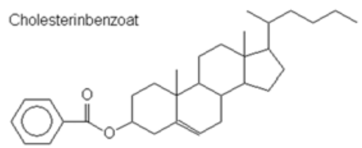
Physical bases of dental material science

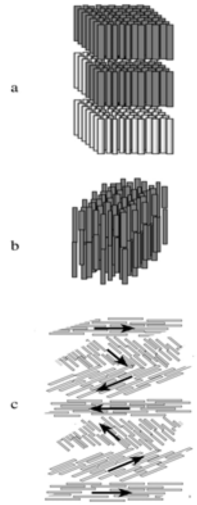
Irén Bárdos-Nagy

Liquid crystals: a mesomorphous state of matter

Thermotropic - liotropic

General properties
- elongated shape of molecules
- relativly long range order stabilized by secondary bonds
- fluidity, deformability
- anisotropy in fluid state



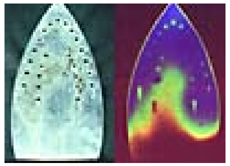


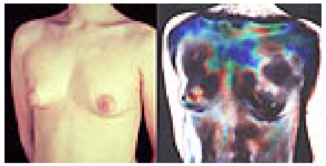
smectic

nematic

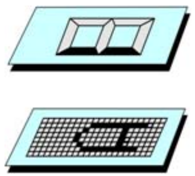
cholesteric

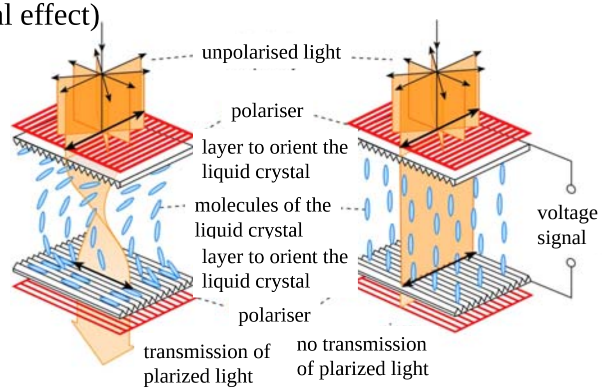
Use of thermotropic liquid crystals



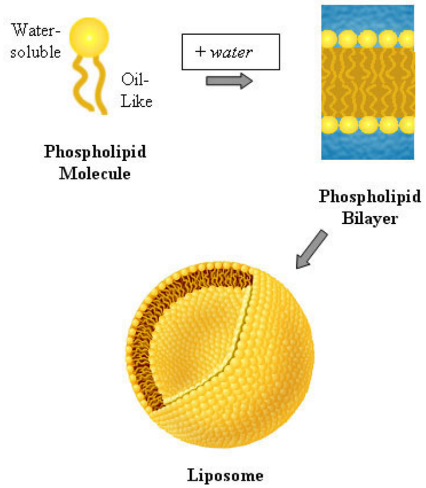


LCD (electro optical effect)

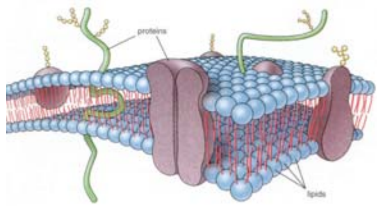


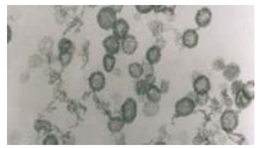


Liotropic liquid crystals



Cellular bi-layer membranes



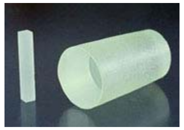


Solid materials

Classification of solid materials

crystalline — amorphous

crystalline → monocrystal, polycrystal



sapphire

calcite

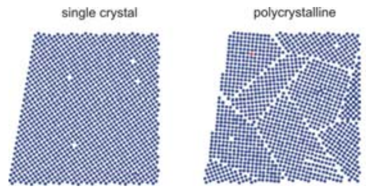
cuprite

porcelain veneer

moldavite

Most important characteristics of crystalline materials

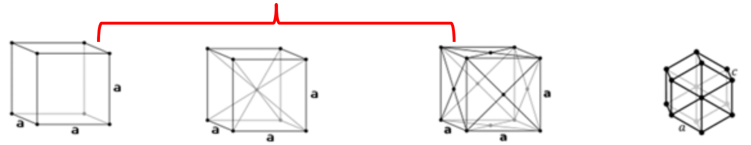
- definite shape and volume
- macroscopic range order (crystals)
- periodic crystal structure, symmetry
- relatively small number of defects in the structure
- low degree of translational motion of the individual building elements
- frequent anisotropy (the physical properties depend on the direction of the measurement)



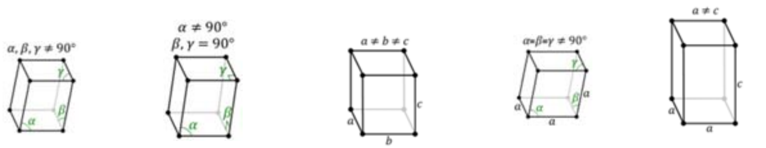
crystal structure: a unique arrangement of atoms or molecules
longe – range order and symmetry
unit cell repeated periodically in 3D

The seven lattice system:

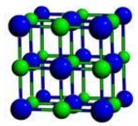
cubic



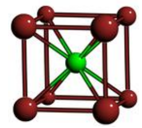
simple cubic | body-centered cubic | face-centered cubic | hexagonal



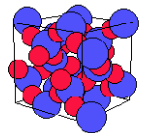
triclinic | monoclinic | orthorhombic | rhombohedral | tetragonal



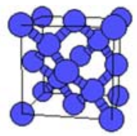
sodium chloride



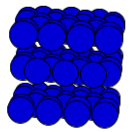
cesium chloride



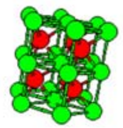
quartz



diamond



graphite



tungsten carbid

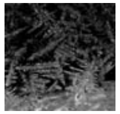
Properties of crystalline materials

type of bond	building units	binding energy (kJ/mol)	melting point	rigidity	conductivity
covalent	atoms	100 – 1000	high	+	-
ionic	ions	200 – 1500	high	+	-
metallic	free electrons and ions	70 – 1000	high	ductile	+
H-bond	molecules	15 – 20	low	+	-
van der Waals	molecules	0.5 – 3	low	soft	-


graphite


fluorapatite


gold


ice


sulfur

Polymorphism - allotropy

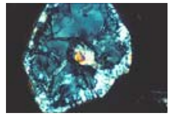
the ability of solid material to exist in more than one form or crystal structure

polymorph forms of SiO_2

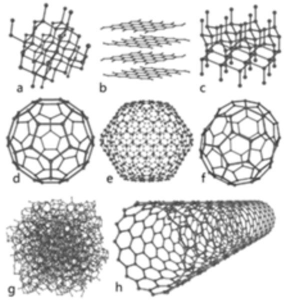

α quartz


tridymite


cristobalite


coesite

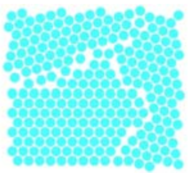
allotrop forms of carbon



a./ diamond
b./ graphite
c./ lonsdaleit
d.-f./ fullerenes
g. amorphous carbone
h./ carbon nanotube

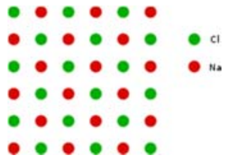
Polycrystalline materials

- no macroscopic range order
- large number of crystallites (grains, microscopic size crystals)
- grain boundaries (interfaces where crystals of different orientations meet)
- large number of crystal defects
- mainly isotrope property



Crystal defects

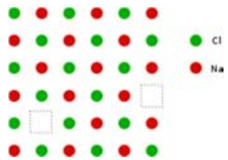
ideal crystal



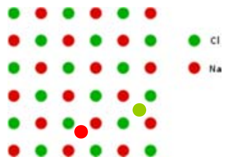
Point defects

a/ thermal

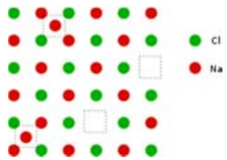
Schottky – defect (vacancy or hole)



interstitium

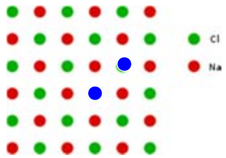


Frenkel – defect (vacancy and interstitia)

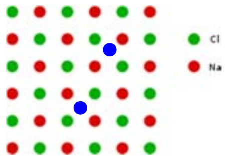


b/ doping

substitutional

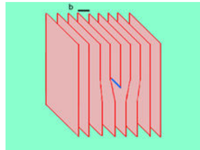


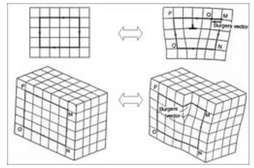
interstitial



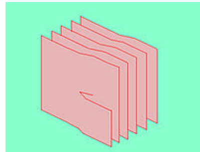
Line defects

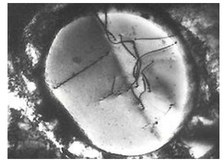
edge dislocation





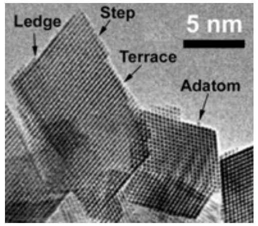
screw dislocation





Transmission electron micrograph of dislocation

Surface defects

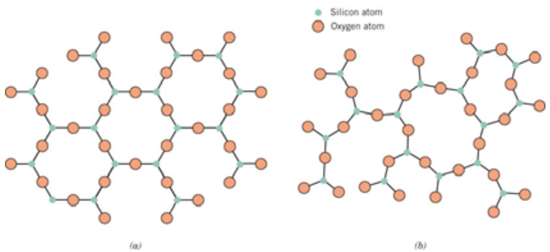


The defects strongly influence the material properties!

Al_2O_3 and $Al_2O_3 + Cr^{3+}$

Properties of amorphous solids:

no longe-range order of the position of atoms



the crystalline and amorphous structure of silica in two dimension

large number of structure defects

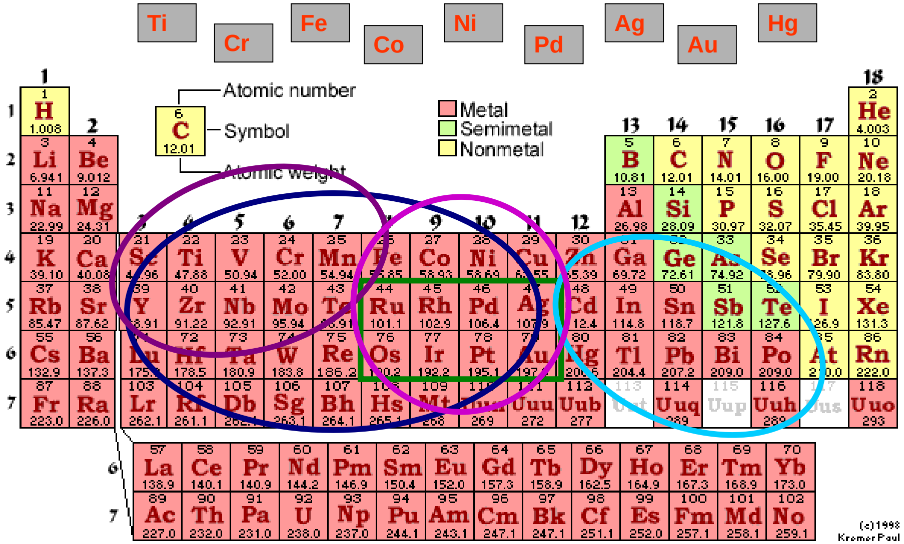
no definite shape (large viscosity liquid, supercooled liquid)

mechanical hardness

glass transition temperature T_g (the amorphous material becomes brittle on cooling or soft on heating)

isotrope property

Crystallization
(metals applied in the dentistry)



high melting-point

precious metals

low melting-point

fragile

ductile


chromium


titanium


iron


nickel


cobalt


palladium


silver


gold

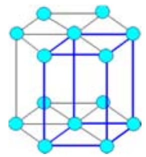

mercury

tin

Properties of metals

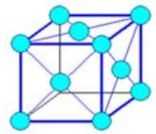
- -solid at room temperature (except Ga and Hg)
- - high luster
- - relatively high density (tightly packed crystal lattice)
- - large strength and toughness
- - ability to be deformed under stress without cleaving (ductile)
- - good electric and thermal conductivity

Submicroscopic structure of metals


hexagonal

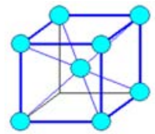
Ti, Cd, Co, Zn

Space filling factor 74 %


face-centered cubic

Ag, Au, Pd, Pt, Al, Cu, Ni

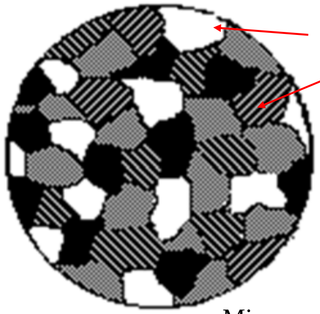
Space filling factor 74 %


body-centered cubic

Fe, Cr

Space filling factor 68 %

Microscopic structure of metals

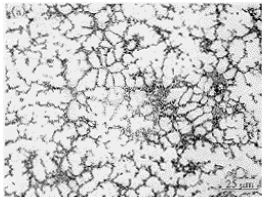


crystallites with different orientation, grains
small homogeneous particles

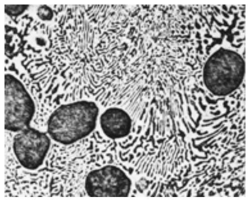
the properties of the material strongly depend on the structure

Stucture analysis: polishing (fine, rough)
chemical etching
microscopic technics

Microscopic view of metal surfaces

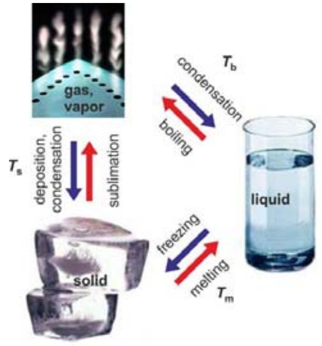


homogeneous

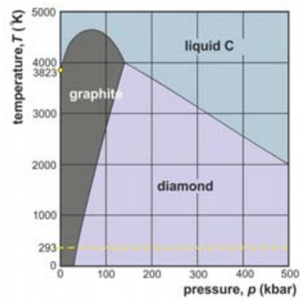


heterogeneous

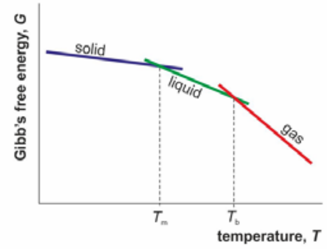
Phase transitions



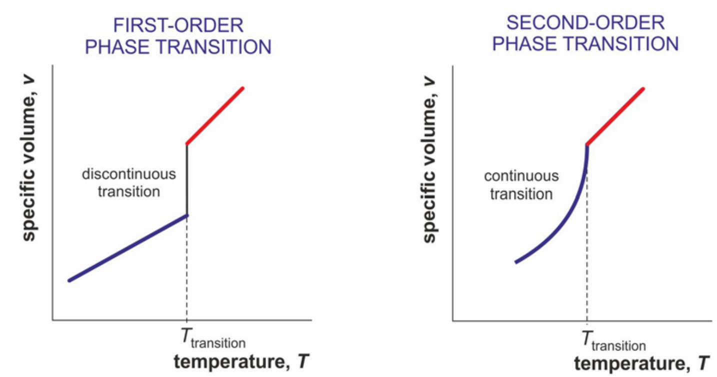
T_m and T_b strongly depend on the type of bond between the particles



$$G = E + pV - TS$$

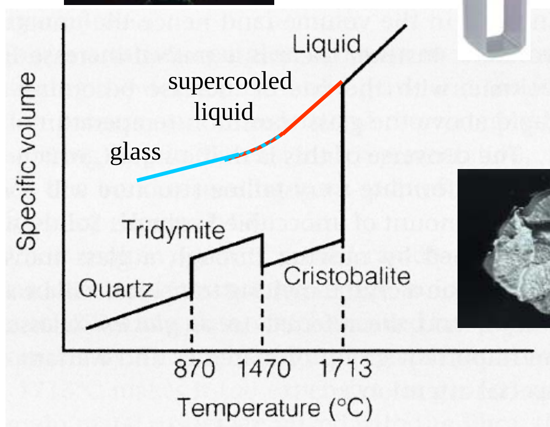


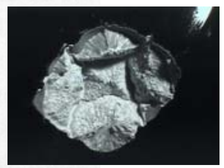
Classification of the phase transitions:



SiO_2

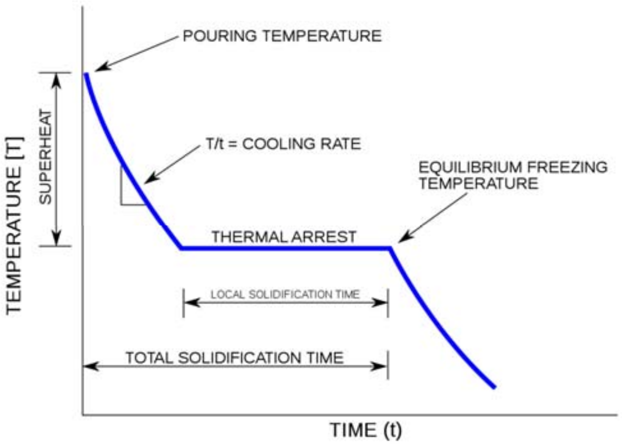
silica glass



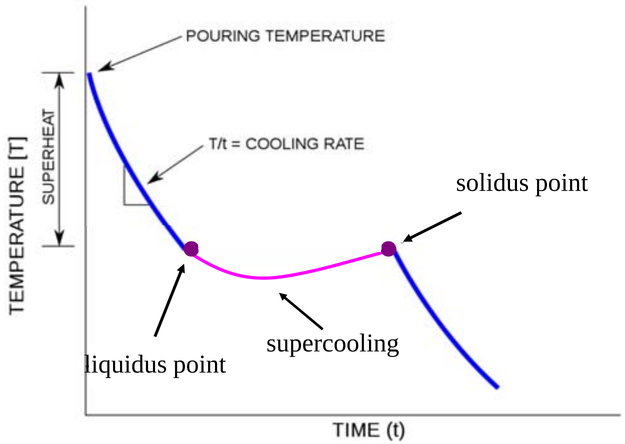


Crystallization (phase transition from liquid to solid phase)

cooling curve



Supercooling (phase transition from liquid to solid phase)



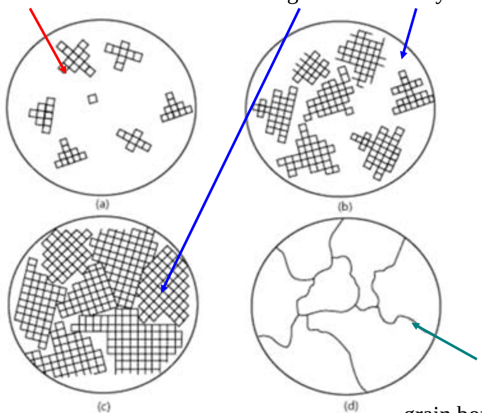
Transition from the liquid to the solid state

two stages: a./ nucleus (seed crystal) formation

b./ crystal growth

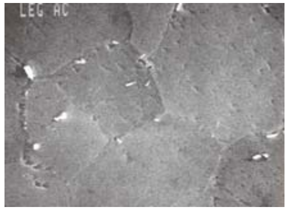
nucleus formation

growth of the crystallites



grain boundaries

dentritic (tree) increase



isotrope increase

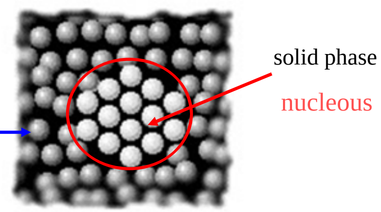
The role of the size and the shape of the grains !!

manganese dentrites on a limestone

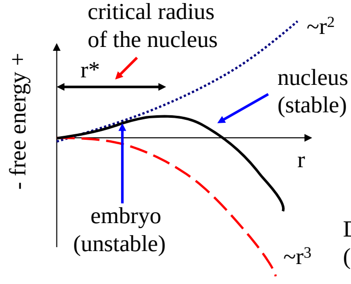
snow crystal

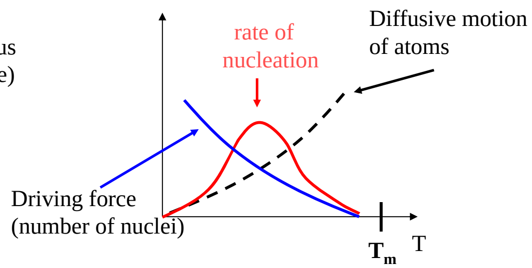
Nucleus formation

a./ homogeneous nucleation



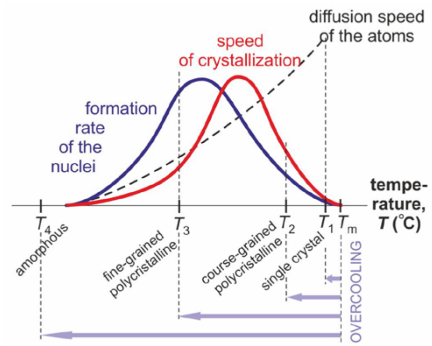
important parameters: the size of the nucleus
the rate of nucleus formation



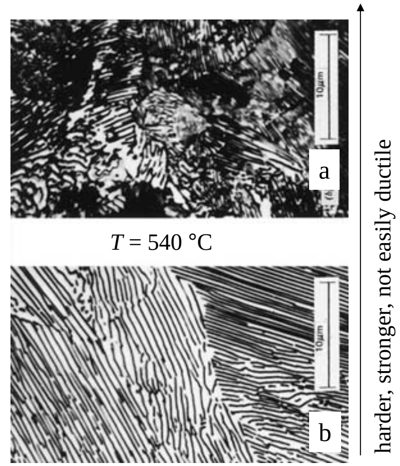


b./ heterogeneous nucleation (on the wall of the dish, impurities, dislocations mainly earlier and faster crystallization)

The growth of the stable nuclei:



fast nucleation and low rate of crystal increase	result	low rate of nucleation and fast increase of crystal size
↓		↓
fine grain structure (a)		rough grain structure (b)



T = 540 °C

T = 690 °C (T_m = 727 °C)

solid – solid state conversions !!

Crystallization ↔ glass formation