

# Physical bases of dental material science

Irén Bárdos-Nagy

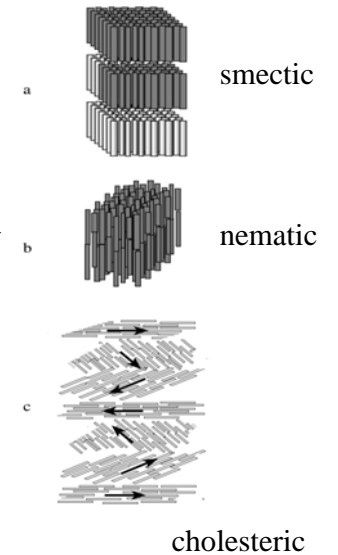
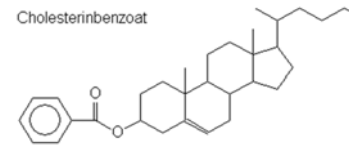
Liquid crystals: a mesomorphous state of matter

Thermotropic - liotropic

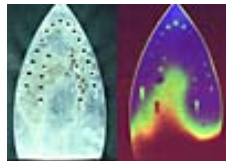
General properties

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

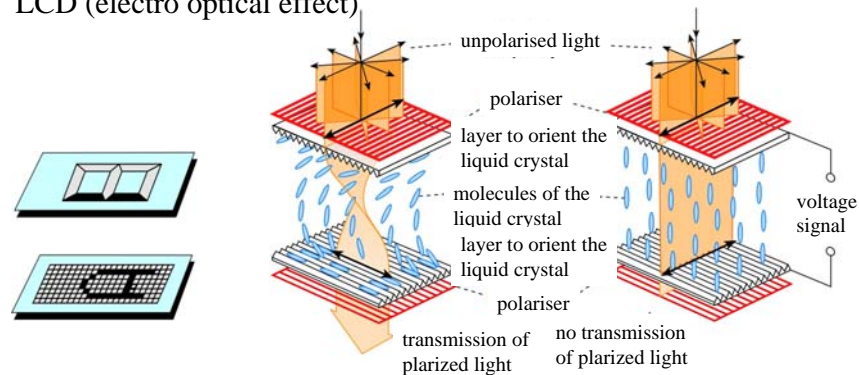
Cholesterinbenzoat



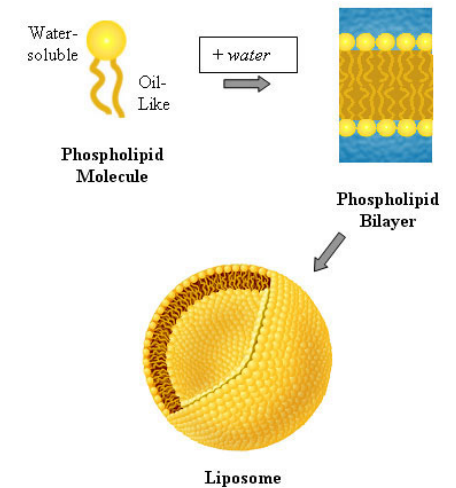
Use of thermotropic liquid crystals



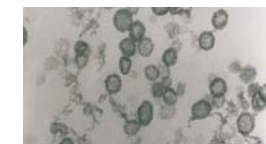
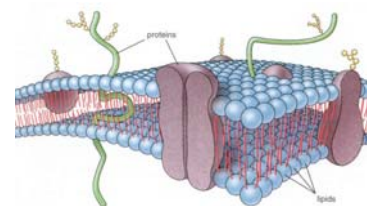
LCD (electro optical effect)



Liotropic liquid crystals

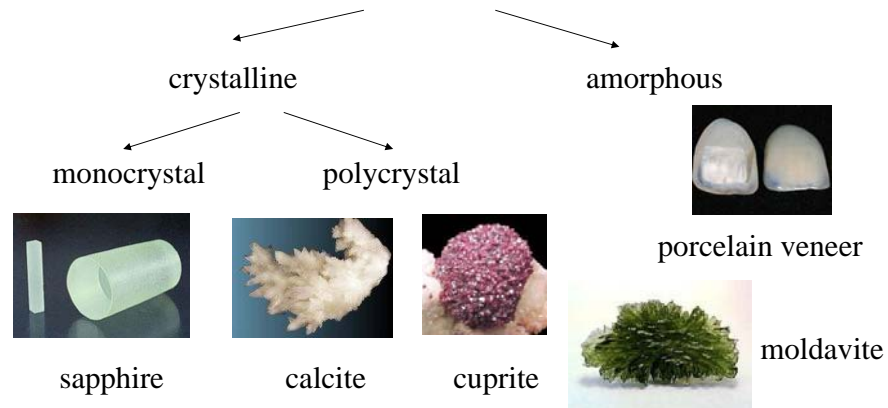


Cellular bi-layer membranes



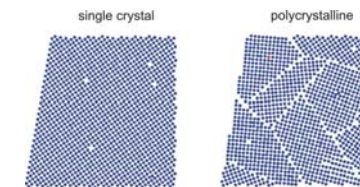
## Solid materials

### Classification of solid materials



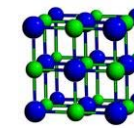
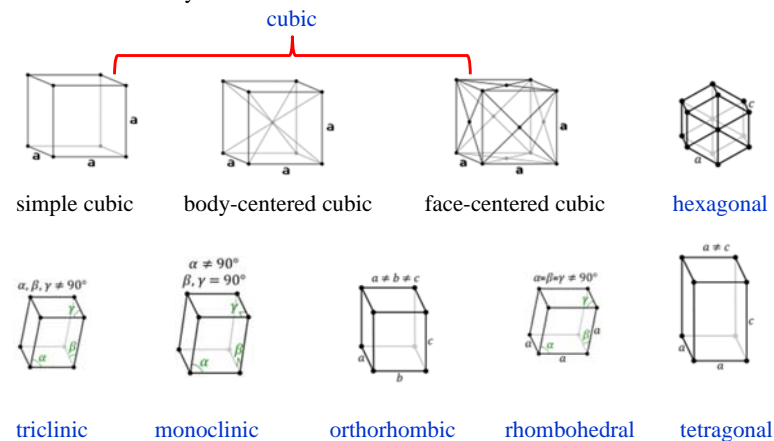
### Most important characteristics of crystalline materials

- 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)

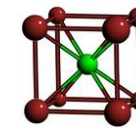


crystal structure: a unique arrangement of atoms or molecules  
long-range order and symmetry  
unit cell repeated periodically in 3D

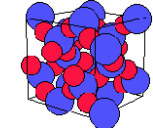
The seven lattice system:



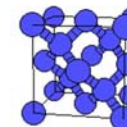
sodium chloride



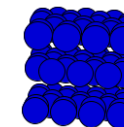
cesium chloride



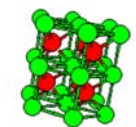
quartz



diamond



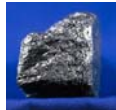
graphite



tungsten carbide

## 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	-



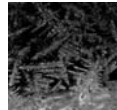
graphite



fluorapatite



gold



ice



sulfur

## Polymorphism - allotropy

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

polymorph forms of  $\text{SiO}_2$



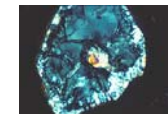
$\alpha$  quartz



tridymite

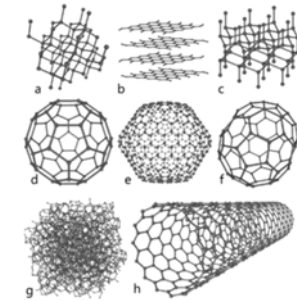


cristobalite



coesite

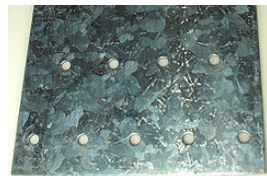
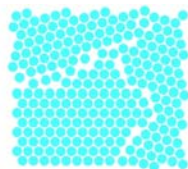
allotrop forms of carbon



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

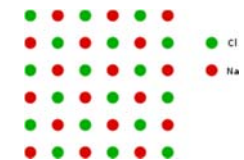
## Polycrystalline materials

- 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

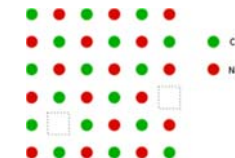
ideal crystal



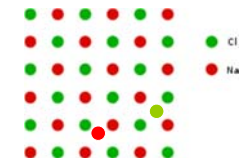
Point defects

a/ thermal

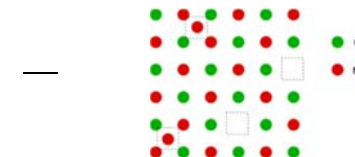
Schottky – defect (vacancy or hole)



interstitium

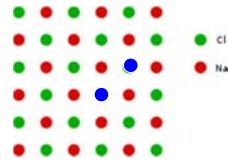


Frenkel – defect (vacancy and interstitia)

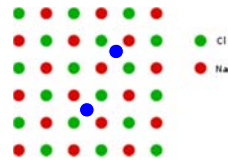


b/ doping

substitutional

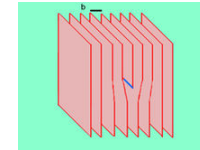


interstitial

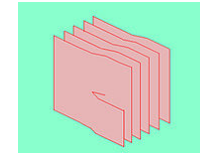


Line defects

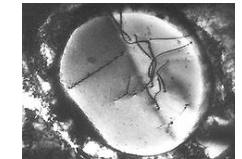
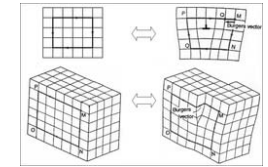
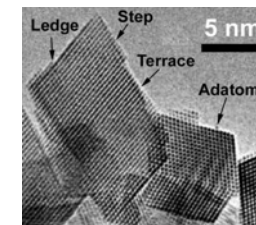
edge dislocation



screw dislocation



Surface defects



Transmission electron micrograph of dislocation

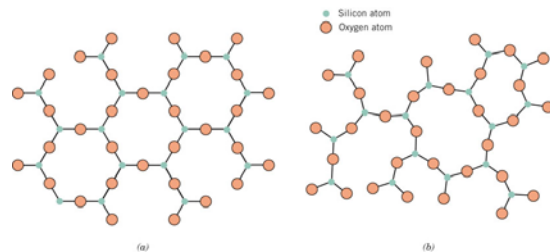
The defects strongly influence the material properties!



$\text{Al}_2\text{O}_3$  and  $\text{Al}_2\text{O}_3 + \text{Cr}^{3+}$

Properties of amorphous solids:

no long-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)

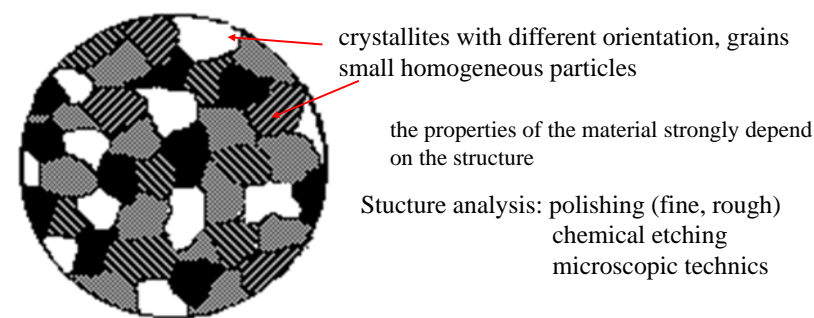
isotrope property

Crystallization  
(metals applied in the dentistry)

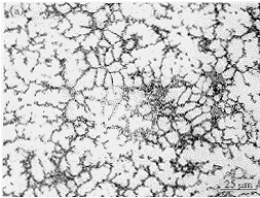




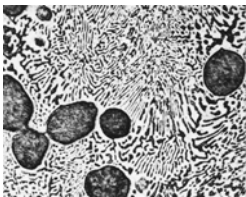
Microscopic structure of metals



Microscopic view of metal surfaces

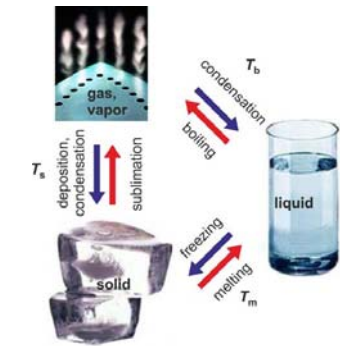


homogeneous

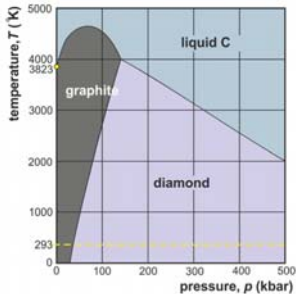


heterogeneous

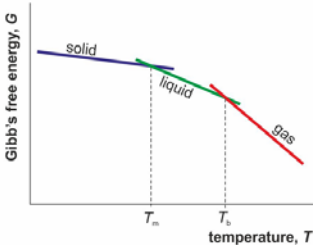
Phase transitions



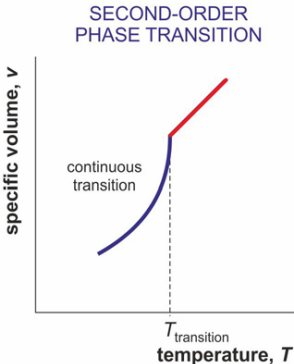
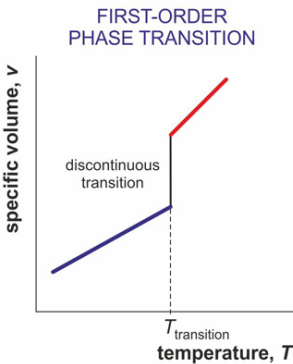
$T_m$  and  $T_b$  strongly depend on the type of bond between the particles



$$G = E + pV - TS$$



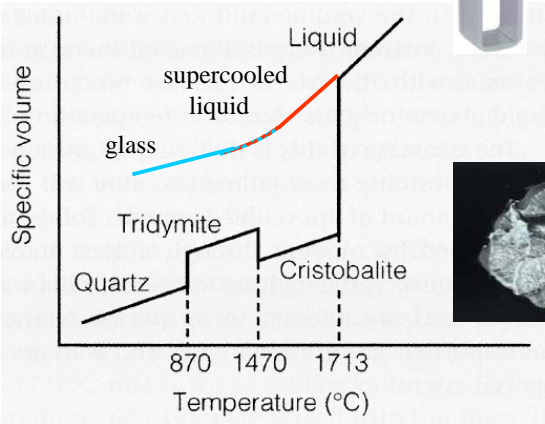
Classification of the phase transitions:



$\text{SiO}_2$

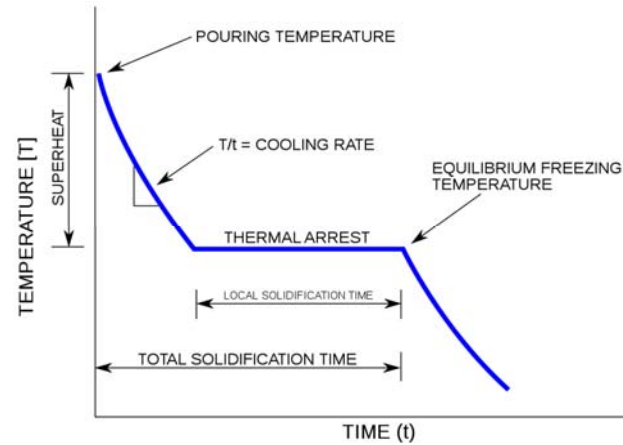


silica glass

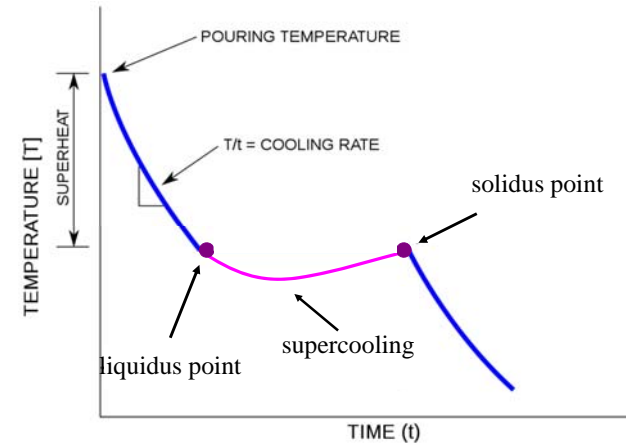


## Crystallization (phase transition from liquid to solid phase)

cooling curve



## Supercooling (phase transition from liquid to solid phase)



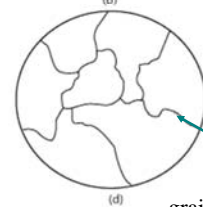
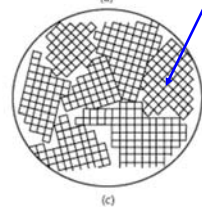
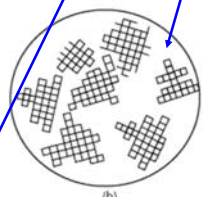
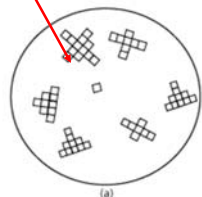
## Transition from the liquid to the solid state

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

b./ crystal growth

nucleus formation

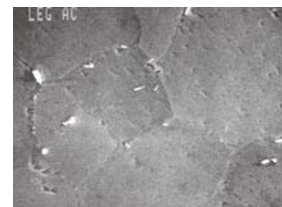
growth of the crystallites



grain boundaries



dendritic (tree) increase



isotrope increase

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



manganese dendrites on a limestone

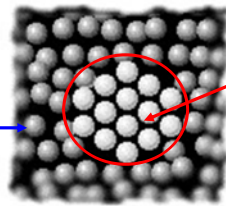


snow crystal

## Nucleus formation

a./ homogeneous nucleation

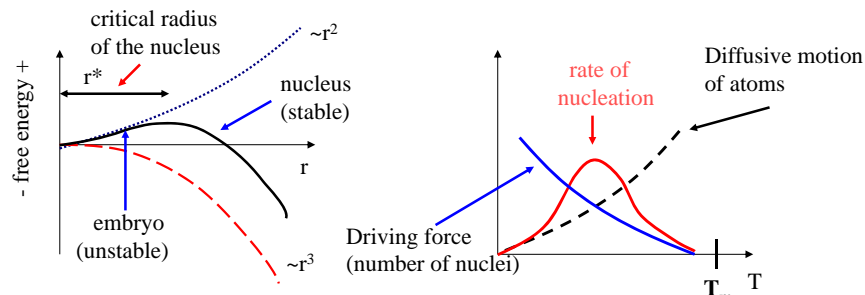
liquid phase



solid phase  
nucleus

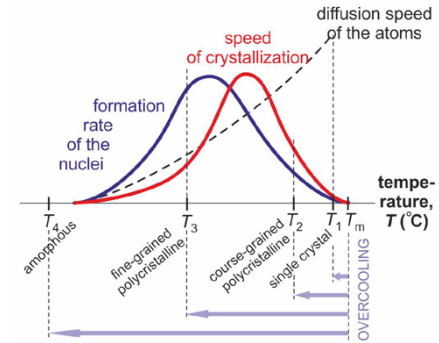
important parameters:

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

low rate of nucleation and fast increase of crystal size

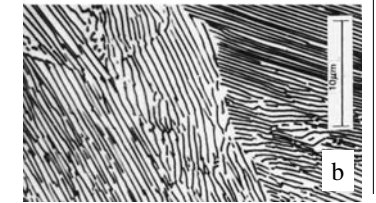
result

fine grain structure  
(a)

rough grain structure  
(b)



$T = 540^{\circ}\text{C}$



$T = 690^{\circ}\text{C}$  ( $T_m = 727^{\circ}\text{C}$ )

solid – solid state conversions !!

harder, stronger, not easily ductile

## Crystallization ↔ glass formation

