Physical bases of dental material science 3.

Structure of matter

Interfacial phenomena

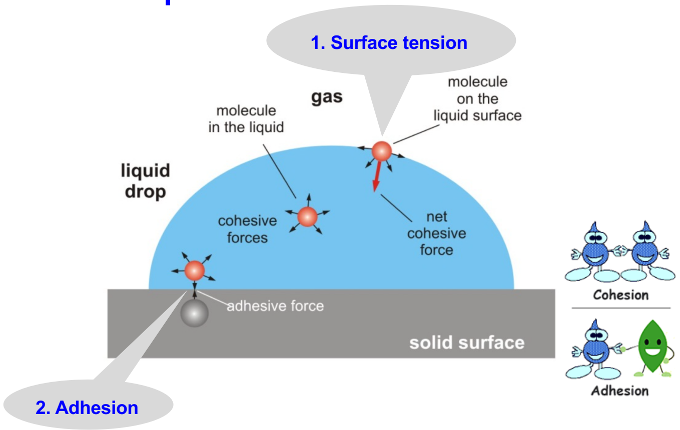
Phase diagram, phase transitions

E-book chapters: 6, 7

Problems: Chapter1: 24, 25, 27, 28, 31

Highlights:
- surface tension
- adhesion – wetting
- phase – phase diagram
- phase transition

Interfacial phenomena



1. Surface tension

Surface tension or specific surface energy (σ):

change in energy with the increase of surface by ΔA

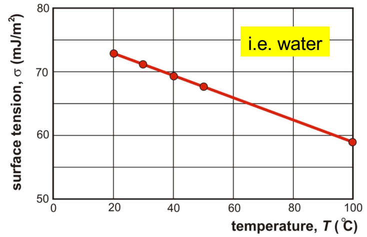
$$\sigma = \frac{\Delta E}{\Delta A} \quad \left(\frac{\mathrm{J}}{\mathrm{m}^2} = \frac{\mathrm{N}}{\mathrm{m}}\right)$$

increase in surface

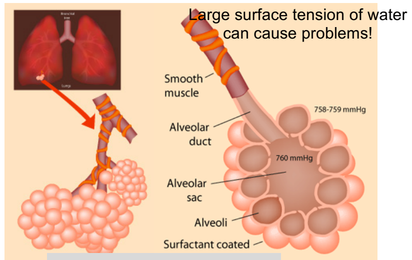
anyag	σ (J/m^2)
water	0,073
blood	0,06
saliva	0,05
paraffin	0,025
alcohol	0,023
dentin	0,092
enamel	0,087
mercury	0,484

* in air, 20°C

Temperature dependence of surface tension:

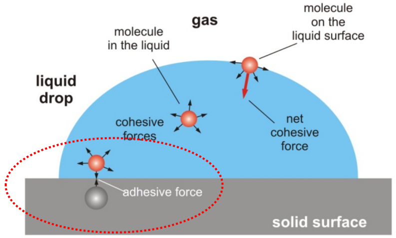


Consequences:



respiratory distress syndrome

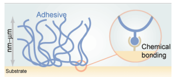
2. Adhesion



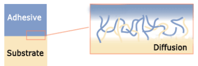
Types:

- chemical (ionic, covalent, H-bond)
- dispersive (van der Waals forces)
- diffusive (materials diffuse into each other)

} molecular level



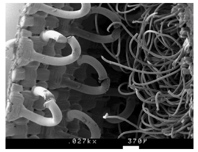
most frequent and general



Further types:

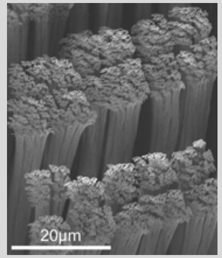
- mechanical
- electrostatic (charged surfaces)

} macroscopic level



In general, the **strength of adhesion** depends on the **size and distance** of touching surfaces

„Super adhesion" of gecko



Quantitative description of adhesion

Specific interfacial energy, (σ):

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

change in energy associated with the increase of surface by ΔA

increase in the interfacial area

Adhesion in dentistry:

- Surface size – acid treatment
- Viscosity
- Wetting (adhesion between solid and liquid)

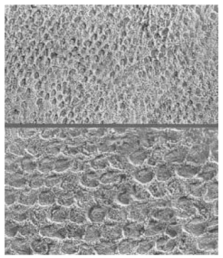
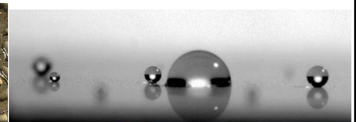
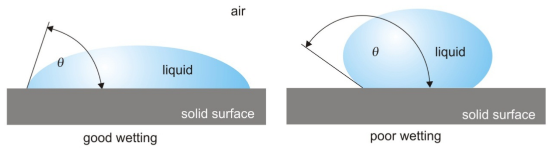


Figure 1. Morphological aspect of the surface of enamel conditioned with 36% phosphoric acid for 20 s. The formation of micropores with type I pattern of conditioning can be observed. (Original magnification: top, 750X; bottom, 1500X).

Wetting

(adhesion between solid and liquid)





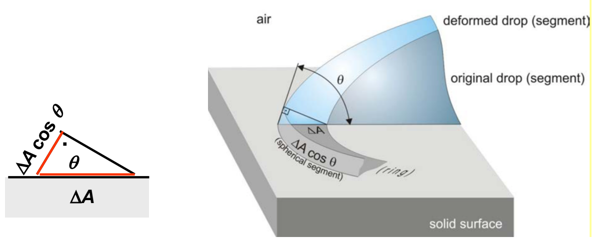
θ: contact angle

Young-equation:

$$\cos\theta = \frac{\sigma_s - \sigma_{s,l}}{\sigma_l}$$

- s : solid body (–air)
- s, l : solid body – liquid
- l : liquid (–air)

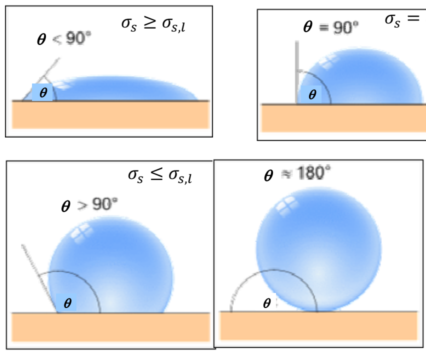
Derivation of Young's equation:



equilibrium = energy minimum ⇒ small change in shape (surface) will not cause any changes in energy

$$\Delta E = \Delta A \cdot \sigma_{s,l} - \Delta A \cdot \sigma_s + \Delta A \cdot \cos\theta \cdot \sigma_l = 0$$

$$\cos\theta = \frac{\sigma_s - \sigma_{s,l}}{\sigma_l}$$



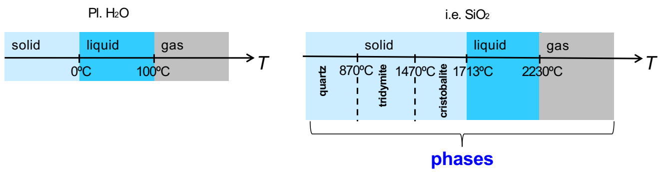
$$\cos\theta = \frac{\sigma_s - \sigma_{s,l}}{\sigma_l}$$

Specific surface energy of some dental materials:

material	σ (mJ/m²)
water	73 (25° C)
saliva	53 (37° C)
dentin	92
enamel	87
PMMA	37
paraffin	25

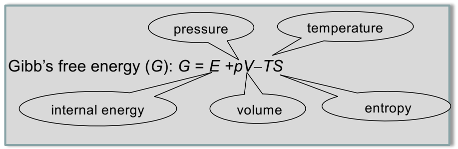
Phase

States of matter:



Phase: physically and chemically homogeneous state of a material

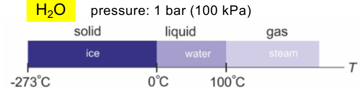
Stabile phase: The phase with the lowest Gibb's free energy at given circumstances.

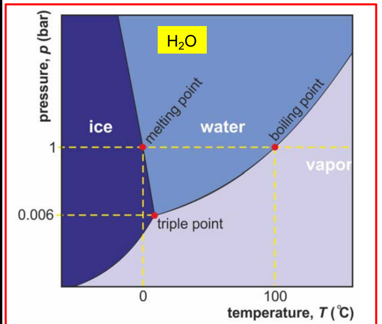


Phase diagram

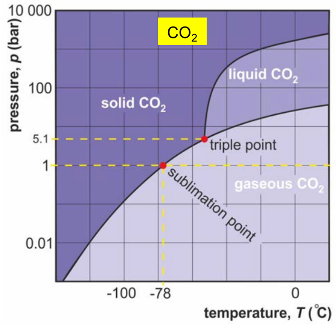
Examples:

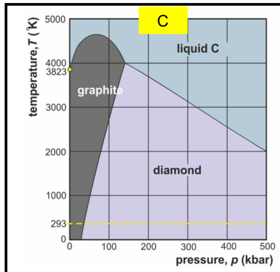
Phase diagram: plotting the stable phases as a function of different parameters (p, T, c, …)

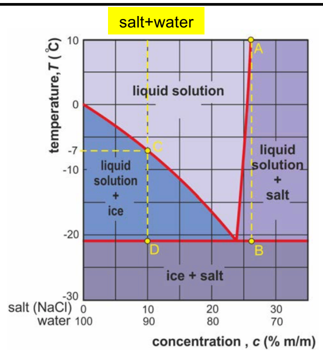


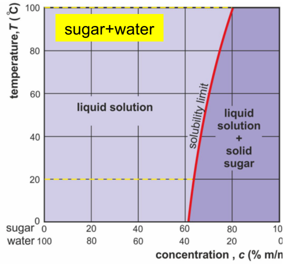


You should know only water's phase diagram for the exam.

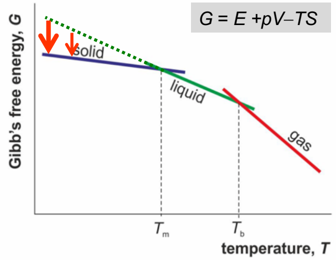


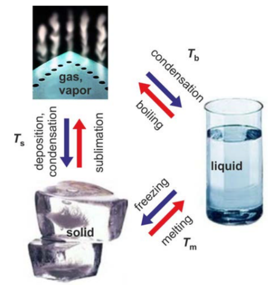






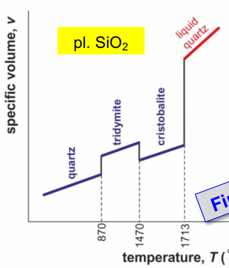
Phase transition

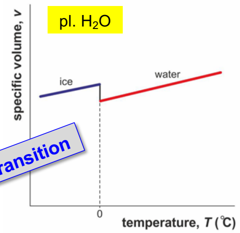




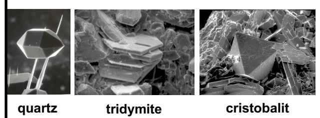
- Driving force: difference in free energy
  - ⇒ the smaller the T (< T_m), the greater the driving force
- Limiting factor: movement of atoms, molecules (diffusion)
  - ⇒ the smaller the T (< T_m), the weaker the movements

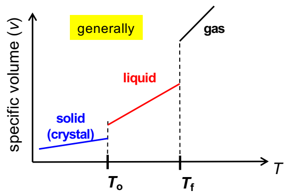
Order of phase transitions

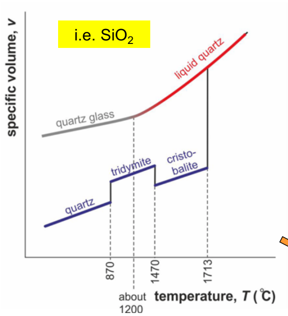


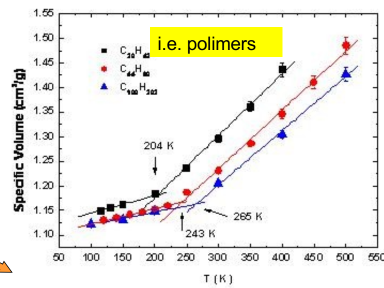


First-order phase transition



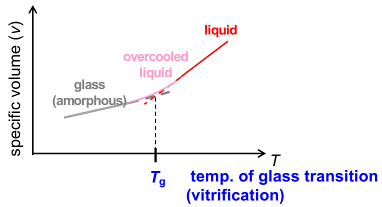




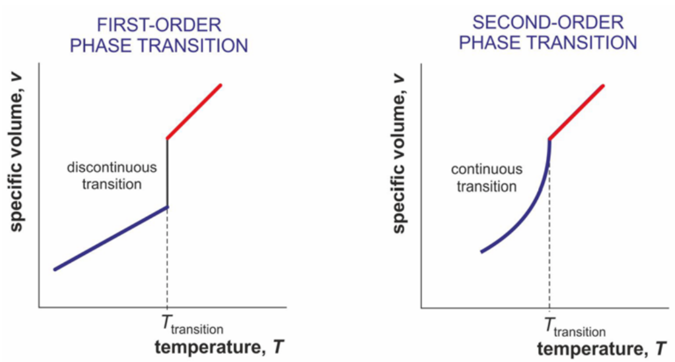


$T_g < T_o$

Second-order phase transition
i.e. vitrification



Summary:



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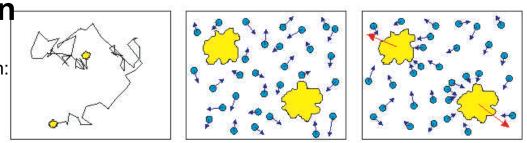
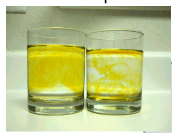
Diffusion

Brownian motion:



Diffusion: equilibration of concentration by random (thermal)



„speed" of diffusion ~ concentration difference
diffusion coefficient

Fick's law:

$$\frac{\Delta \nu}{\Delta t} = -D \cdot A \cdot \frac{\Delta c}{\Delta x}$$

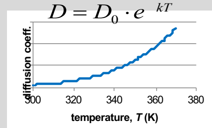
D: diffusion coefficient (m^2/s)

Diffusing molecule	medium	*D* (m^2/s)
O_2	air	$\approx 10^{-5}$
	water	$\approx 10^{-9}$
	glass	$\approx 10^{-50}$
He	glass	$\approx 10^{-18}$

Einstein-Stokes equation:
(for spherical particles)

$$D = \frac{kT}{6\pi\eta r}$$

$$D = D_0 \cdot e^{-\frac{\Delta\varepsilon}{kT}}$$



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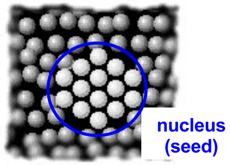
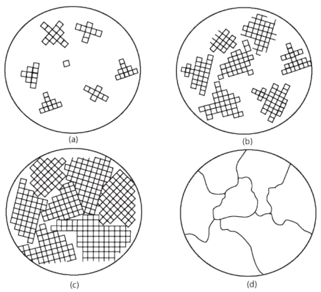
Kinetics of phase transitions (i.e. crystallization)

Overcooling! $T < T_m$

1. Nucleation



2. Growth



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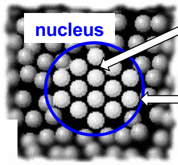
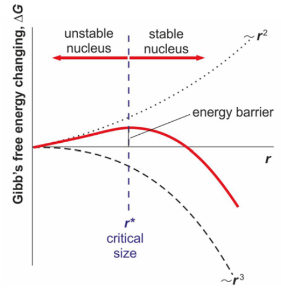
1. Nucleation

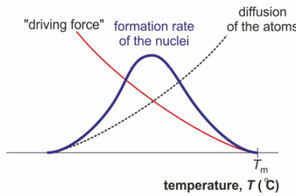


ordered structure ⇒ decrease in energy (~ volume) r^3

interface ⇒ increase in energy (~ surface) r^2

$T < T_o$





(⇒ overcooling)

- **homogenous nucleation:** inside the same material
- **heterogeneous nucleation:** on solid surfaces (i.e. wall of container, impurity particles)

faster!

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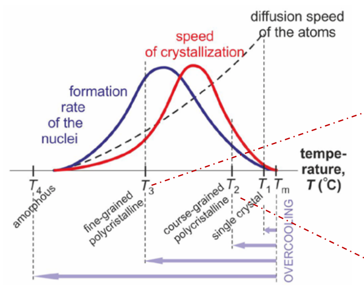
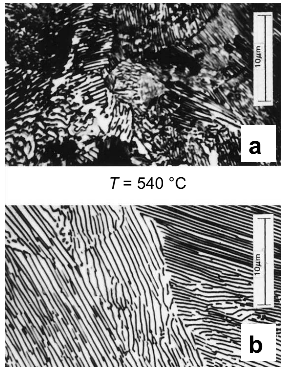
2. Crystal growth

Shape and size of grains ⇒ properties!



Example:



T = 540 °C

T = 690 °C (T_o = 727 °C)

harder, stronger, less deformable

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