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

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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

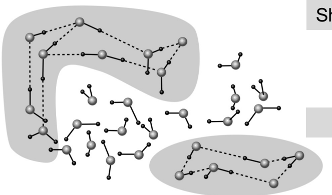
particle movement versus inter-particle bonds

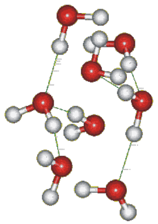
↓

Short range, dynamic order

↓

isotropic





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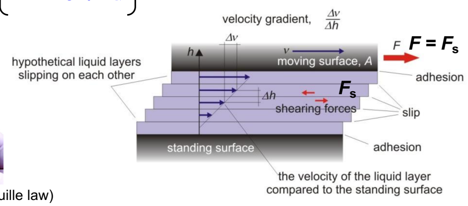
Viscosity (η) ⟺ (Fluidity ($1/\eta$))

(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)

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

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

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

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Rotational viscometer:

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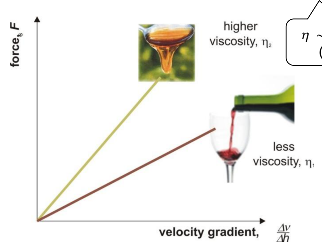
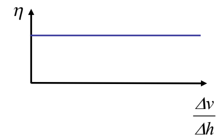
Newton's law of viscosity: $F_s = \eta \cdot A \cdot \frac{\Delta v}{\Delta h}$

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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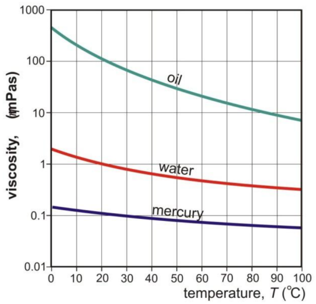
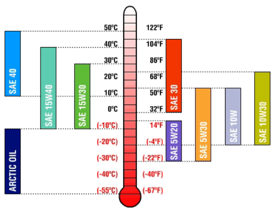
η depends on:
- material quality
- temperature





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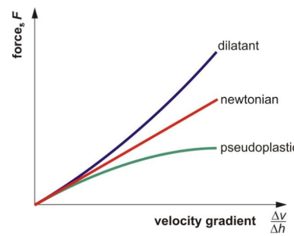
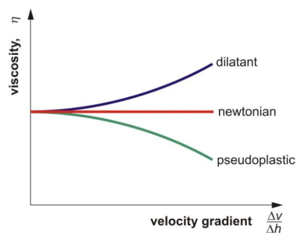
η depends on: • shear forces/velocity gradient





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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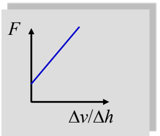
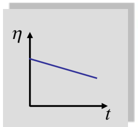
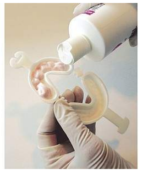
Bingham-fluid:

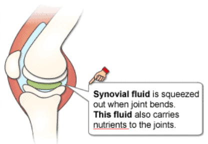


η depends on: • time of mechanical stress

Thixotropic fluid:

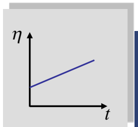


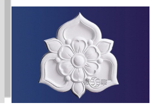




some dental impression materials

Rheopex fluid:





Not to confuse them with dilatant and pseudoplastic fluids!

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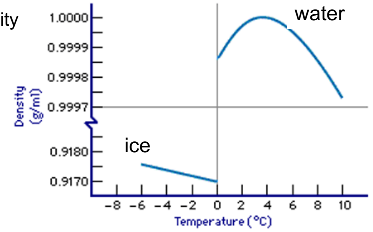
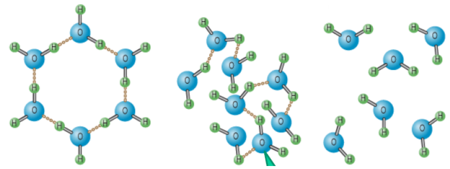
Water

- fluid in a large range of temperature
- relatively low density (1 g/cm³)
- Newtonian fluid with low viscosity





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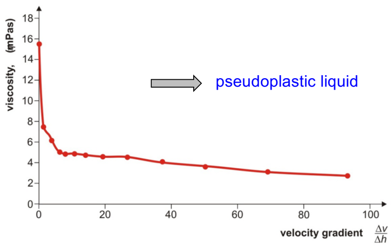
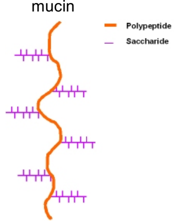
Saliva

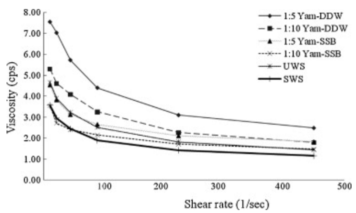


pseudoplastic liquid

mucin



saliva substitutes:



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Solid materials

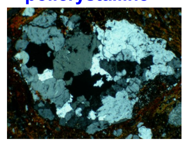
(crystal = solid body)

crystalline

amorphous

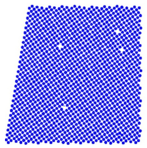
single crystal

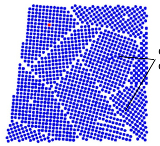
policrystalline



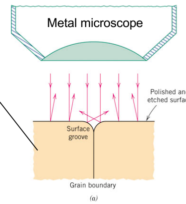
single crystal

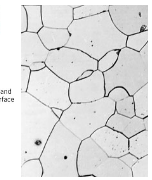
polycrystalline





crystallites or grains





anisotropic ↔ isotropic

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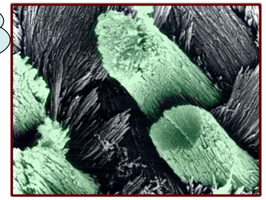
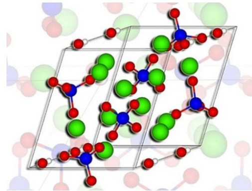
Apatite

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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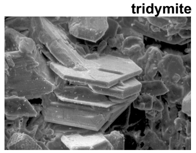
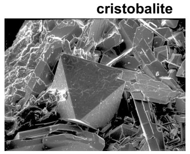
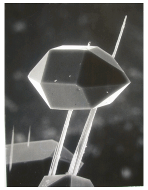
Polymorphism

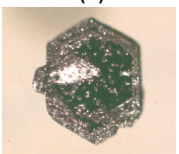
Examples: **SiO_2**

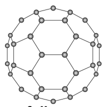


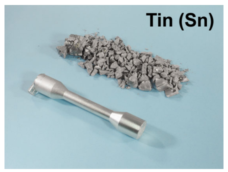


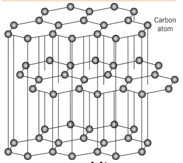


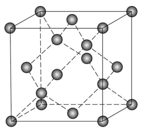
carbon (C)

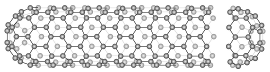












polymorphism of elements = allotropy 15

Crystal defects

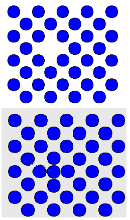
- **point defects**
  - **thermal defect**
    - **vacancy (Schottky-defect)**
    - **interstitial defect**
  - **Impurity (dopant)**
    - **substitutional impurity atom**
    - **interstitial impurity atom**

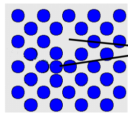
(alloys !!)

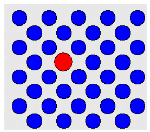
$$n_S = N \cdot e^{-\frac{\varepsilon_S}{kT}}$$

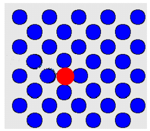
No. of Schottky-defects

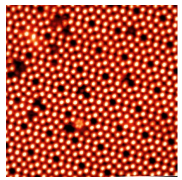
Frenkel-defect











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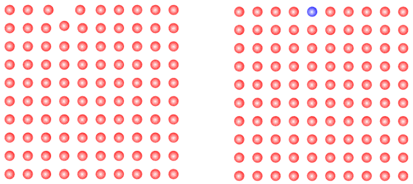
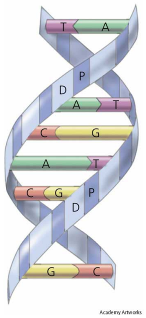
Generation and diffusion of point defects:

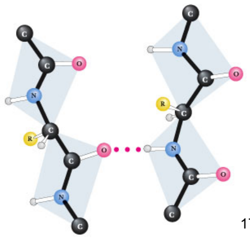


Thermal defects in biomolecules



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

No. of broken H-bonds



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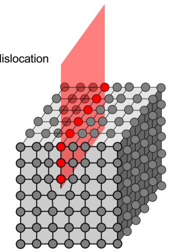
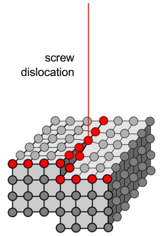
- Line defects
  - edge dislocation
  - screw dislocation

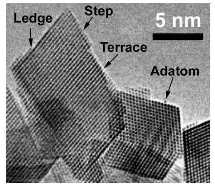
edge dislocation

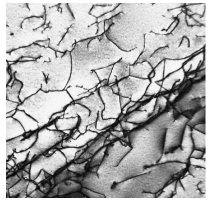


screw dislocation



- planar defects





dislocations in titanium alloy

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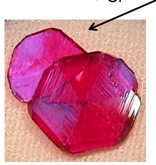
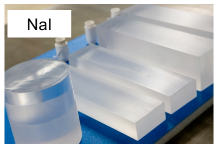
Lattice defects strongly influence the properties!

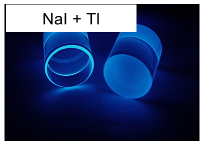
i.e. optical properties

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.

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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

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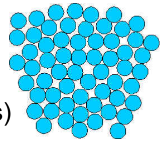
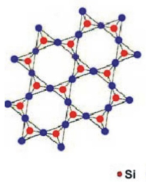
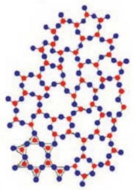
Amorphous materials = glass, glassy materials

- 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, ...

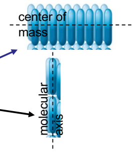


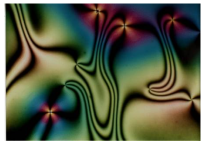


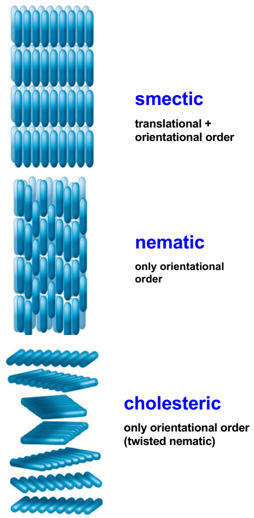
❖ (Medical Biophysics I/3.4.2.)

Liquid crystals

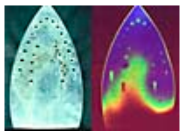
- anisodimensional molecules
- mesophasic
- partially ordered structure
  - Translational order
  - Orientational order
- fluid
- optically anisotropic
- structure can change according to environment
  - temperature can change the order: *thermotropic liquid crystals*
  - concentration: *lyotropic liquid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

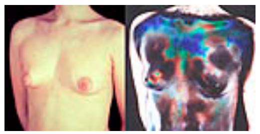


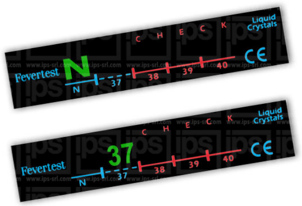




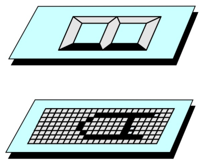
Contact thermography
(thermo-optical effect)

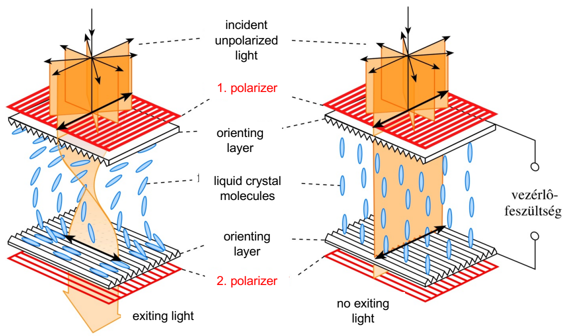




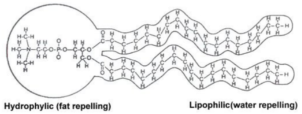


LCD
(electro-optical effect)

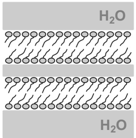




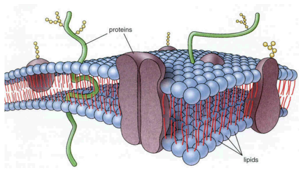
Lyotropic liquid crystals

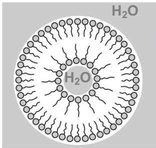


Shape of phospholipid molecule



lamellar





liposome