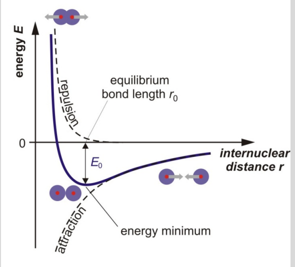
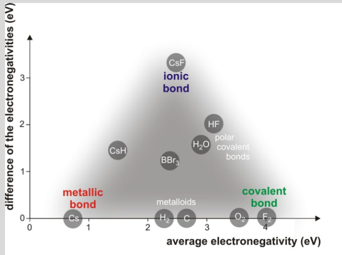
Repetition

Atomic interactions

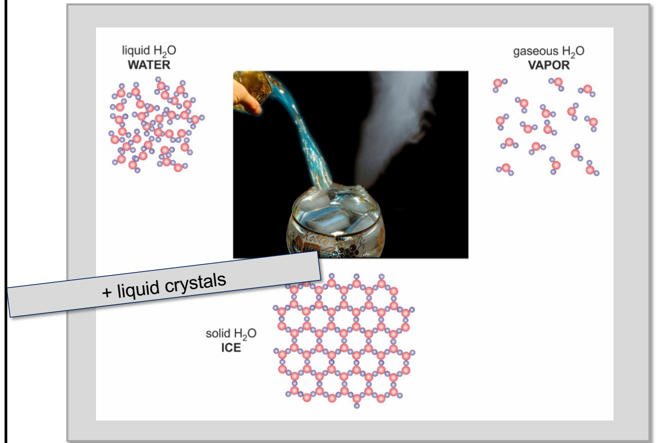


Bond types



1

States of matter

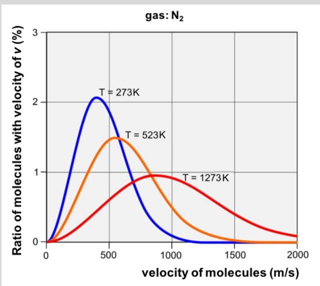


2

Gases

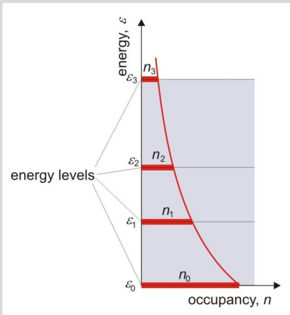
Interpretation of temperature:

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



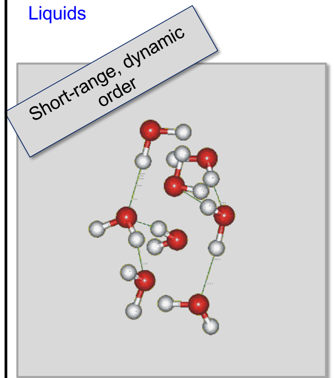
Boltzmann-distribution:

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



3

Liquids



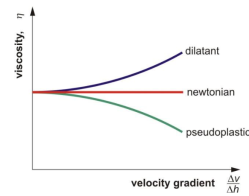
Viscosity:

$$F_s = \eta \cdot A \cdot \frac{\Delta v}{\Delta h}$$

viscosity (coefficient of internal friction)

depends on:

- temperature
- velocity gradient
- time of mechanical stress



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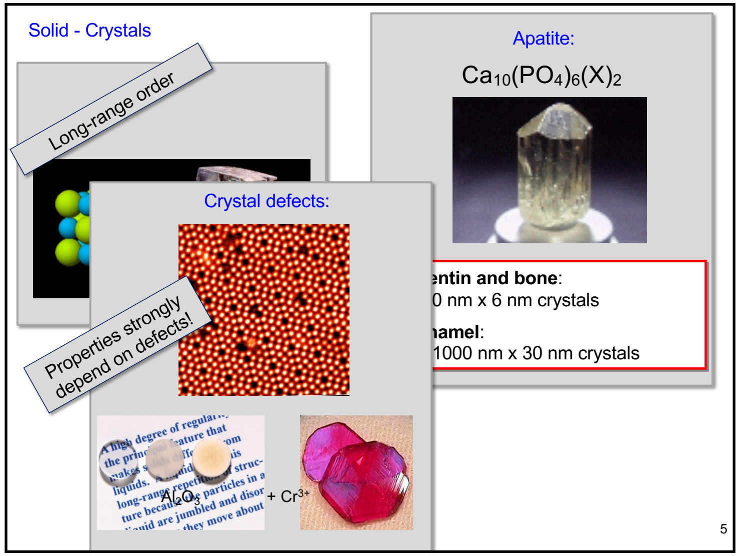
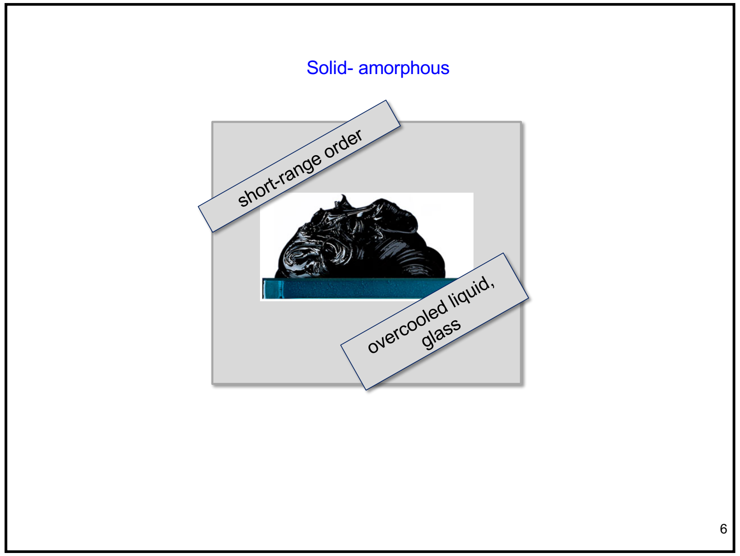
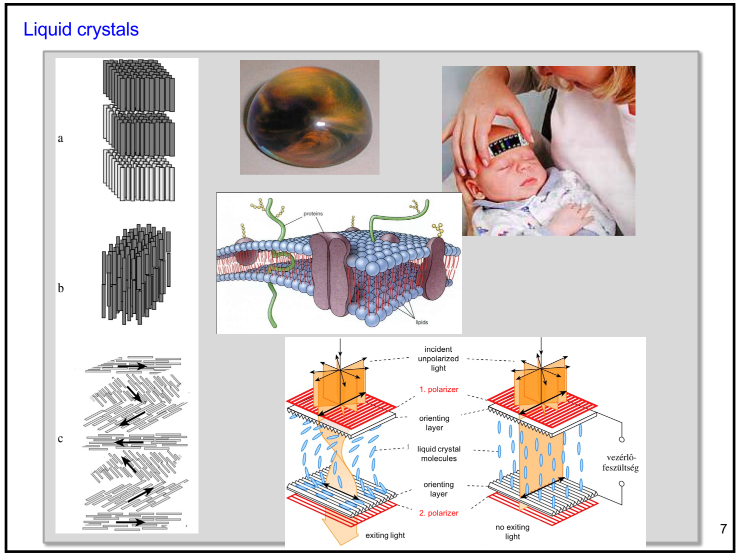

Solid - Crystals
Long-range order
Apatite:
$Ca_{10}(PO_4)_6(X)_2$
Crystal defects:
entin and bone:
0 nm x 6 nm crystals
namel:
1000 nm x 30 nm crystals
Properties strongly depend on defects!
Al_2O_3 + Cr^{3+}
5

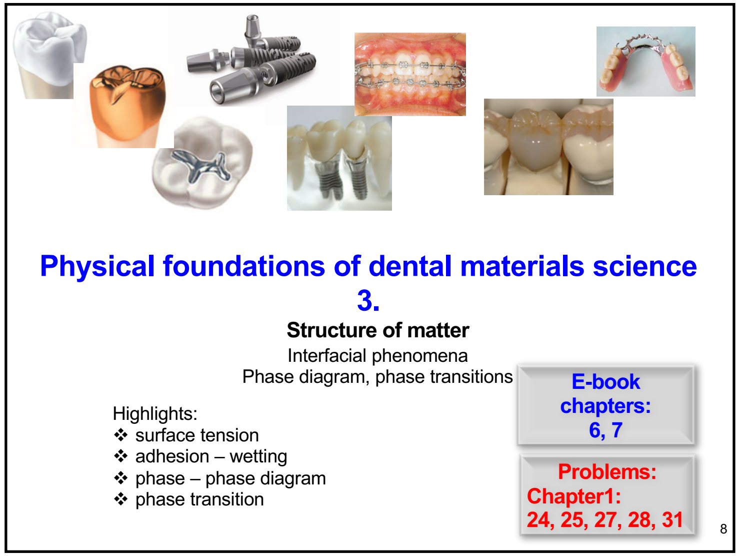
5


Solid- amorphous
short-range order
overcooled liquid, glass
6

6


Liquid crystals
a
b
c
incident unpolarized light
1. polarizer
orienting layer
liquid crystal molecules
orienting layer
2. polarizer
exiting light
no exiting light
vezérlő-feszültség
7

7


Physical foundations of dental materials science 3.
Structure of matter
Interfacial phenomena
Phase diagram, phase transitions
Highlights:
❖ surface tension
❖ adhesion – wetting
❖ phase – phase diagram
❖ phase transition
E-book chapters: 6, 7
Problems: Chapter1: 24, 25, 27, 28, 31
8

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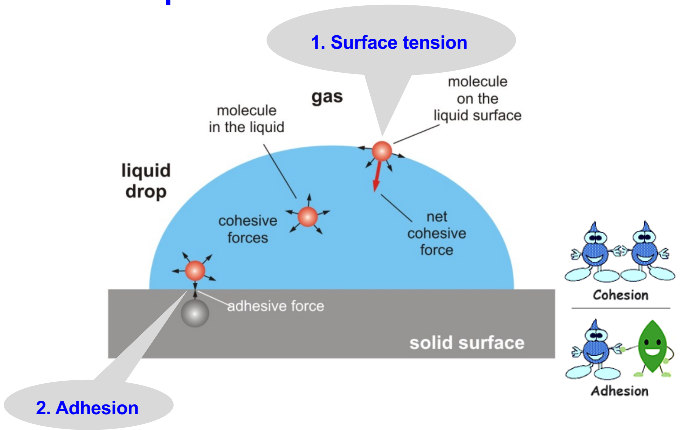
Interfacial phenomena



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1. Surface tension

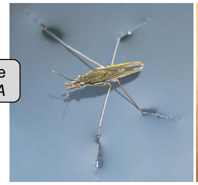
Surface tension or specific surface energy (σ): change in energy with the increase of surface by ΔA

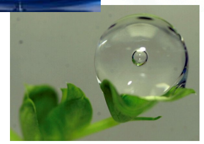
$$\sigma = \frac{\Delta E}{\Delta A} \quad \left(\frac{J}{m^2} = \frac{N}{m}\right)$$

increase in surface

anyag	σ (J/m²)
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





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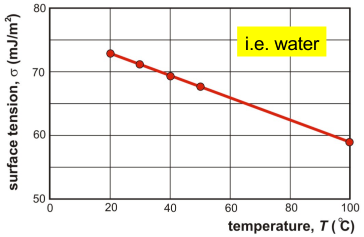
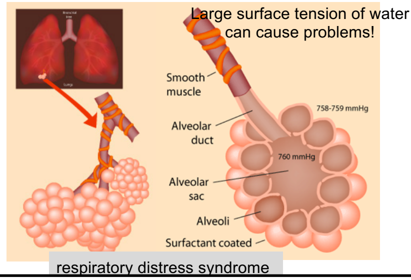
Temperature dependence of surface tension:



Consequences:



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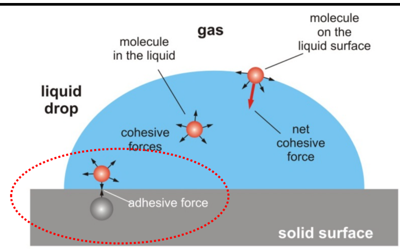
2. Adhesion

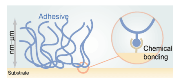


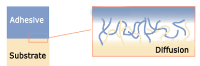
Types:

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

} molecular level

most frequent and general





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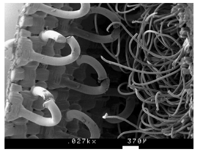
Further types:

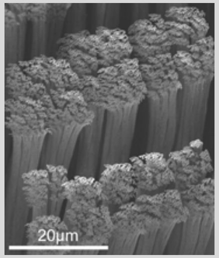
- mechanical
- electrostatic (charged surfaces)

} macroscopic level



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

„Super adhesion" of gecko



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Quantitative description of adhesion

Specific interfacial energy, (σ):

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

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)

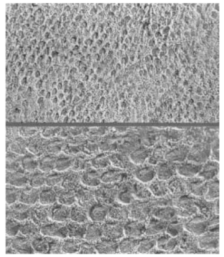

Figure 1. Morphological aspect of the surface of enamel conditioned with 36% phosphoric acid for 20 s. The formation of micropores with type I pattern of conditioning can be observed. (Original magnification: top, 750X; bottom, 1500X).

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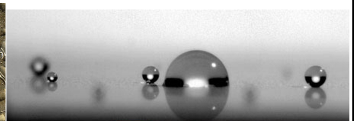
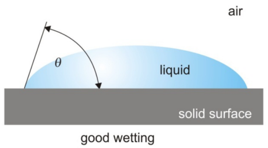
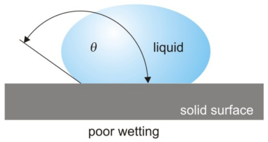
Wetting

(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)

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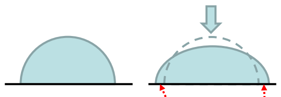
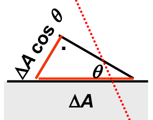
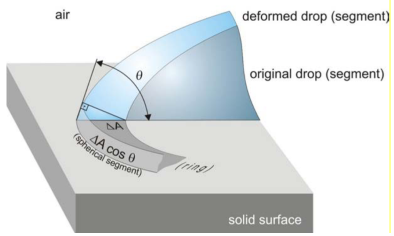
Derivation of Young's equation:







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

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

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

σ_s: solid – gas interface
$\sigma_{s,l}$: solid – liquid interface
σ_l: liquid – gas interface

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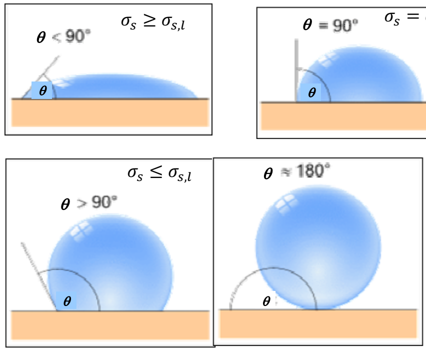

$$\cos\theta = \frac{\sigma_s - \sigma_{s,l}}{\sigma_l}$$

Specific surface energy of some dental materials:

material	σ (mJ/m^2)
water	73 (25° C)
saliva	53 (37° C)
dentin	92
enamel	87
PMMA	37
paraffin	25

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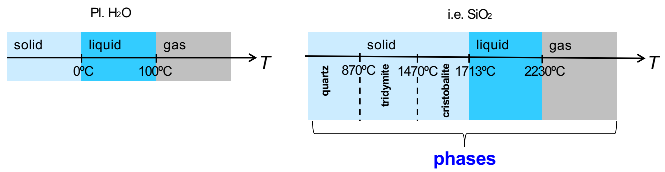
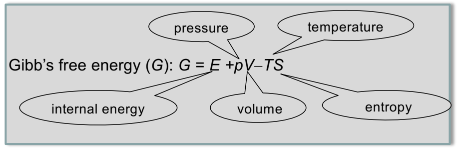
Phase

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.



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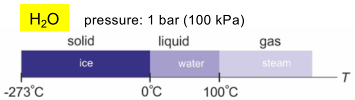
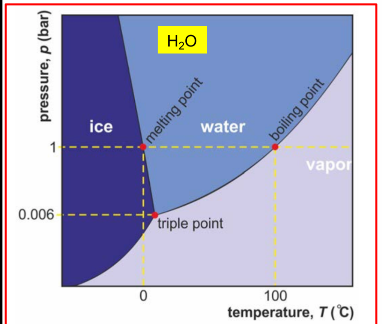
Phase diagram

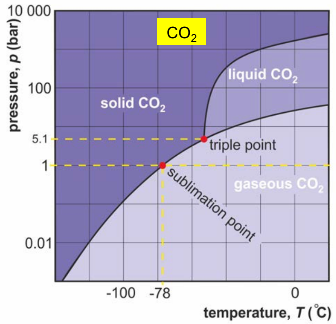
Examples:

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.



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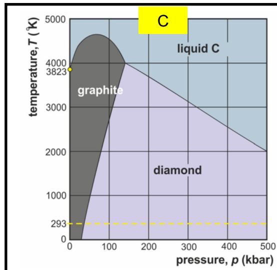

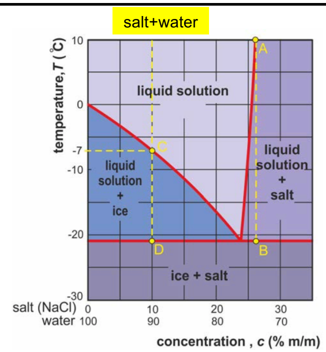

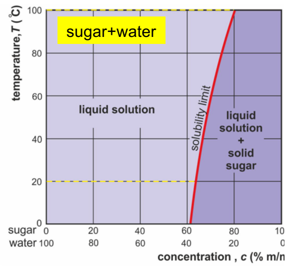

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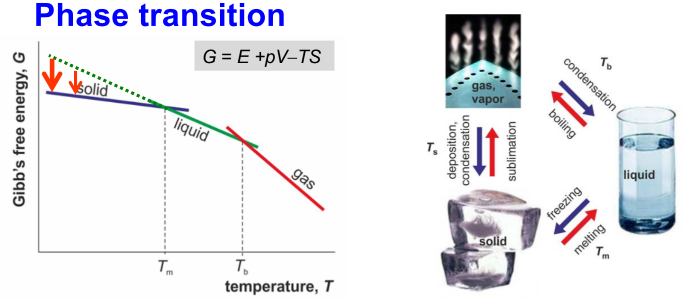
Phase transition



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

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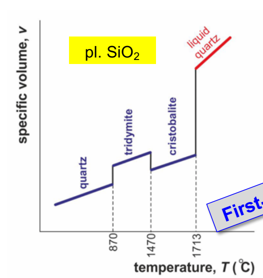
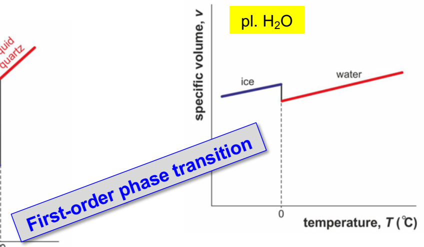
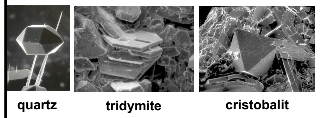
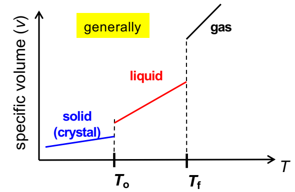
Order of phase transitions









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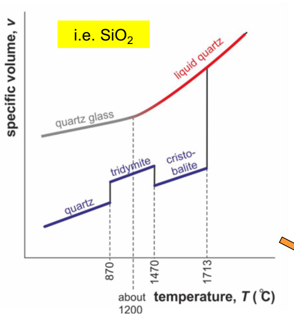
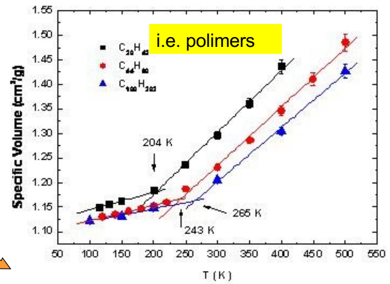
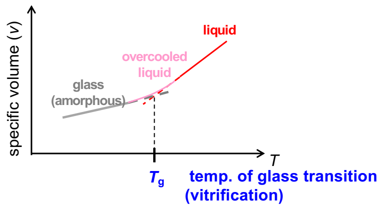




$T_g < T_o$

Second-order phase transition
i.e. vitrification



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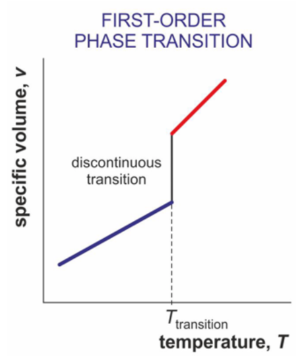
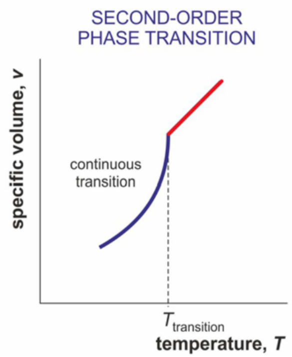
Summary:





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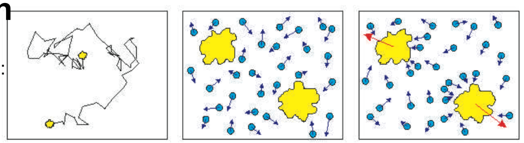
Diffusion

Brownian motion:



Diffusion: equilibration of concentration by random (thermal)

„speed" of diffusion ~ concentration difference / diffusion coefficient

Fick's law:

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

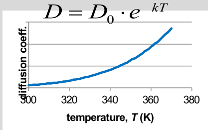
D: diffusion coefficient (m^2/s)

Einstein-Stokes equation:
(for spherical particles)

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

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

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



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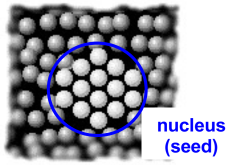
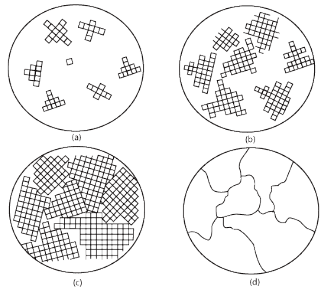
Kinetics of phase transitions (i.e. crystallization)

Overcooling! $T < T_m$

1. Nucleation



2. Growth



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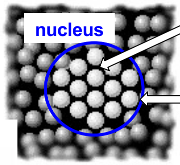
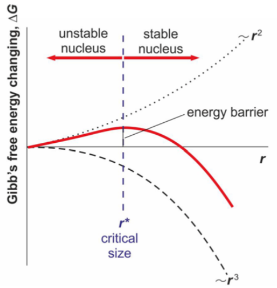
1. Nucleation

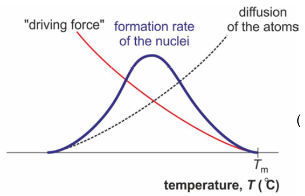


ordered structure
⇒ decrease in energy
(~ volume)
r^3

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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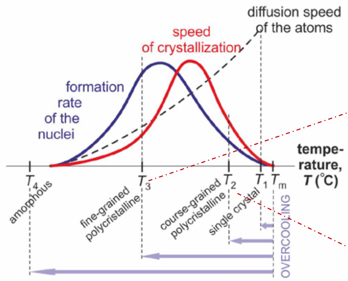
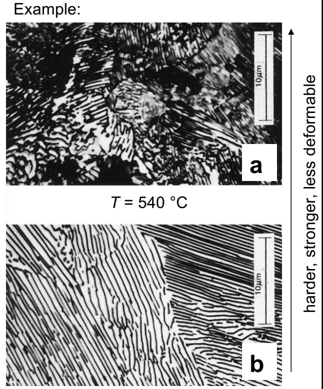
2. Crystal growth

Shape and size of grains ⇒ properties!



Example:



$T = 540$ °C

$T = 690$ °C ($T_o = 727$ °C)

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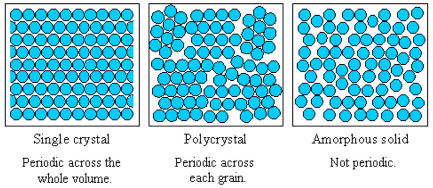
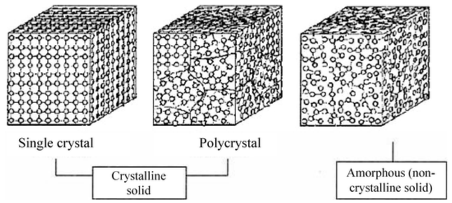


Single crystal: uninterrupted atomic order across the whole crystal.

Polycristal: macroscopically homogeneous but microscopically heterogeneous. Atomic order is interrupted at grain boundaries.

Amorphous: Macroscopically homogeneous, but no atomic order present. (It is like a frozen liquid state)



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