Physical Bases of Dental Material Science 2.

Structure of matter

Liquids, solids, liquid crystals

Highlights:
- Viscosity
- Water and saliva
- Crystals - apatite
- Polymorphism
- Crystal defects
- Amorphous materials
- Liquid crystals (Material found in Medical Biophysics!)

E-book Chapters: 4, 5
Medical Biophysics I/3.4.2.

Problems:
Chapter 1.:
22, 23, 32, 33, 34, 35

States of matter - Phases

T

	solid	liquid	gas
definite volume	+	+	-
stable shape	+	-	-

Fluids versus **Solids**

indefinite shape:
Shape does not recover after deformation, lack of restoring forces.

definite shape:
Shape recovers after deformation, due to restoring forces.

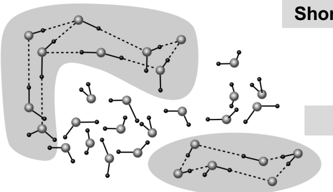
Fluids

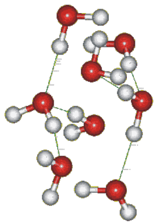
INTERACTIONS
REPULSIVE = ATTRACTIVE

particle movement versus inter-particle bonds

⇩

Short range, dynamic order





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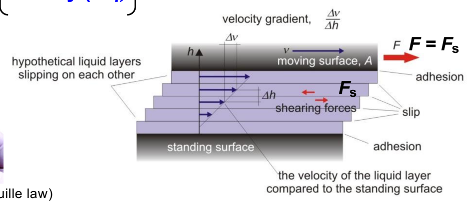
isotropic

Viscosity (η) ⟺ Fluidity ($1/\eta$)

(later: Hagen-Poiseuille law)



Newton's law of viscosity:

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

viscosity (coefficient of internal friction)

$[\eta] = \mathrm{Pa \cdot s}$

Another form of Newton's law:

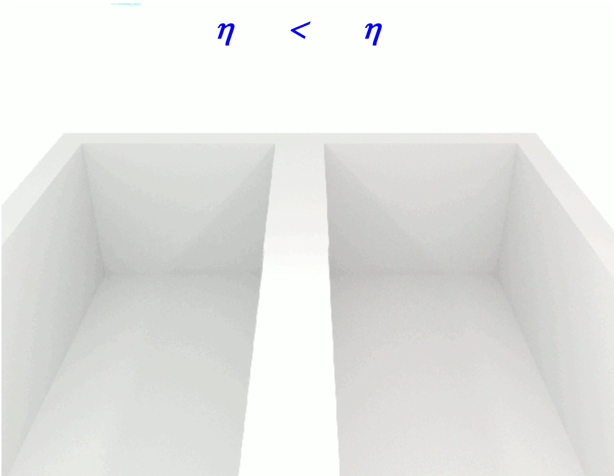
$$\sigma_{shear} = \frac{F_s}{A} = \eta \cdot \frac{\Delta v}{\Delta h} \quad g_v$$

shear stress — velocity gradient

$$\sigma_{shear} = \eta g_v$$

Which one has higher viscosity?

$\eta \quad < \quad \eta$



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Rotational viscometer:

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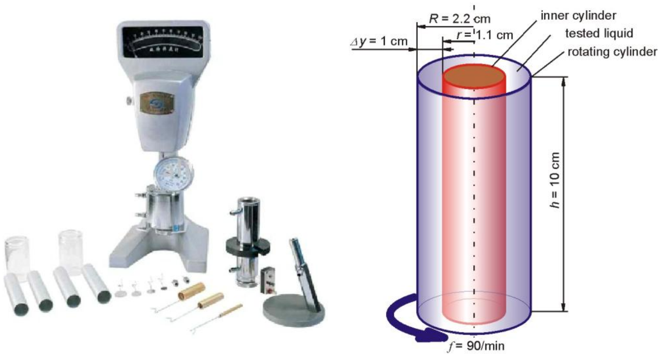
Figure schematically shows the structure of a rotational viscometer. The inner cylinder is still and the outer is rotated. The radius of the outer cylinder R = 2.2 cm, the inner cylinder r = 1.2 cm. The cylinder's height is h = 10 cm. The tested liquid between cylinders is glycerine. Layer thickness is $\Delta y = R - r$ = 1cm. Calculate the force that is necessary for uniform rotation of the cylinder does 90 revolutions per minute? (viscosity of the glycerine η = 1500 mPas. The flow is laminar.)



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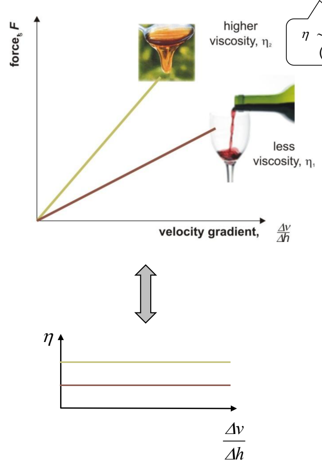
Newton's law of viscosity: $F_s = \eta \cdot A \cdot \frac{\Delta v}{\Delta h}$

η ~ is the slope (constant)



material	η (mPas)
air	0,019 (20° C)
water	1 (20° C)
saliva substitute (USA patent)	2–10
glycerol	1500 (20° C)
ethyl methacrylate monomer	0,5 (25° C)
ethylene glycol dimethacrylate monomer	3,4 (25° C)
zinc phosphate	95 000 (25° C)
zinc oxide -eugenol	100 000 (37° C)
silicone	60 000-1 200 000 (37° C)

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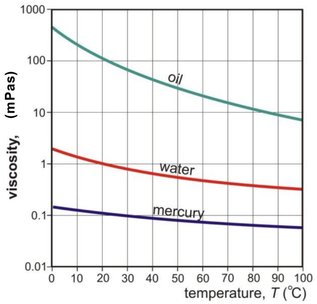
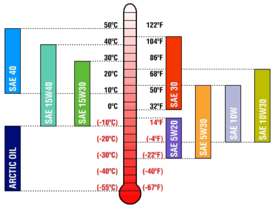
η **depends on:**
- material quality
- temperature





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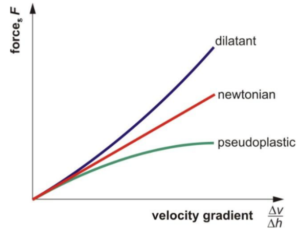
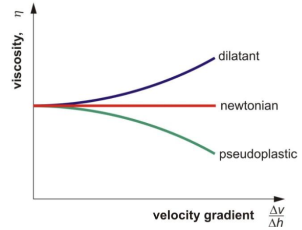
η **depends on:** 1. shear forces/velocity gradient





liquids

- Newtonian fluids
  - i.e. water, oil
- Non-Newtonian fluids
  - pseudoplastic: i.e. saliva, blood, polycarboxylate cements, elastomer impression materials
  - dilatant: i.e. dental composite resins

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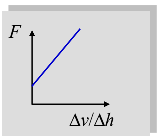
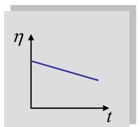
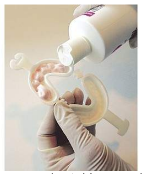
Bingham-fluid:

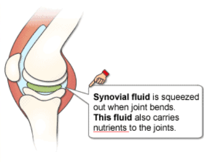


η **depends on:** 2. time of mechanical stress

Thixotropic fluid:

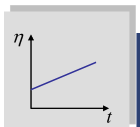


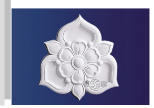




some dental impression materials

Rheopex fluid:





Not to confuse them with dilatant and pseudoplastic fluids!

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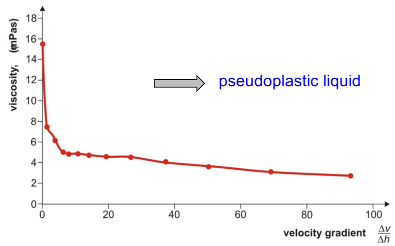
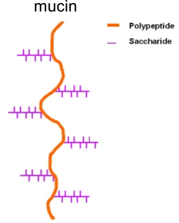
Saliva

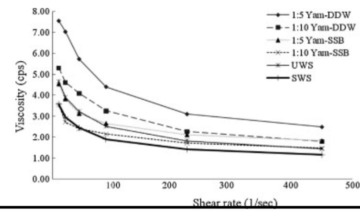


→ pseudoplastic liquid

mucin



saliva substitutes:



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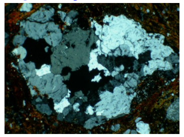
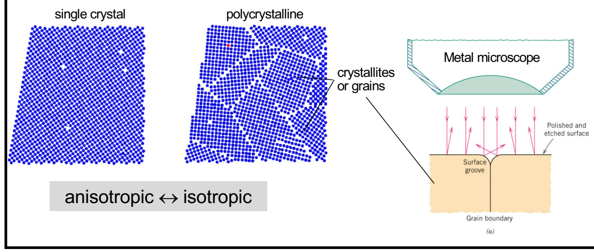
Solid materials

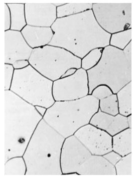
(crystal = solid body)

crystalline — amorphous

single crystal — policrystalline







anisotropic ↔ isotropic

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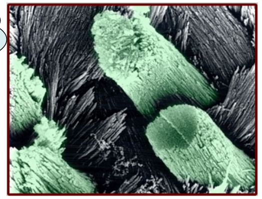
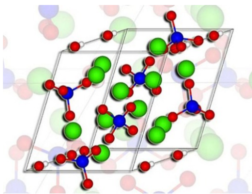
Apatite

OH$^-$: hydroxyapatite
F$^-$: fluorapatite

$Ca_{10}(PO_4)_6(X)_2$ hexagonal ioncrystal

$Ca_5(PO_4)_3X$





Dentin, bone: 20-60 nm x 6 nm crystals

Enamel: 500-1000 nm x 30 nm crystals

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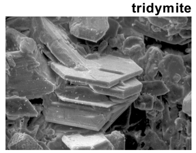
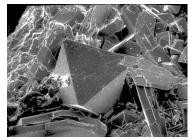
Polymorphism

Examples: SiO_2

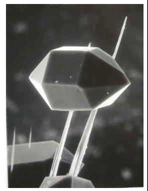
tridymite



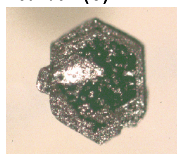
cristobalite

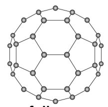


quartz



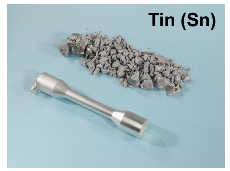
carbon (C)

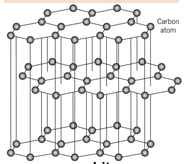




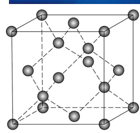
fullerene

Tin (Sn)

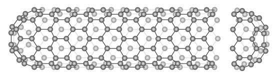




graphite



diamond



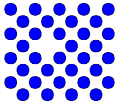
nanotube

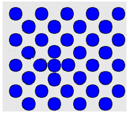
polymorphism of elements = **allotropy** 16

Crystal defects

- point defects
  - thermal defect
    - vacancy (Schottky-defect)
    - interstitial defect
  - Impurity (dopant)
    - substitutional impurity atom
    - interstitial impurity atom

(alloys !!)

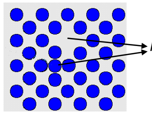


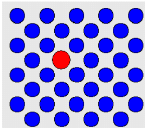


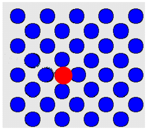
$$n_S = N \cdot e^{-\frac{\varepsilon_S}{kT}}$$

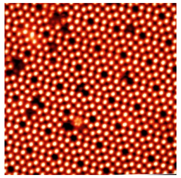
No. of Schottky-defects

Frenkel-defect





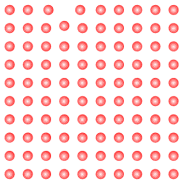


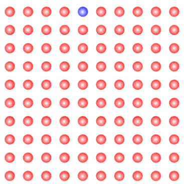


0.9 eV energy is necessary to produce a vacancy in copper.
a) How many percnt is the ratio of vacancies in the crystal at 1000°C?

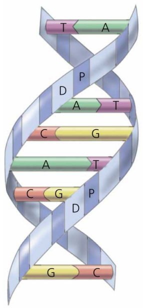
$$n_S = N \cdot e^{-\frac{\varepsilon_S}{kT}}$$

Generation and diffusion of point defects:



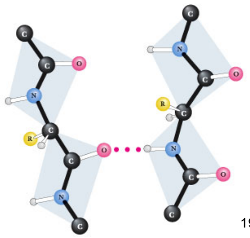


Thermal defects in biomolecules

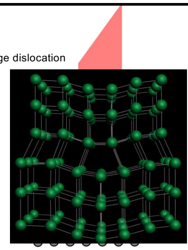


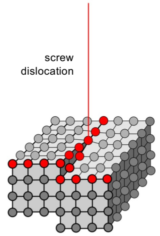
$$n_{S_0} = N \cdot e^{-\frac{\varepsilon_S}{kT}}$$

No. of broken H-bonds

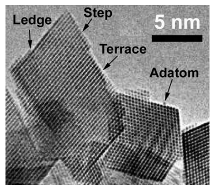


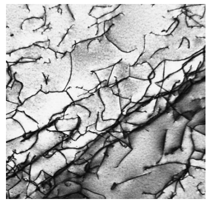
- Line defects
  - edge dislocation
  - screw dislocation





- planar defects



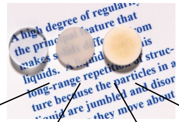


dislocations in titanium alloy

Lattice defects strongly influence the properties!

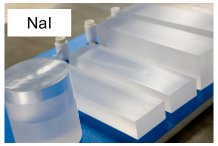
i.e. optical properties

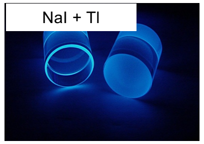
Al_2O_3



+ Cr^{3+} + V^{2+} Fe^{2+} +Ti^{4+}+Fe^{2+}





Emits light when irradiated by X-ray!

Scintillation crystals for detecting X-ray and gamma rays.

i.e. mechanical properties



i.e. chemicl properties

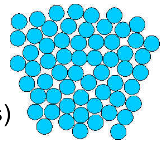
$Ca_{10}(PO_4)_6(OH)_2$ ⟺ $Ca_{10}(PO_4)_6F_2$

hydroxyapatite   fluorapatite

Lower solubility in acids.

i.e. electronic properties ⇒ doped semiconductors

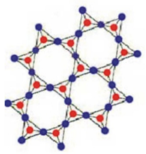
Amorphous materials = glass, glassy materials

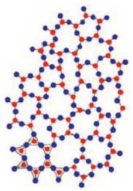
- short distance order
- many defects
- no defined shape (flows) (extreme high viscosity, thus flow is extremely slow)
- hard materials
- isotropic

i.e. glass, synthetic resins, wax, asphalt, ...

crystalline SiO_2



amorphous SiO_2



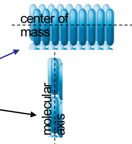
•Si •O

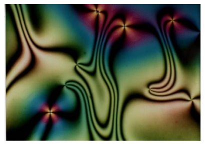
pitch drop experiment

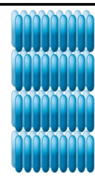
❖ (Medical Biophysics I/3.4.2.)

Liquid crystals

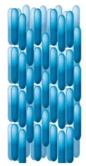
- anisodimensional molecules
- mesophase
- partially ordered structure
  - Translational order
  - Orientational order
- fluid
- optically anisotropic
- structure can change according to environment
  - temperature can change the order: *thermotropic liquid crystals*
  - concentration: *lyotropic liquid crystals*



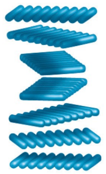




smectic
translational + orientational order

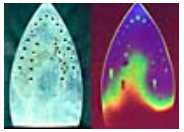


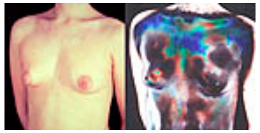
nematic
only orientational order

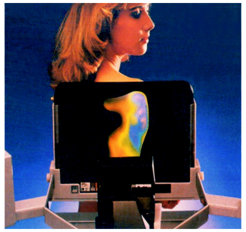


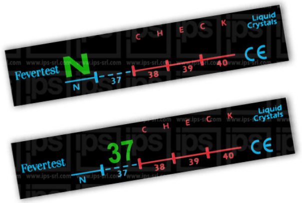
cholesteric
only orientational order (twisted nematic)

Contact thermography
(thermo-optical effect)

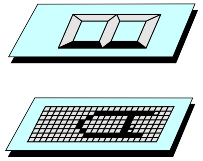


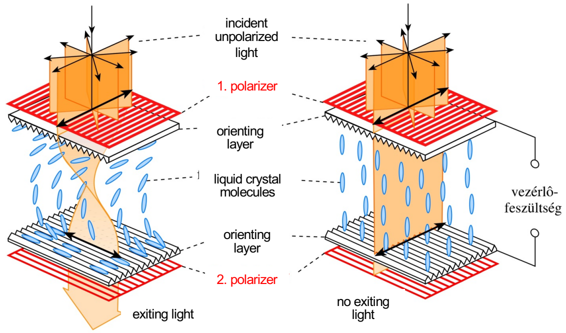




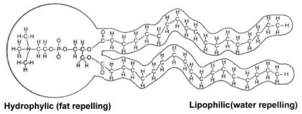


LCD
(electro-optical effect)

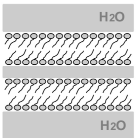




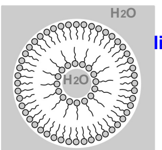
Lyotropic liquid crystals



Shape of phospholipid molecule



lamellar



liposome