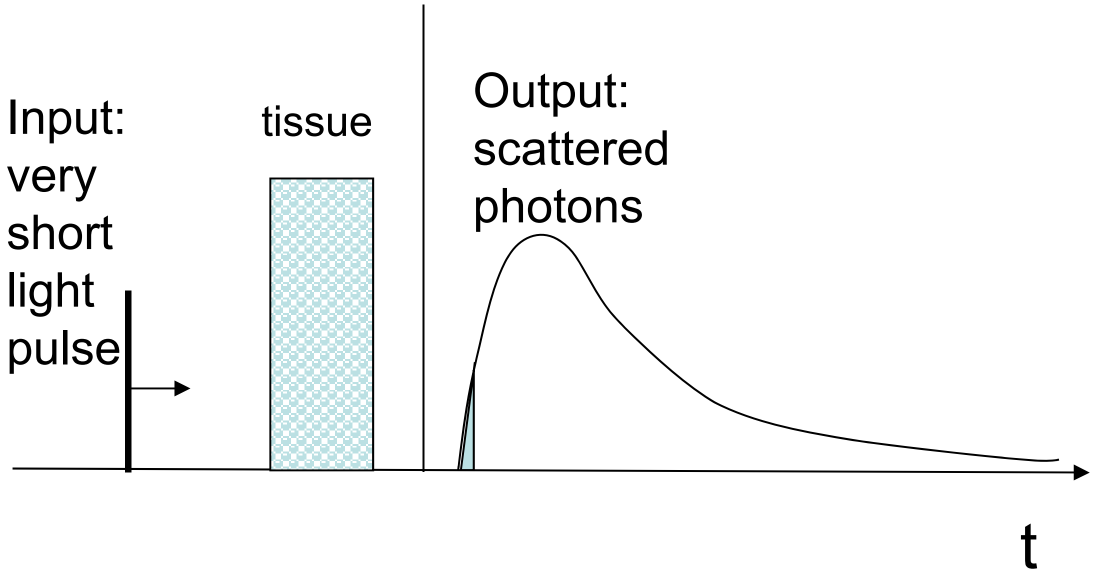


Can add polarizers:



Turbid Media

- **The earliest arriving photons have traveled the straightest path**
  - Can we select only the earliest photons?
- **Time gating methods**
  - Streak camera
  - Time-to amplitude converters
  - Coherence gates
  - Nonlinear optical gates
    - Kerr gate
    - Second harmonic generation
    - Raman amplification

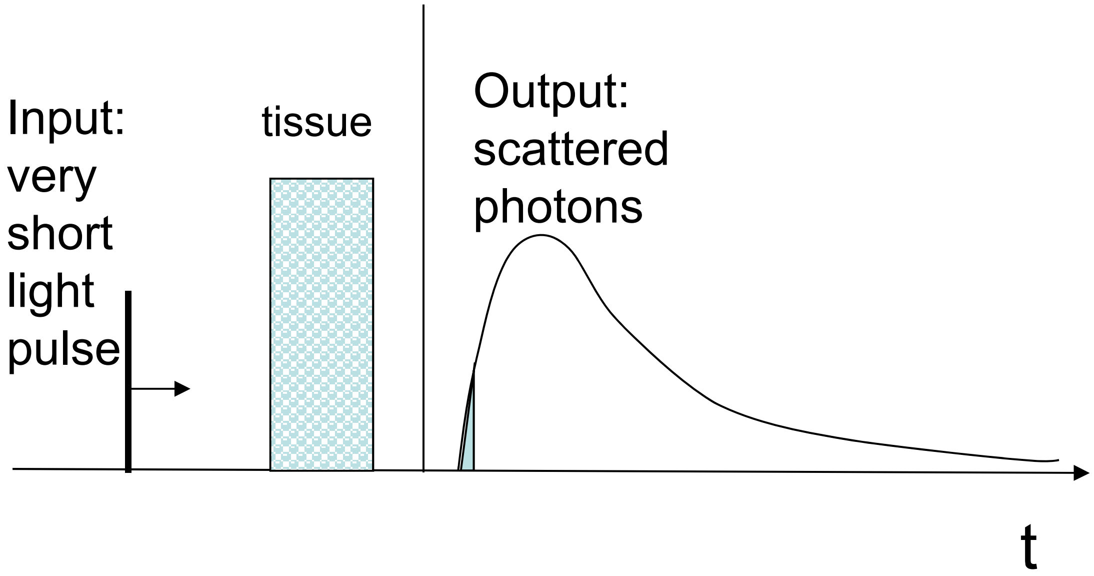


Turbid Media

- **But, are there enough unscattered photons??**
  - Beer's law can also tell us how many photons remain unscattered after a given distance in tissue:

$$I_U = I_0 e^{-\mu_s' L}$$

  - A typical value for many tissues: $\mu_s' \sim 10\ cm^{-1}$
  - $\Rightarrow$ for optical mammography there are very few unscattered photons



Turbid Media

How can we image with diffuse light?

- **The "forward" problem**
  - Asks: if we know the light going in, and we know what the hidden object is, can we calculate what reaches the surface in different locations?
- **The "inverse" problem**
  - Asks: if we know the light going in, and we measure the light coming out at various locations, what can we say about the hidden object?
- **Methods**
  - Monte Carlo
  - Diffusion Approxiamtion
  - Time Domain vs. Frequency domain

Turbid Media

How do we solve an inverse problem?

- **Sometimes done as an iteration of forward calculations:**
  1. Must make assumptions about the optical properties of the surrounding tissue
  2. Make an initial "guess" about the location, size and optical properties of the lesion.
  3. Do a forward propagation calculation and see how those results compare with the measurements.
  4. Re-estimate the properties of the lesion based on the difference, and recalculate the forward problem.
  5. Repeat many times!!!

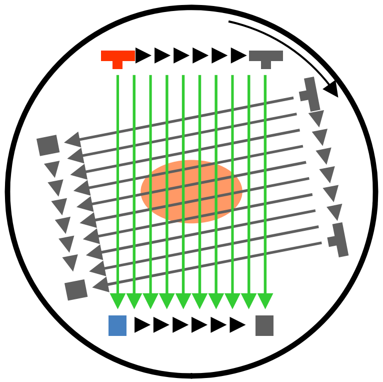
Diffuse Optical tomography (DOT)

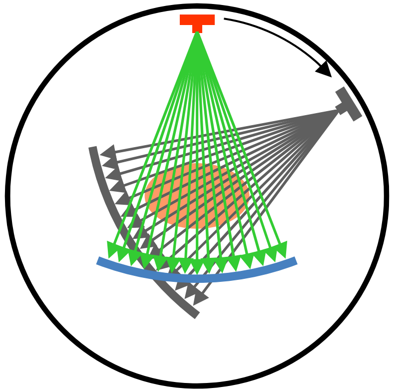
• Year discovered:	~1988
• Form of radiation:	Near-infrared light (non-ionizing)
• Energy/wavelength of radiation:	~1 eV / 600–1000 nm
• Imaging principle:	Interaction (absorption, elastic scattering) of light w/ tissue
• Imaging volume:	~10^3 cm^3
• Resolution:	Low (~1cm)
• Applications:	Perfusion, functional imaging

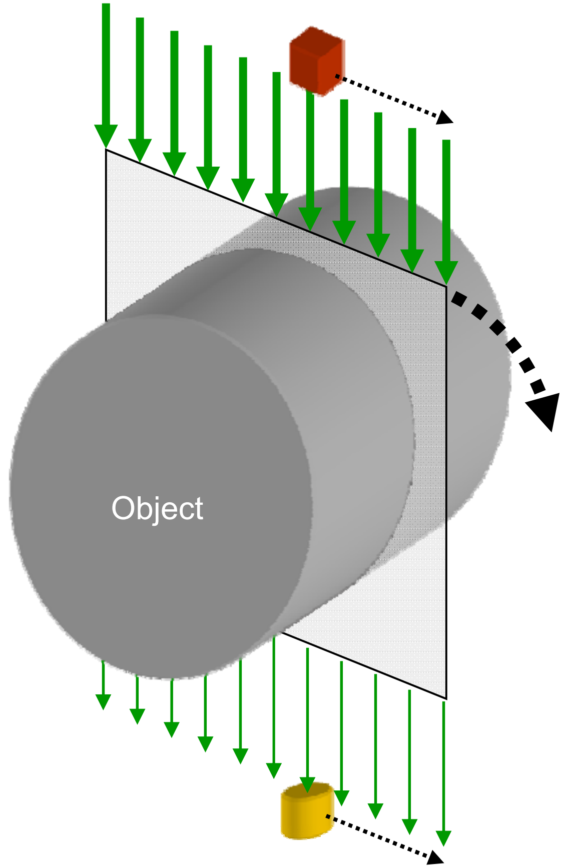
Diffuse Optical tomography (DOT)

DOT and CT

- **Superficial Similarities**
  - Generation: x-ray tube
  - Detection: Detector arrays (ion.-chambers, scint. + photodiode)
  - Computer reconstruction of 2D slices/ 3D volumetric images
- **Essential Differences**
  - No scattering!

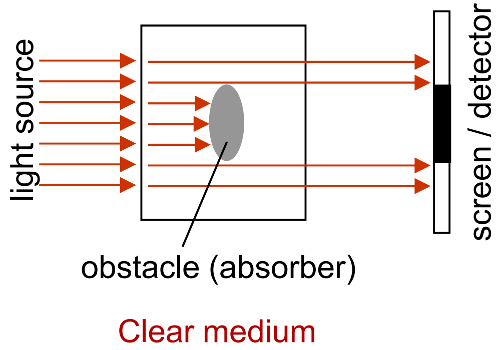


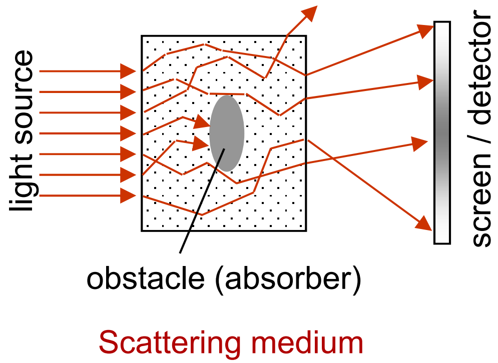


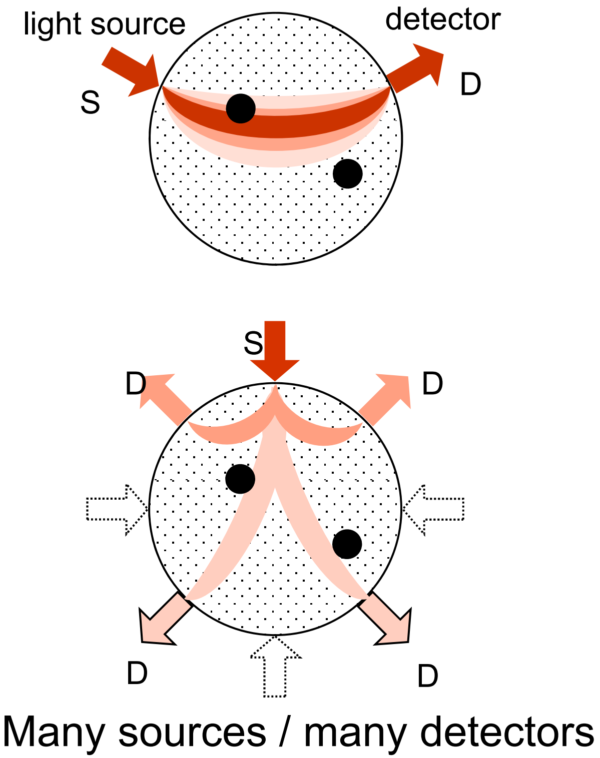


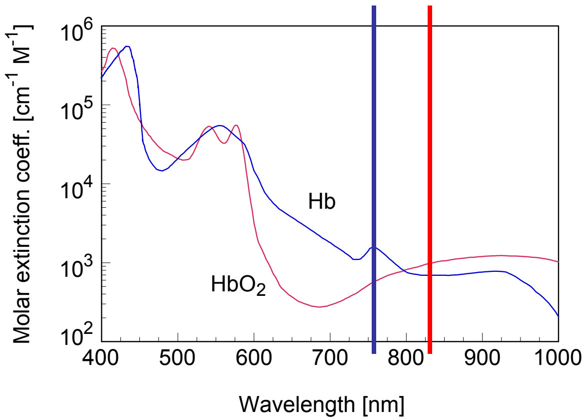
Diffuse Optical tomography (DOT)

- **Principles of DOT**
  - Scattering dominated
  - Limited penetration depth (~cm), low res. (mm-cm)
  - Economic, functional (hemodynamics)



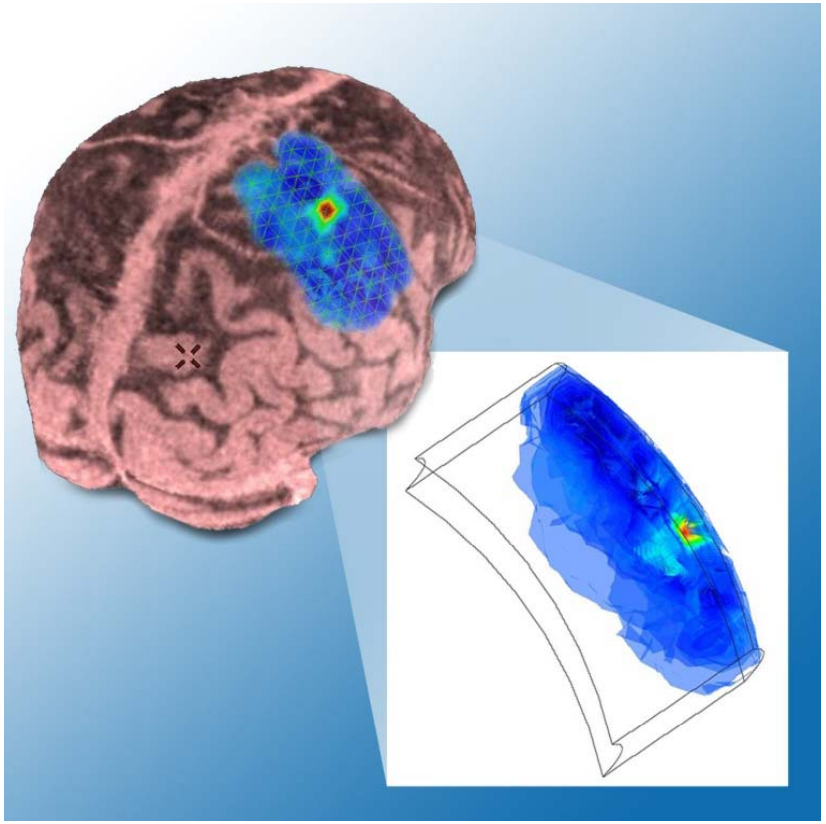


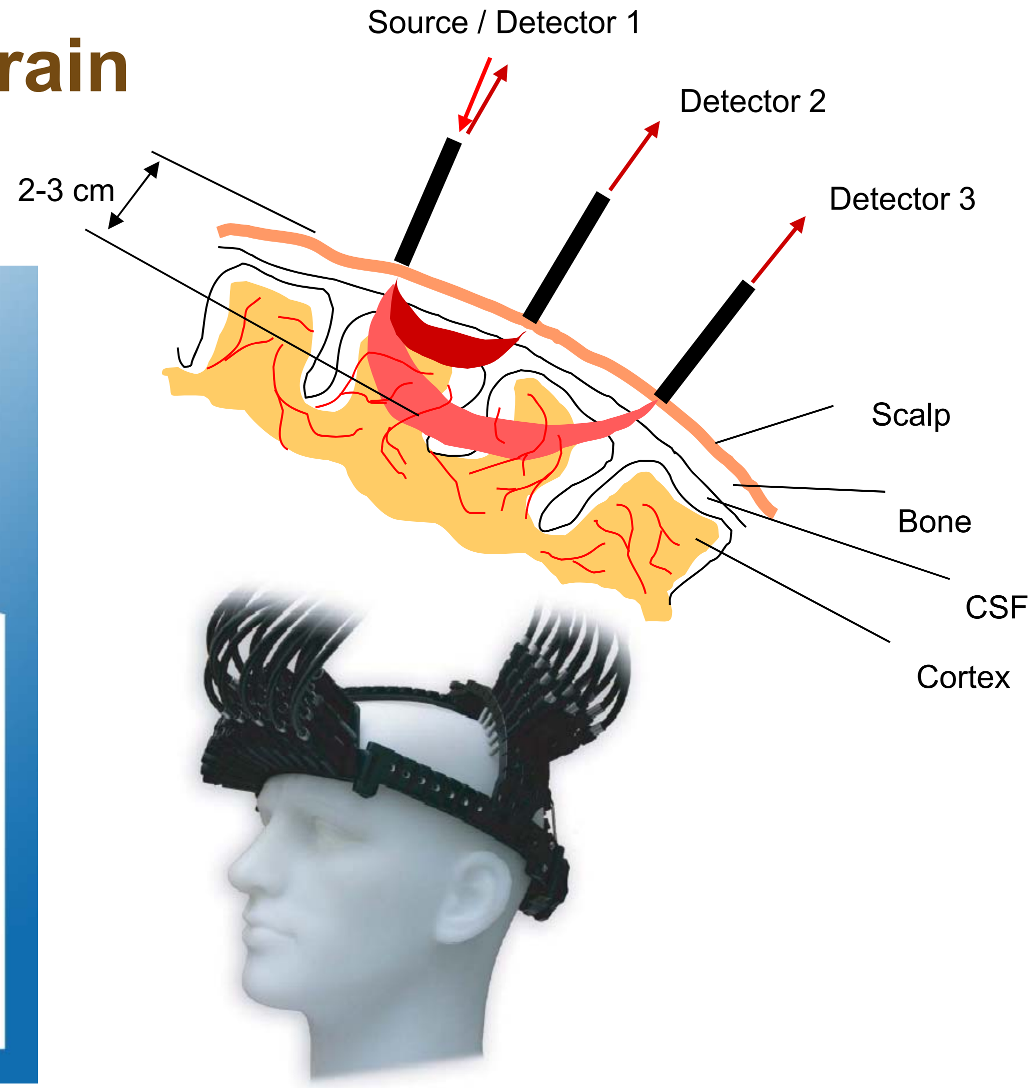




Diffuse Optical tomography (DOT)

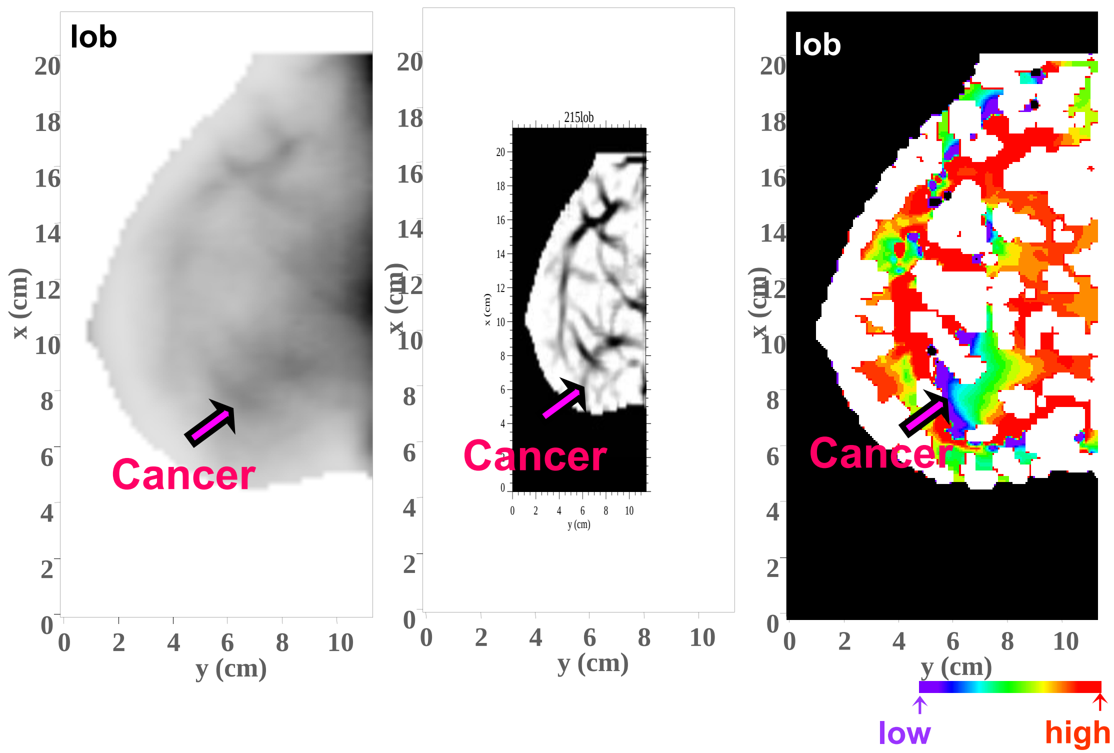
- DOT Applications - Brain

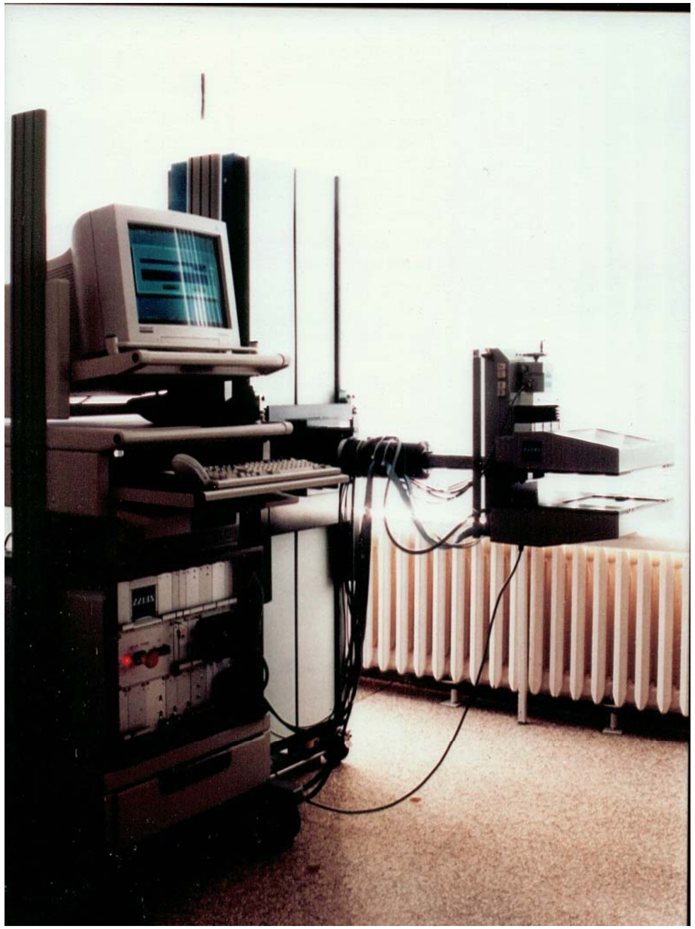




Diffuse Optical tomography (DOT)

- **DOT Applications - Breast**





Atomic spectroscopy

- **Atomic spectroscopy**
  - Not very relevant to medical applications.
    - Flames, electrical discharges (especially in gases)
  - However, one method may prove useful → Laser-induced breakdown spectroscopy (LIBS)
- **Laser-induced breakdown spectroscopy (LIBS)**
  - Atomic emission spectroscopy
  - Highly energetic laser pulse focused to form a plasma
  - Emit light of characteristic frequencies
  - LIBS at surface of skin could be used to sense heavy metal contamination