

## Physical bases of dental material science

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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:

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

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

There is CO<sub>2</sub> gas in a 20 l tank. At 25 C° temperature the pressure in the tank is 2\*10<sup>5</sup> Pa. How many moles of CO<sub>2</sub> gas are in the tank. How large is the total mass and the density of the gas?

$$pV = \nu RT$$

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

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

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

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

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

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 N<sub>2</sub> molecules) is 28 g/mol (0.028 kg/mol). How large is the kinetic energy of one molecule?

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

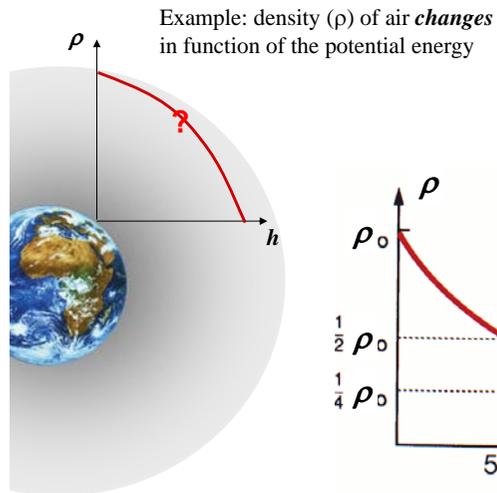
$$\bar{v} = \sqrt{\frac{3 \cdot k \cdot T}{m}}$$

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

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

## Gas phase (ideal gas)

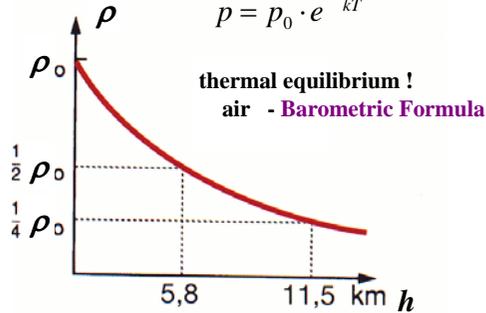
in a force field – gravitation



$$\rho = \rho_0 \cdot e^{-\frac{mgh}{kT}}$$

$$p = \text{const} \cdot \rho$$

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



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  $\varepsilon_i$

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

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

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

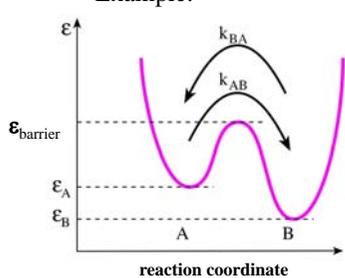
- the number of particles is smaller at the levels of higher energy
- on the same level, the number is smaller at higher temperatures
- the lowest energy level has the highest number of population

## 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...

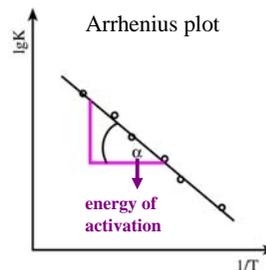


Example:



$$k_{AB} = \text{const} \cdot e^{-\frac{\varepsilon_{\text{barrier}} - \varepsilon_A}{kT}}$$

$$K = \frac{n_A}{n_B} = e^{-\frac{\varepsilon_A - \varepsilon_B}{kT}}$$



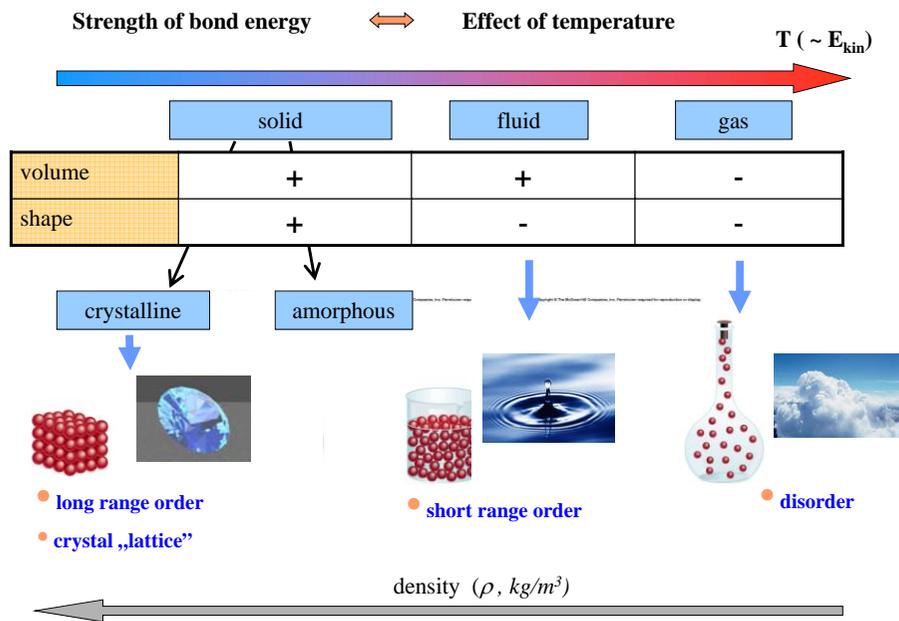
At which altitude decreases the oxygen concentration by half of the sea level if the temperature is 0°C? Suppose that the atmosphere is in rest!

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

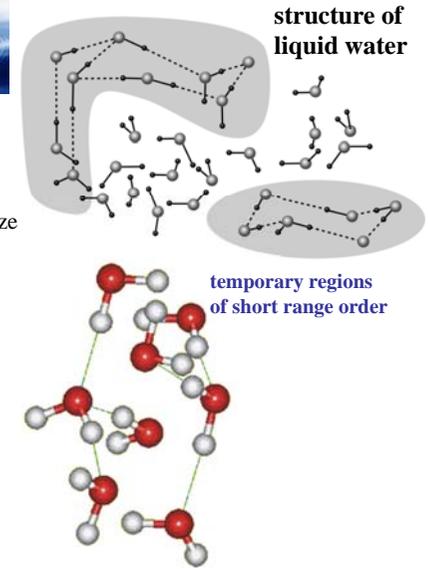
$$n = n_0 \cdot e^{-\frac{mgh}{kT}} = n_0 \cdot e^{-\frac{Mgh}{RT}}$$

$$n = n_0 / 2$$

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

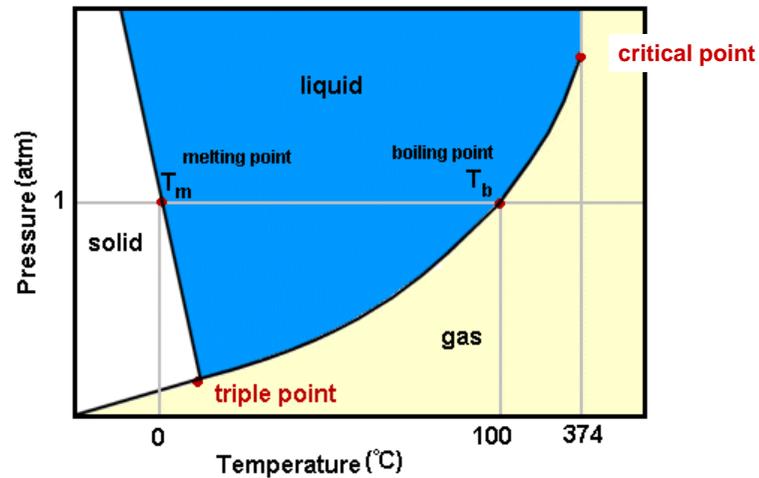


## Fluids

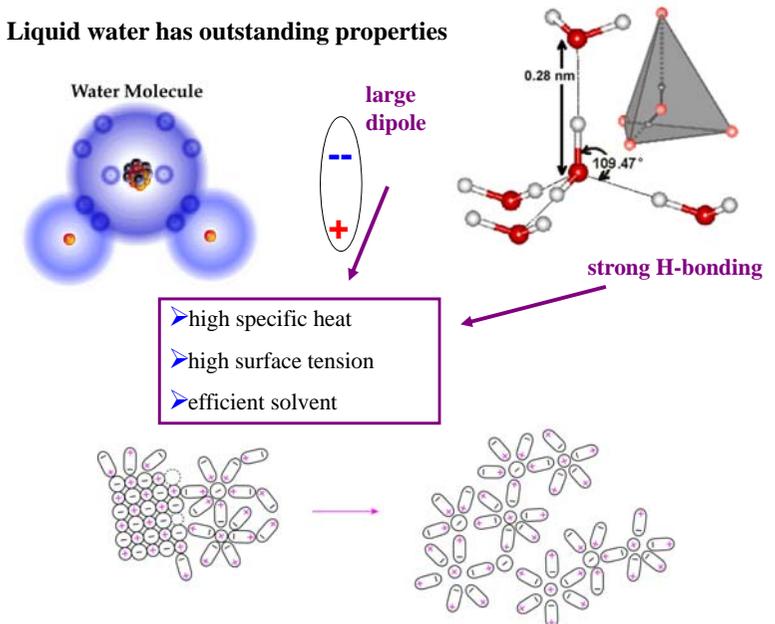


- Temporary regions of short range order within a few molecules ~10 nm domain size
- High concentration of structural defects
- Constant volume
- No firm shape - liquid
- High motional freedom of particles
- Isotropy

Phase diagram of water



Liquid water has outstanding properties

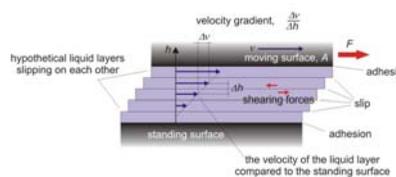


# Important properties of fluids

## 1. Viscosity ( $\eta$ )

– an intrinsic mechanical property

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



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

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

$$\left(\frac{F}{A}\right) \text{ Shear stress}$$

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

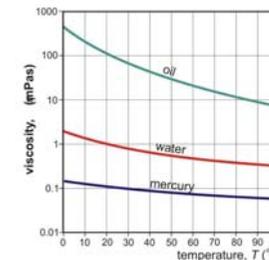
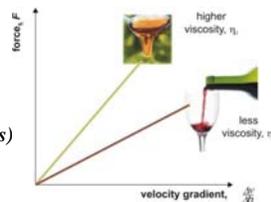
laminar flow

**Newton's law – viscosity is a constant**

$\eta$  depends on - the temperature  
- the magnitude of F/A

( $\eta$  is a constant only up to a certain magnitude of the shear stress)

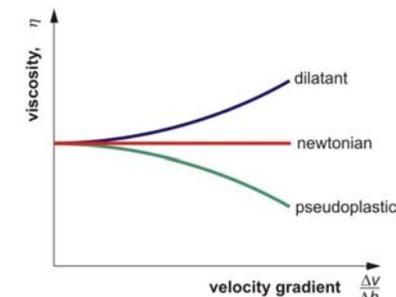
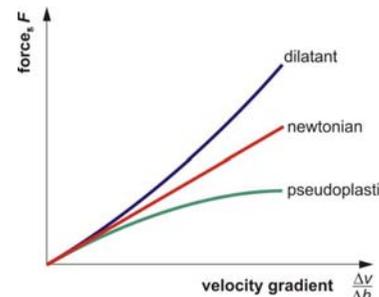
fluidity  $\sim 1/\eta$



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 ( $\eta$  decreases in time)

rheopectic ( $\eta$  increases in time)

### Viscosity of fluids/materials of dental applications

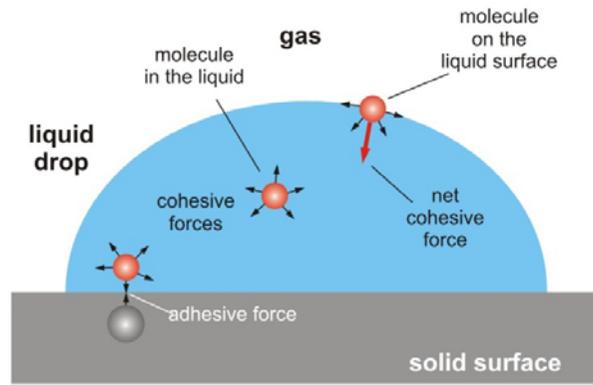
material	$\eta$ (mPas)
liquid water	1 (20°C)
glycerol	60 (20°C)
methylmethacrylate monomer	0,5 (25°C)
ethylene glycol dimethacrylate monomer	3,4 (25°C)
Zn-phosphate	95 000 (25°C)
Zinc oxide eugenol dental cement	100 000 (37°C)
silicon	60 000-1 200 000 (37°C)

To move a 20 cm<sup>2</sup> glass plate in a fluid with 100 1/s velocity gradient 1 mN force is required. How large is the viscosity of the fluid?

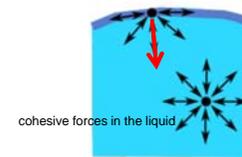
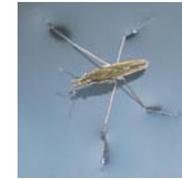
$$F = \eta * A * \frac{\Delta v}{\Delta h}$$

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

## 2. Properties of fluid interfaces



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



energy  $\Delta E$  is required to increase the surface by an area  $\Delta A$

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

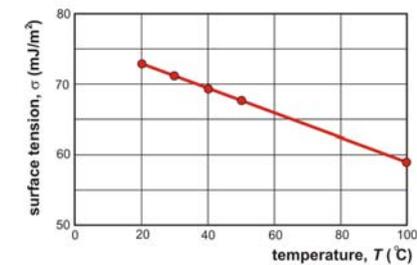
surface tension

### 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	$\sigma$ (J/m <sup>2</sup> )
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

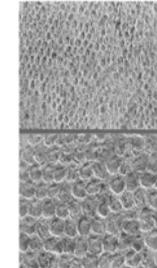
Classification of adhesion forces:

mechanical  
chemical  
electrostatic  
dispersive  
diffusive

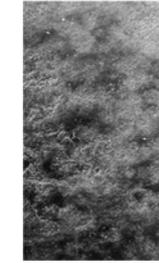
} adhesion forces ~ area



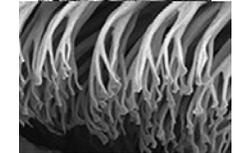
velcro



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 typical pattern of conditioning can be observed. (Digital magnification: x40,000, bottom, 1982).

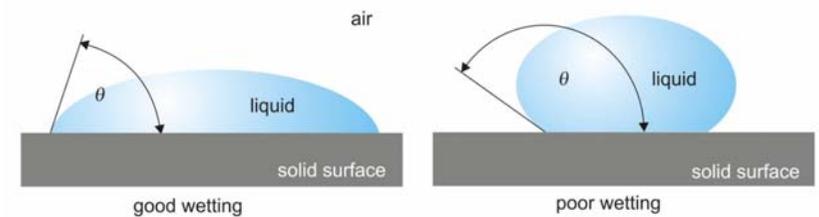
## Wetting



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

What the shape of the drop depends on?

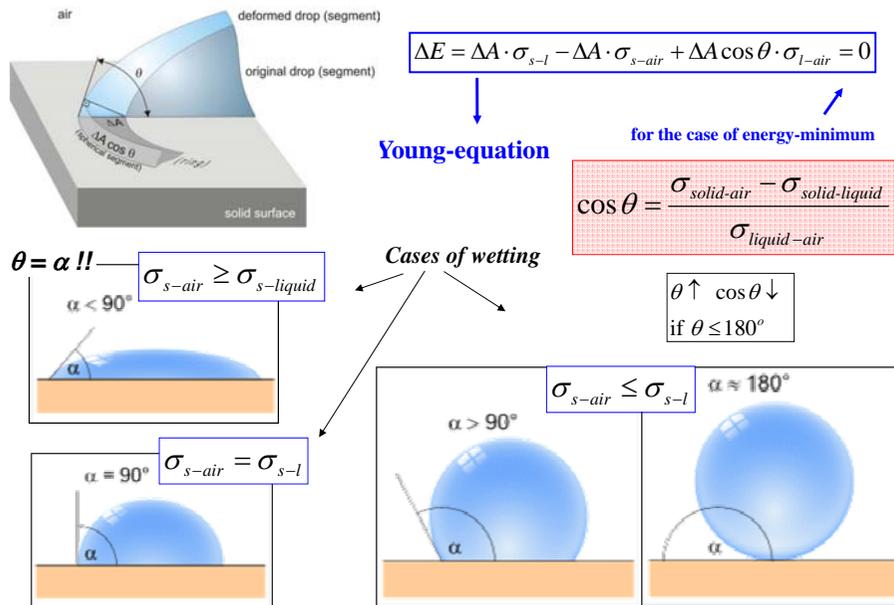
How can we characterise the shape of the drop?



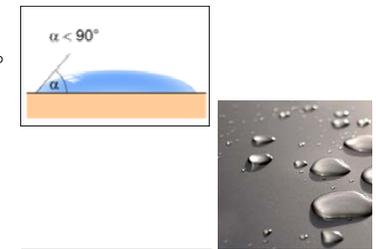
**θ : Contact angle (wetting angle)**

Basic issue: what is energetically more favorable?

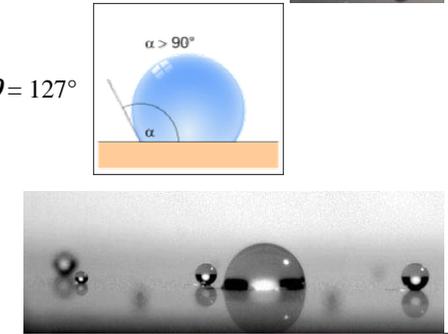
To form a solid-liquid or a solid-air interface?



e.g. liquid = water : 73 mJ/m<sup>2</sup>  
 solid = glass: 130 mJ/m<sup>2</sup>  
 glass - water: 60 mJ/m<sup>2</sup> }  $\theta = 16,5^\circ$



e.g. Liquid = Hg: 500 mJ/m<sup>2</sup>  
 solid = glass: 130 mJ/m<sup>2</sup>  
 glass - Hg: 430 mJ/m<sup>2</sup> }  $\theta = 127^\circ$



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/m<sup>2</sup>, glass-air 90 mJ/m<sup>2</sup>.

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

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

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

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