Physical basis of dental material science 10.

Thermal and optical properties

Thermal properties

• **temperature: proportional to the internal energy of the material.**
(unit: K, °C in physics K is used mainly)

• **Heat uptake/loss – exchange between the object and the enviroment.**

Heat capacity (C):
(energy that increases the temperature by 1 K)

$$C = \frac{\Delta Q}{\Delta T}$$

ΔQ – exchanged thermal energy
n – no. of mols
m – mass
ΔT – temperature change

molar heat capacity (c_v):
(heat capacity for one mol)

$$c_v = \frac{C}{v}$$

c_p –measured at constant pressure
c_V – measured at constant volume

specific heat capacity (c):
(heat capacity for unit mass)

$$c = \frac{C}{m}$$

$$c_p > c_V$$

Specific heat capacity

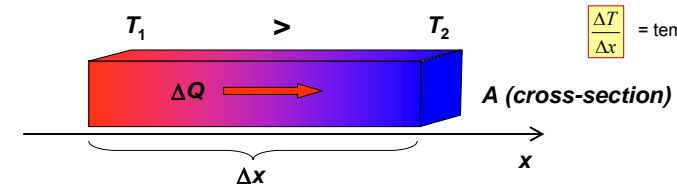High specific heat of the water is important from the viewpoint of the life!
(thermal stability)

specific heat capacity of some dental materials:

material	c (J/(kg·K))
Enamel	750
Dentin	1260
Water	**4190**
Amalgam	210
Gold	126
Porcelain	1100
Glass	800
PMMA	1460
ZnPO$_4$	500

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thermal conduction

$$\Delta t = T_2 - T_1$$

T_1 > T_2

$$\frac{\Delta T}{\Delta x}$$ = temperature gradient

ΔQ

A (cross-section)

Δx

x

How is the energy transported?

lattice oscillation

In metals e.g. motion of the free electrones.

time increases

Thermal conductivity

Fourier-law

$$\frac{\Delta Q}{\Delta t} = -\lambda A \frac{\Delta T}{\Delta x}$$

λ — **thermal conductivity**
$J/(s \cdot m^2 \cdot K/m) = W/(m \cdot K)$

Characterizes well the phenomenon in the case of stationary flow!

(stationary – the parameters are constant in time)

Thermal conductivity of some dental material:

material	λ (W/(mK))
Enamel	0.9
Dentin	0.6
Water	0.44
Amalgam	23
Gold	300
Porcelain	1
Glass	0.6-1.4
Acrylate	0.2
PMMA	0.2-0.3
$ZnPO_4$	1.2

Non-stationary case

$$D = \frac{\lambda}{c_p \rho}$$

D — thermal **diffusivity** (m^2/s)
(may be different in the different points of the material)

ρ — density
c_p – specific heat capacity at constant pressure

Thermal diffusivity of some dental materials:

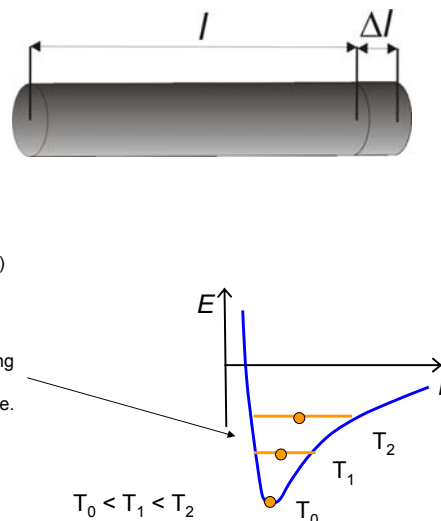| material	λ (W/(mK))	D (10^{-6} m²/s)
Enamel	0.9	0.5
Dentin	0.6	0.2
Water	0.44	0.14
Amalgam	23	9.6
Gold	300	118
Porcelain	1	0.4
Glass	0.6-1.4	0.3-0.7
Acrylate	0.2	0.1
PMMA	0.2-0.3	0.12
$ZnPO_4$	1.2	0.3

Thermal expansion

Linear expansion:

$$\frac{\Delta l}{l_0} = \alpha \, \Delta T$$

$$l = l_0 (1 + \alpha) \, \Delta T$$

α — **coefficient of thermal expansion** (1/K)

Increasing temperature results increasing oscillation of particles.
This may be observed as increasing size.

$T_0 < T_1 < T_2$
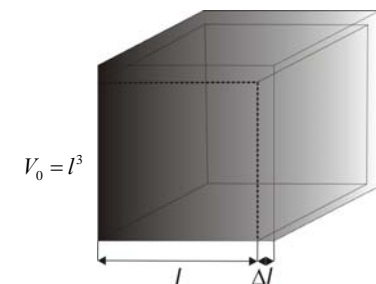

Volumetric thermal expansion

$$\frac{\Delta V}{V_0} = \beta \, \Delta T$$

$$V = V_0 (1 + \beta) \, \Delta T$$

β — **volumetric thermal expansion coefficient** (1/K)

for isotropic materials:

$$\beta \approx 3\alpha$$

$V_0 = l^3$

Isotropic: properties are independent from the direction

The coefficient of thermal expansion of some dental materials :

Material	α (10^{-6} 1/K)
Enamel	11.4
dentin	8.3
Gold	14,2
Gold alloys	11-16
Amalgam	≈ 25
Porcelain	4-16
Acrylate	90
Glass	8
PMMA	90-160
Silicon	100-200
gypsum	15-20
wax	300-500

different expansion $\Longrightarrow$ stress!

Conservative dentistry!

Optical properties

What is the light?

- electromagnetic wave
- propagation of the energy (radiation)
- propagates in straightline
- Interact to the material

Sources: Sun - thermal radiation
luminescence (cold light)

Egyptian mythology.
The Sun as the
source of the light.

What is the electromagnetic wave?

wave: propagating oscillation.

E

λ

at a given moment

direction of propagation

in a given point

H

E T

time

E – strenght of the electric field
H – strength of the magnetic field
λ - wavelength
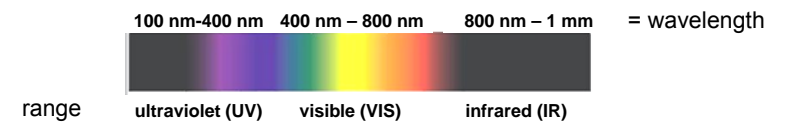T - period

speed of the wave

$$c = f \cdot \lambda$$

f – frequency = 1/T (T – period)

$$c = \frac{c_0}{n}$$

speed in vacuum
~ $3 \cdot 10^8$ m/s

refractive index of the material (absolute)

spectrum: distribution of the energy versus the frequency (or wavelength)

100 nm-400 nm   400 nm – 800 nm   800 nm – 1 mm   = wavelength

range   ultraviolet (UV)   visible (VIS)   infrared (IR)
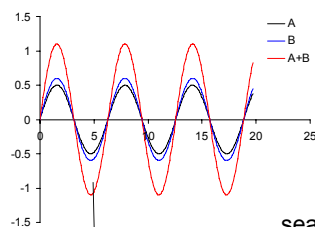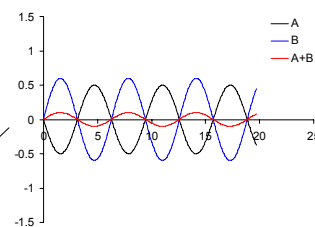
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• **wave phenomena**   **superposition** of 2 or more waves: the amplitudes are summed.
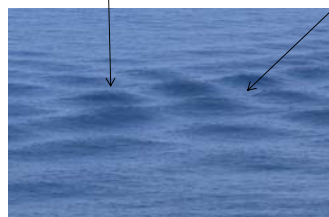
positive (constructive) interference
(same phase: see below)

negative (destructive) interference
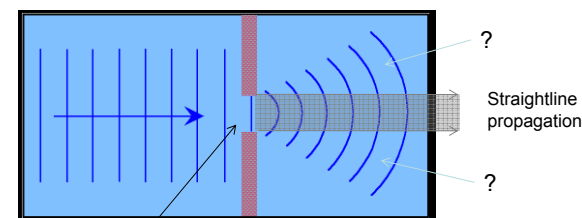(opposite phase: see below)

sea waves

Interference pattern
Stable constructive
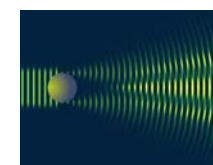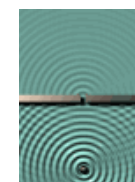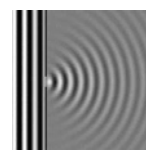and destructive
interference points

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Diffraction

?

Straightline
propagation

?

slit (size is close to the wavelength)

may be any barrier

Slide (Diffraction and interference)

Diffraction and interference

monochromatic light
(practically only 1 wavelangth)

white light
(whole spectrum)
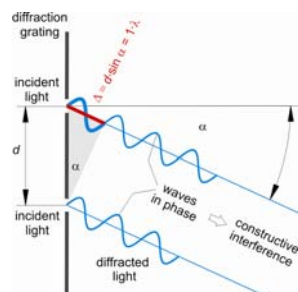
Spots are the points of
constractive interference.

Depends on the wavelength!

$$d \cdot \sin \alpha = k \cdot \lambda$$

(k =0, 1, 2 …)

diffraction
grating

incident
light

d

incident
light

diffracted
light

waves
in phase ⇨ constructive interference

The direction of the constructive
interference depends ont the
wavelength!

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Photon

Photoelectric effect

vacuum

electrons

light

alkali metal

$$\varepsilon = A + E_e$$

A – work function
E_e – kinetic energy of electrons

Planck constant

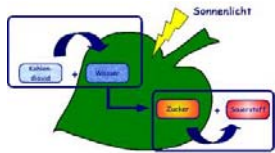$$\varepsilon = h \cdot f$$

photonenergy

frequency

Threshold frequency exists.
Below this frequency there are no free electrons.

Energy is quantized and the
quantum is the photon.

Energy transport

Photosynthesis is the base of the life.

Chloroplast absorbs the light energy and stores in molecules as chemical energy.

Solar cell converts the light energy into electric one.

The absorbed energy in the skin results reddening.

Crude oil contains the stored energy of the Sun.

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Intensity (J)

Energy propagates in the radiation.

light
ΔP

ΔA

Intensity characterizes the strength of the radiation.

$$J = \frac{\Delta P}{\Delta A} \qquad \left(\frac{W}{m^2}\right)$$

ΔA – surface of the area.
ΔP – Power of the radiation propagating thrue the whole.
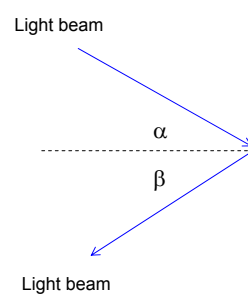Power: energy during unit time

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Geometrical optics

• **light propagates in straightline.**

reflection

Light beam

α

β

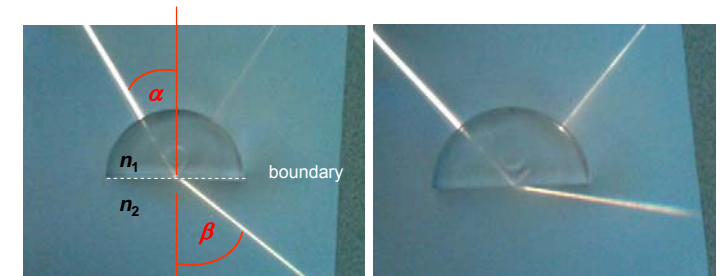$$\alpha = \beta$$

Light beam

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Refraction

Snell's law:

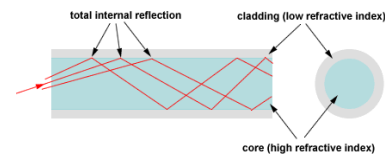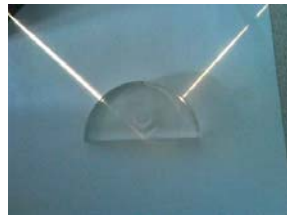$$\frac{\sin \alpha}{\sin \beta} = \frac{c_1}{c_2} = \frac{n_2}{n_1} = n_{21}$$

(relative) refractive index
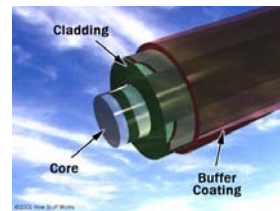
α

n_1

boundary

n_2

β

határszög

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Application of the total internal reflection

total internal reflection   cladding (low refractive index)

core (high refractive index)

optical fiber

Application of the total internal reflection
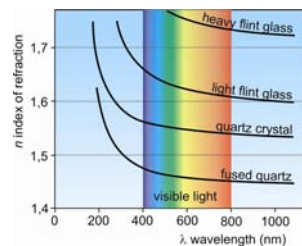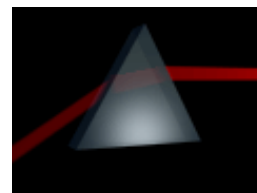
mirage:

dentistry

endoscopy

Dispersion of the light
(n depends on the wavelength)

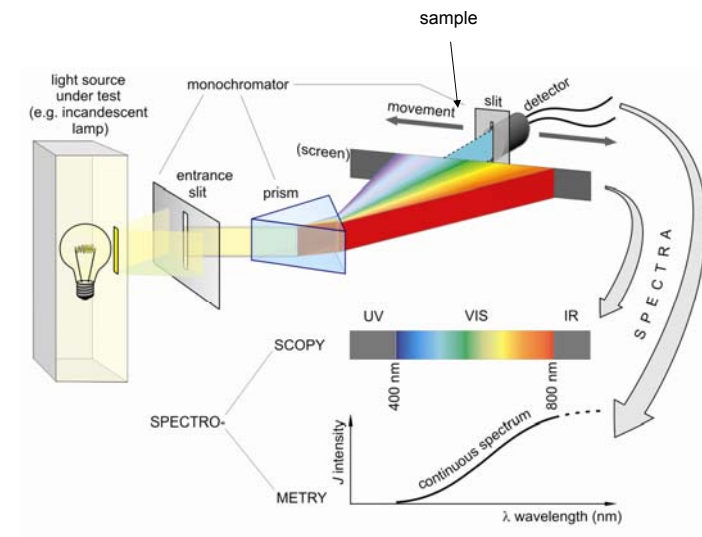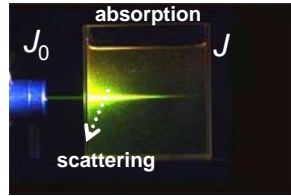$n(\lambda)$

monochromatic light
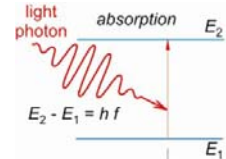

white light

rainbow

Spectroscopy and spectrometry

sample

Interaction to the matter

Consequence
$$J < J_0$$

absorption

J_0 J

scattering

Attenuation: decreasing intensity

attenuation = scattering + absorption

Inhomogenity of the refractive index in the material!

light photon   *absorption* E_2

$E_2 - E_1 = h\,f$

E_1

Light scattering

elastic scattering
(λ, f, ε are constant)

inelastic scattering
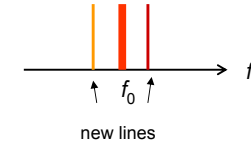(λ, f, ε are not constant)

Rayleigh-scattering
particle size $<< \lambda$

$$\text{scattered intensity} \sim \frac{1}{\lambda^4}$$

blue sky: blue is scattered better.
(wavelength is shorter)

Raman-scattering

f_0 f

new lines

Mie-scattering
size of the scattering particle $\geq \lambda$
(no strong λ dependency)
(white clouds)

Attenuation law

if the scattering is negligible

attenuation ~ absorption
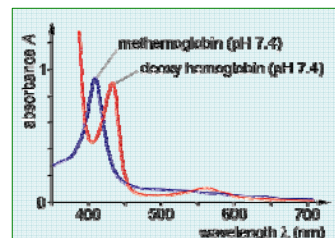
transmission

$$\bar{T} = \frac{J}{J_0}\,(\cdot 100\,\%)$$

absorbance

$$A = \lg\frac{J_0}{J}$$

attenuation coefficient

$$J = J_0 \cdot e^{-\mu \cdot x}$$

absorption spektrum: A(λ)

methemoglobin (pH 7.4)
deoxy hemoglobin (pH 7.4)

absorbance A

400   500   600   700
wavelength λ (nm)

Attenuation law

J

$\mu_4 > \mu_3 > \mu_2 > \mu_1$ transparent

J_0

μ_2

$J_0/2$

μ_3

$J = J_0\,e^{-\mu \cdot x}$

μ_4

opaque

D x

layer thickness

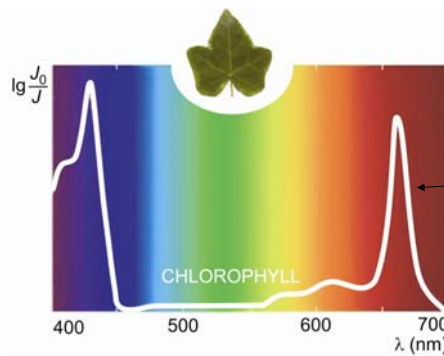**penetration depth (δ):**

$$\delta = \frac{1}{\mu}$$

half-value thickness (D):

$$D = \frac{\ln 2}{\mu}$$

absorption spectra

CHLOROPHYLL

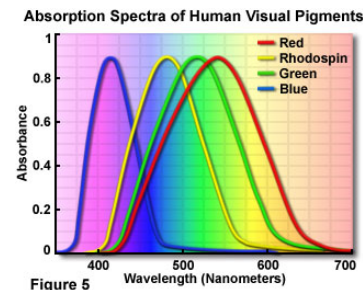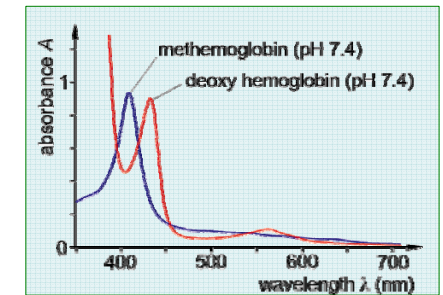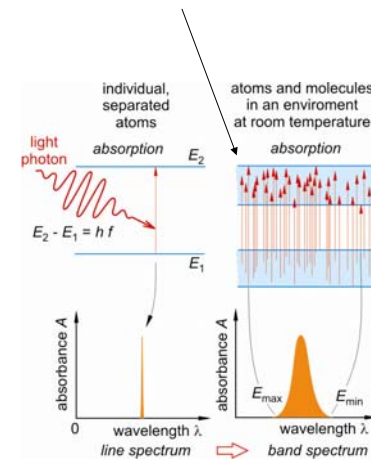Green color of the plants is due to the absorption in red.

The colour of a material depends on the absorption.

Color vision

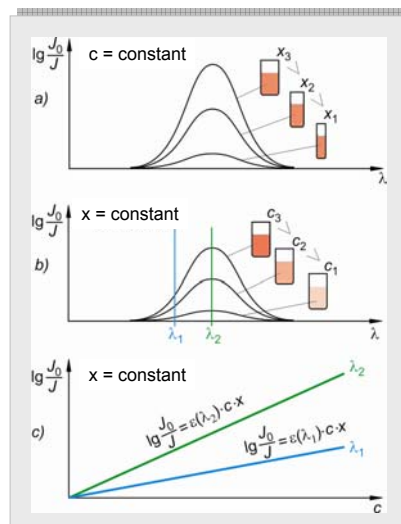**Absorption Spectra of Human Visual Pigments**

Figure 5

Line and band spectra

The energy state of the electrons depends on the envireoment a little bit.

Materials in solvent usually have band spectrum.

individual, separated atoms — absorption — E_2

atoms and molecules in an enviroment at room temperature — absorption

$E_2 - E_1 = h\,f$

E_1

E_{max} E_{min}

wavelength λ
line spectrum $\Longrightarrow$ band spectrum

methemoglobin (pH 7.4)
deoxy hemoglobin (pH 7.4)

Application of the attenuation

a) $\lg\frac{J_0}{J}$ c = constant

b) $\lg\frac{J_0}{J}$ x = constant

c) $\lg\frac{J_0}{J}$ x = constant

$\lg\frac{J_0}{J} = \varepsilon(\lambda_2)\cdot c\cdot x$

$\lg\frac{J_0}{J} = \varepsilon(\lambda_1)\cdot c\cdot x$

Lambert-Beer law:

$$A = \varepsilon(\lambda)\cdot c\cdot x$$

Possibility to measure the concentration.