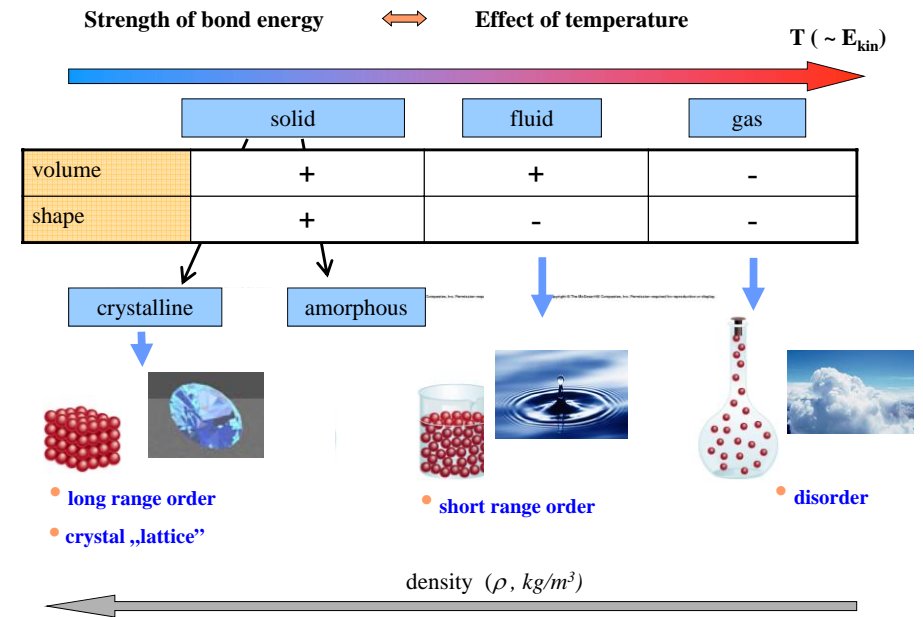


Physical bases of dental material science

Irén Bárdos-Nagy



Density of materials used in Dentistry

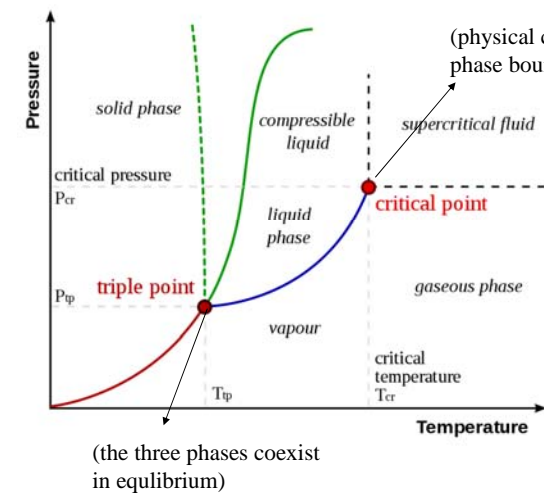
$$1 \frac{kg}{m^3} = \frac{10^3 g}{(10^2)^3 cm^3} = \frac{10^3 g}{10^6 cm^3} = 10^{-3} \frac{g}{cm^3}$$

Broad scale of materials – broad scale of structures and properties

material	ρ (g/cm ³)
dental enamel	2,2
dentine	1,9
water	1
amalgam	≈ 12
gold	19,3
gold-alloys	12-17
Pd-Ag alloys	10-12
Co-Cr alloys	8-9
Ni-Cr alloys	≈ 8
glass	2,2-2,7
ceramic	1,6-3,9
porcelain	2,2-2,4
gypsum (CaSO ₄ ·x2H ₂ O)	2,31-2,76
PMMA poly(methylmethacrylate)	≈ 1,2
silicon poly(dimethylsiloxane)	≈ 1,4

A typical phase diagram

phase diagram: graphical presentation of stable phases as a function of different parameters



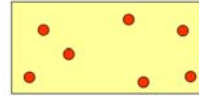
simultaneous transition of Ar from solid to liquid and to gas

Classes of materials

Gas phase (ideal gas)

characteristics

- filling the container – no volume in itself
- disorder
- composed of independent particles
- isotropy



Macroscopic properties/parameters

p, V, ν, T

R – universal gas constant
 $R = 8.314 \text{ J/mol} \cdot \text{K}$

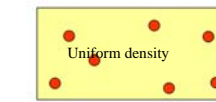
$$pV = \nu RT$$

Equation of state

↑
mole number

Gas phase (ideal gas) without force field

Microscopic description



Macroscopic properties/parameters

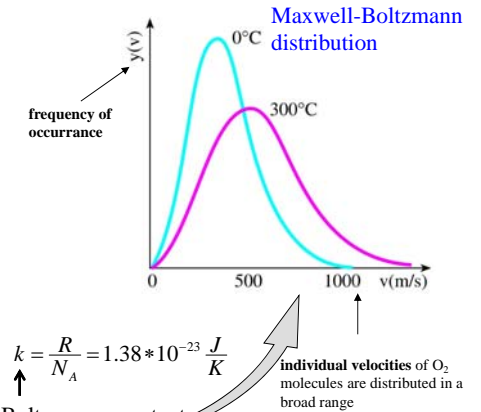
$$pV = \nu RT$$

$$\frac{1}{2} m \bar{v}^2 = \frac{3}{2} kT$$

average kinetic energy

$$k = \frac{R}{N_A} = 1.38 \cdot 10^{-23} \frac{\text{J}}{\text{K}}$$

Boltzmann constant



The ionization energy of the sodium atom is 496 kJ/mol. How large energy is necessary in eV to ionize one atom?

The ionization energy of a single atom:

$$\varepsilon_i = \frac{E_i}{NA} = \frac{496000}{6 \cdot 10^{23}} = 8,27 \cdot 10^{-19} (\text{J} / \text{atom}) = \frac{8,27 \cdot 10^{-19}}{1,6 \cdot 10^{-19}} = 5,15 \text{ eV} / \text{atom}$$

where E_i is the molar ionization energy, NA is the Avogadro number.

There is CO_2 gas in a 20 l tank. At 25 °C temperature the pressure in the tank is $2 \cdot 10^5 \text{ Pa}$. How many moles of CO_2 gas are in the tank. How large is the total mass and the density of the gas?

$$pV = \nu RT$$

$$\nu = \frac{p \cdot V}{R \cdot T}$$

$$\nu = \frac{2 \cdot 10^5 \cdot 20 \cdot 10^{-3}}{8,31 \cdot 298} = 1,62 (\text{mol})$$

$$m = \nu \cdot M = 1,62 \cdot 44 = 71,07 (\text{g})$$

$$\rho = \frac{m}{V} = \frac{71,07}{20000} = 0,0035 (\text{g} / \text{cm}^3)$$

$$\text{specific volume} = \frac{V}{m} = \frac{20000}{71,07} = 281,4 (\text{cm}^3 / \text{g})$$

Calculate the velocity of the molecules in the nitrogen gas at room temperature (20 C°)!
 Suppose the same velocities! The molar mass of the nitrogen (considering that the particles are N₂ molecules) is 28 g/mol (0.028 kg/mol). How large is the kinetic energy of one molecule?

$$\frac{1}{2} m \bar{v}^2 = \frac{3}{2} kT$$

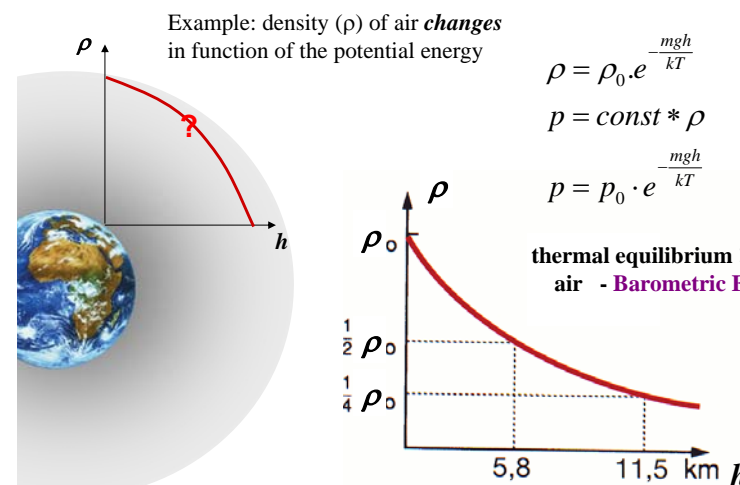
$$\bar{v} = \sqrt{\frac{3 \cdot k \cdot T}{m}}$$

$$\bar{v} = \sqrt{\frac{3 \cdot 1,38 \cdot 10^{-23} \cdot 293}{0,028 / 6 \cdot 10^{23}}} = 509,8 (m/s)$$

$$\varepsilon_{\text{kin}} = \frac{3 \cdot k \cdot T}{2} = \frac{1}{2} m \cdot v^2 = \frac{3 \cdot 1,38 \cdot 10^{-23} \cdot 293}{2} = \frac{1}{2} \frac{0,028 \cdot 509,8^2}{6 \cdot 10^{23}} = 6,04 \cdot 10^{-21} (J / molecule) = 0,038 (eV)$$

Gas phase (ideal gas)

in a force field – gravitation



less and less particles are found (in the same volume) at the levels of higher potential energy (at higher altitudes)

The Barometric formula is a special case of a general law

Boltzmann distribution

Distribution of particles on the levels of potential energy ε_i

$$\left. \begin{array}{l} n_i \\ n_0 \end{array} \right\} \begin{array}{l} \varepsilon_i \\ \varepsilon_0 \end{array} \Delta \varepsilon$$

$$n_i = n_0 \cdot e^{-\frac{\varepsilon_i - \varepsilon_0}{kT}}$$

$$n_i = n_0 \cdot e^{-\frac{\varepsilon_i}{kT}} = n_0 \cdot e^{-\frac{\Delta \varepsilon}{kT}} = n_0 \cdot e^{-\frac{\Delta E}{RT}} \quad \left(\begin{array}{l} \Delta E = \Delta \varepsilon \cdot N_A \\ R = k \cdot N_A \end{array} \right)$$

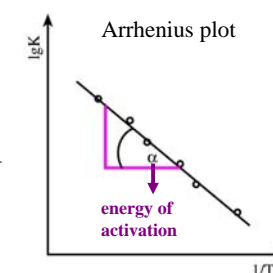
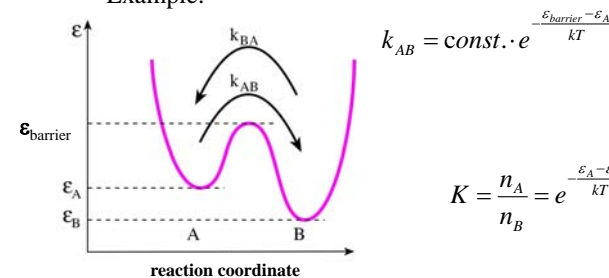
- the number of particles is smaller at the levels of higher energy
- on the same level, the number is smaller at higher temperatures
- the lowest energy level has the highest number of population

Wide range of applications

- barometric formula
- thermal emission of metals
- Nernst equation
- ~~equilibrium and rate of chemical reactions~~
- concentration of thermal defects in ordered, structured systems
- conductivity of semiconductors...



Example:



At which altitude decreases the oxygen concentration by half of the sea level if the temperature is 0°C? Suppose that the atmosphere is in rest!

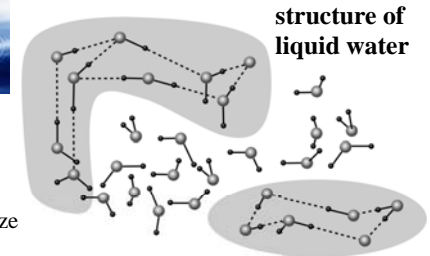
$$p = p_0 \cdot e^{-\frac{mgh}{kT}}$$

$$n = n_0 \cdot e^{-\frac{mgh}{kT}} = n_0 \cdot e^{-\frac{Mgh}{RT}}$$

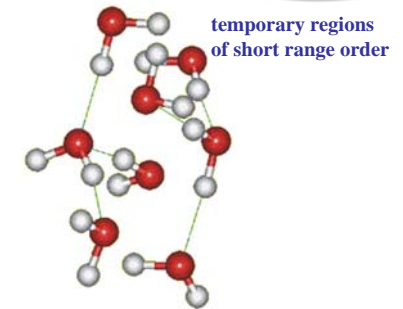
$$n = n_0 / 2$$

$$h = -\frac{RT \cdot \ln \frac{1}{2}}{M \cdot g} = -\frac{8,31 \cdot 273 \cdot (-0,693)}{0,032 \cdot 9,81} = 5010(m)$$

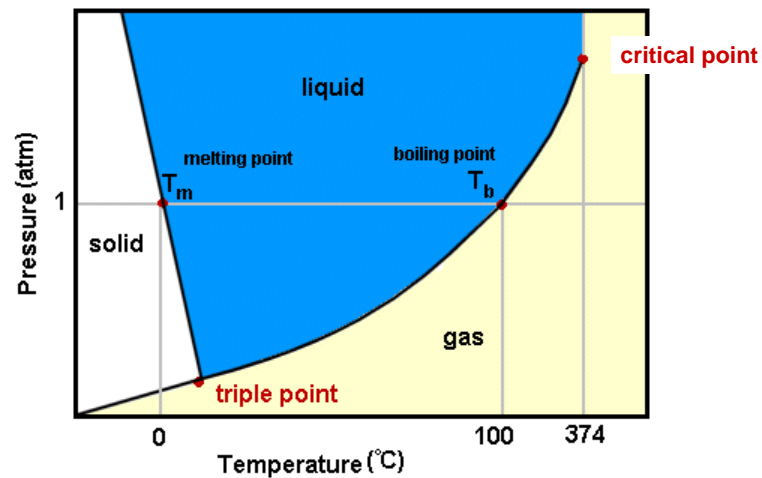
Fluids



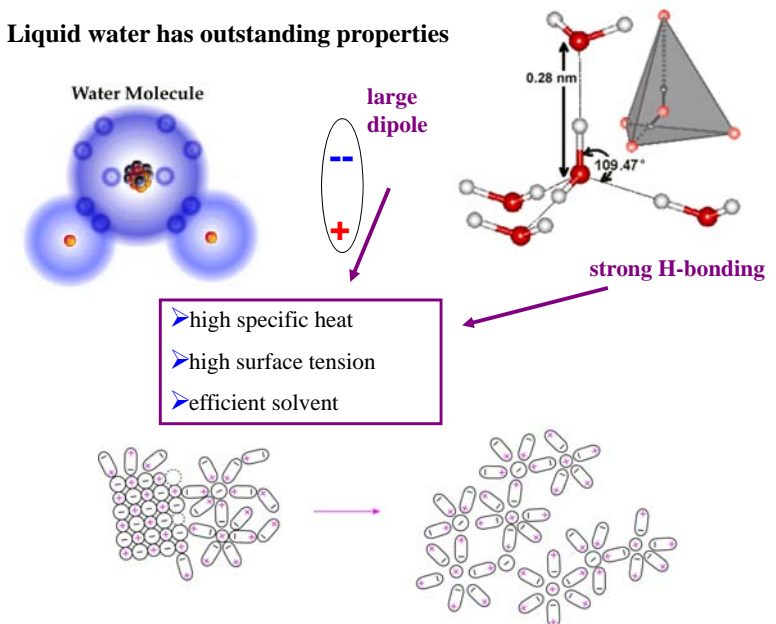
- Temporary regions of short range order within a few molecules ~10 nm domain size
- High concentration of structural defects
- Constant volume
- No firm shape - liquid
- High motional freedom of particles
- Isotropy



Phase diagram of water



Liquid water has outstanding properties

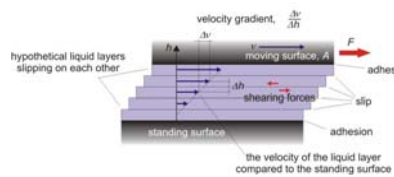


Important properties of fluids

1. Viscosity (η)

– an intrinsic mechanical property

Resistance to shearing motion: frictional force between adjacent layers as they slide past one another



laminar flow

Newton's law – viscosity is a constant

η depends on - the temperature
- the magnitude of F/A

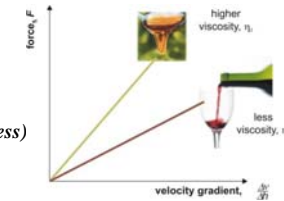
(η is a constant only up to a certain magnitude of the shear stress)

fluidity $\sim 1/\eta$

$$F = \eta * A * \frac{\Delta v}{\Delta h}$$

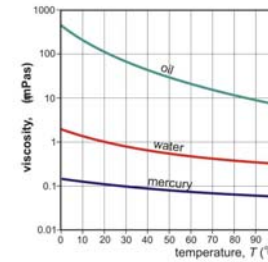
$$[\eta] = Pa * s$$

$$\sigma_s = \frac{F}{A} = \eta * \frac{\Delta v}{\Delta h} = \eta * g_v \quad [Pa]$$



$$\left(\frac{F}{A} \right)$$

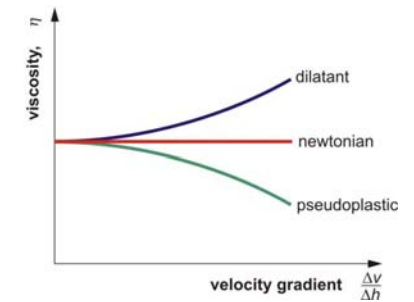
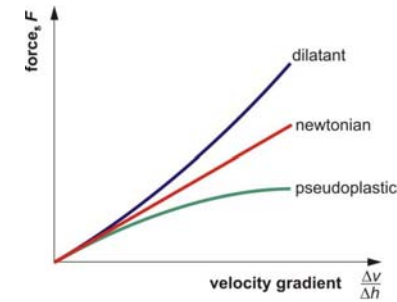
Shear stress



viscosity of some material as the function of temperature

exponential decrease (Boltzmann distribution)

Non-Newtonian fluids: the viscosity depends on the velocity gradient (not constant)



Time dependence of viscosity (chemical and/or physical change in the structure)

thixotropic (η decreases in time)

rheopectic (η increases in time)

Viscosity of fluids/materials of dental applications

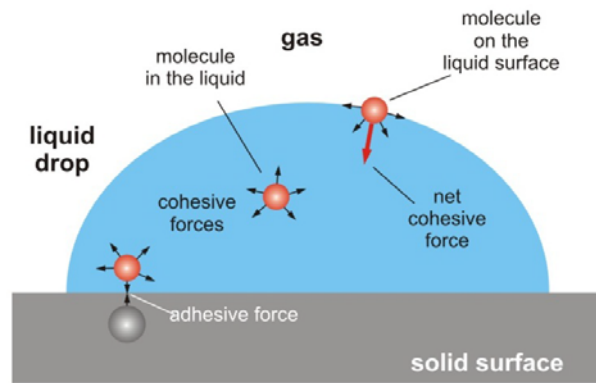
material	η (mPas)
liquid water	1 (20°C)
glycerol	60 (20°C)
methylmethacrylate monomer	0,5 (25°C)
ethylene glycol dimethacrylate monomer	3,4 (25°C)
Zn-phosphate	95 000 (25°C)
Zinc oxide eugenol dental cement	100 000 (37°C)
silicon	60 000-1 200 000 (37°C)

To move a 20 cm² glass plate in a fluid with 100 1/s velocity gradient 1 mN force is required. How large is the viscosity of the fluid?

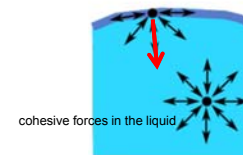
$$F = \eta * A * \frac{\Delta v}{\Delta h}$$

$$\eta = \frac{F}{A \cdot g_v} = \frac{0,001}{20 \cdot 10^{-4} \cdot 100} = 5 \cdot 10^{-3} (Pas)$$

2. Properties of fluid interfaces



2.1. Fluid-air (gas) interfaces – surface tension (surface energy)



energy ΔE is required to increase the surface by an area ΔA

$$\sigma = \frac{\Delta E}{\Delta A} \quad \left(\frac{\text{J}}{\text{m}^2} = \frac{\text{N}}{\text{m}} \right)$$

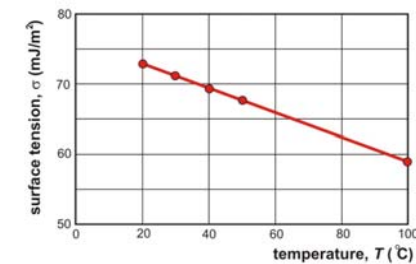
surface tension

Surface tension of materials in air

$$\sigma = \frac{\Delta E}{\Delta A} \quad \left(\frac{\text{J}}{\text{m}^2} = \frac{\text{N}}{\text{m}} \right)$$

material	$\sigma (\text{J/m}^2)$
liquid water	0,073
blood	0,06
saliva	0,05
paraffin	0,025
alcohol	0,023
dentine	0,092
enamel	0,087
Hg	0,484
PMMA	0,037

Temperature dependence of water surface tension



The spherical shape of a liquid drop is due to the surface tension

2.2. Liquid-solid interfaces

Adhesion



Interfacial energy of the boundary between two materials
the energy changes when the area of the boundary changes

interfacial energy < surface energy of the two material



attraction between the two materials



aggregation
adhesion

Classification of adhesion forces:

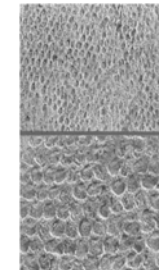
mechanical
chemical
electrostatic
dispersive
diffusive



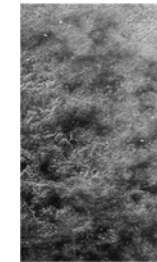
adhesion forces ~ area



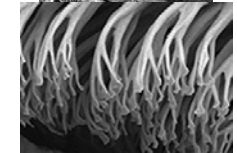
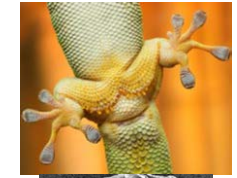
velcro



chemically purified
surface of enamel



wetted surface of enamel



gecko's foot

Figure 1. Morphological aspect of the surface of enamel conditioned with 30% phosphoric acid for 20s. The formation of micropores with type I pattern of conditioning can be observed. (Original magnification: top, 750X; bottom, 1500X).

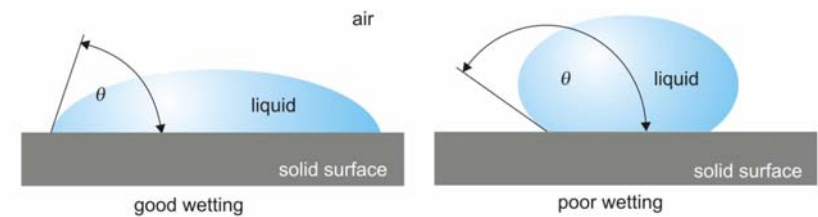
Wetting



Water drops on different materials (metal, glass, wax)

What the shape of the drop depends on?

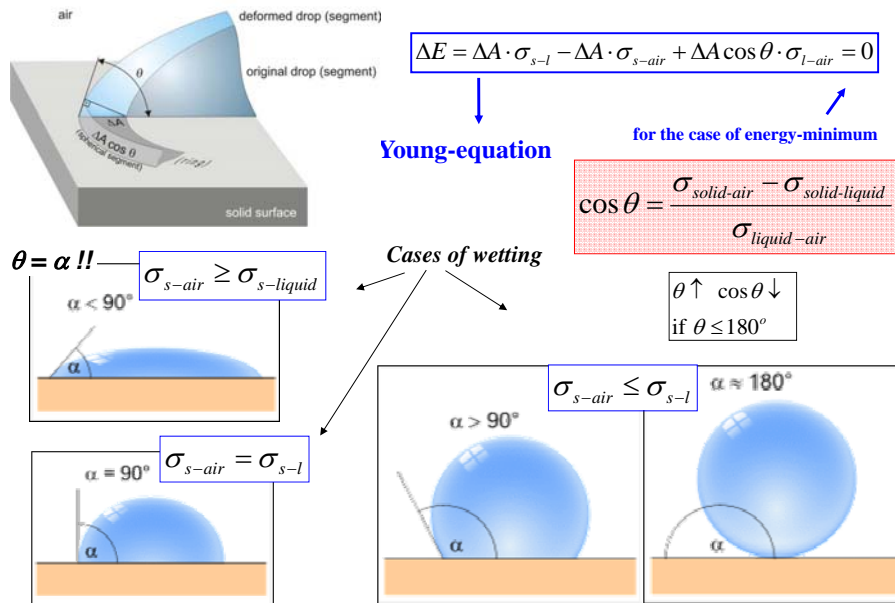
How can we characterise the shape of the drop?



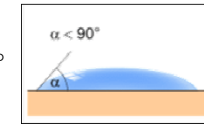
θ : Contact angle (wetting angle)

Basic issue: what is energetically more favorable?

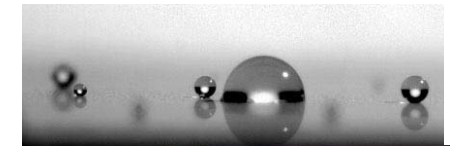
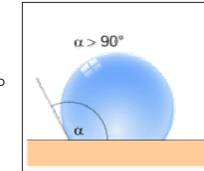
To form a solid-liquid or a solid-air interface?



e.g. liquid = water : 73 mJ/m²
solid = glass: 130 mJ/m²
glass - water: 60 mJ/m² } $\theta = 16,5^\circ$



e.g. Liquid = Hg: 500 mJ/m²
solid = glass: 130 mJ/m²
glass - Hg: 430 mJ/m² } $\theta = 127^\circ$



Contact angle of a mercury drop is 140° on glass. How large is the interfacial tension of the glass-mercury boundary? Other surface tension values: mercury-air 480 mJ/m², glass-air 90 mJ/m².

$$\cos \theta = \frac{\sigma_{solid-air} - \sigma_{solid-liquid}}{\sigma_{liquid-air}}$$

$$\sigma_{solid-air} - \sigma_{liquid-air} \cdot \cos \theta = \sigma_{solid-liquid}$$

$$90 - 480 \cdot \cos 140 = \sigma_{solid-liquid}$$

$$458(mJ / m^2) = \sigma_{solid-liquid}$$