Physical Bases of Dental Material Science

Introduction

Important informations

- **Tutor:** Zsolt Mártonfalvi, PhD (martonfalvi.zsolt@med.semmelweis-univ.hu)
- Department of Biophysics and Radiation Biology, left elevators, 2nd floor
  Head: Prof. Miklós Kellermayer
- http://biofiz.semmelweis.hu
- Pdf format e -book (Physical bases of dental material science)
- Exam: written test composed of three sections:
  1) Definitions, 2) Calculations, 3)Theory

Further readings:

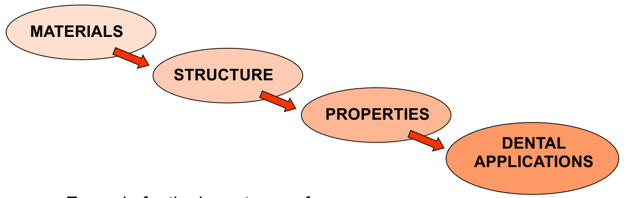
- W.D. Callister: *Materials Science and Engineering*. An Introduction (7th ed.), Wiley&Sons, 2007
- K.J. Anusavice: Phillips' *Science of Dental Materials* (11th ed.), Saunders, 2003
- Damjanovich, Fidy, Szöllősi: *Medical Biophysics*, Medicina, Budapest, 2009

Lectures

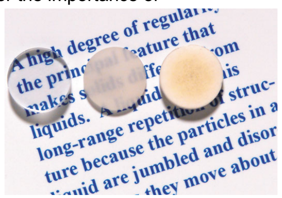
1	Atomic interactions, bonds. Multiatomic systems, gases. Interpretation of temperature, Boltzmann-distribution. (Zsolt Mártonfalvi)	10.09.2017
2	Fluids, solids, liquid crystals. (Zsolt Mártonfalvi)	17.09.2017
3	Cohesion, adhesion, interfacial phenomena. Phase, phasediagram, phase transitions. (Zsolt Mártonfalvi)	24.09.2017
4	Crystallisation. Metals, alloys, ceramics. (Zsolt Mártonfalvi)	01.10.2017
5	Polymers, composites. (Zsolt Mártonfalvi)	08.10.2017
6	Methods for structural examination (diffraction, microscopic, spectroscopic methods) *Extra workday for October 22.* (Zsolt Mártonfalvi)	13.10.2017
7	Mechanical properties of materials 1. Elasticity. (Zsolt Mártonfalvi)	15.10.2017
8	Mechanical properties of materials 2. Plasticity, hardness. (Zsolt Mártonfalvi)	29.10.2017
9	Mechanical properties of materials 3. Rheological properties, viscoelasticity. (Károly Módos)	05.11.2017
10	Optical, electrical and thermal properties of materials. (Károly Módos)	12.11.2017
11	Comparison of the properties of dental materials based on their structure. (Károly Módos)	19.11.2017
12	Bases of biomechanics. Structure, mechanical and other properties of dental tissues. (Zsolt Mártonfalvi)	26.11.2017
13	Physical bases of implantology. (*Guest lecturer: Attila Szűcs*) (Zsolt Mártonfalvi)	03.12.2017
14	Physical bases of orthodontics. (*guest lecturer: Bálint Nemes*) (Zsolt Mártonfalvi)	10.12.2017

How to start? – How to proceed?

The way how the lectures proceed



Example for the importance of structure:



All are Al_2O_3 !

How to study?

Preferably prior to lecture!

- download handout, read it
- read book chapter
- question marks (?)

1. introduction

0,5-1 h

2. processing → understanding

2-3 h

- Learn definitions, laws, quantities precisely
- practical applications

3. repetition, memorizing

0,5-1 h

Communicate!

- lecture: take notes! – make questions
- read again the book chapter, understanding, remarks
- do the calculations

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Physical Bases of Dental Material Science 1.

Structure of matter

Atomic interaction, multiatomic sytem - gases

E-book chapters: 1, 2, 3

Highlights:
- ❖ Interactions
- ❖ Energy curve of atomic and molecular interactions
- ❖ A Interpretation of temperature
- ❖ Boltzmann-distribution

Problems: Chapter 1, 2, 3.: 1, 3, 9, 10, 13, 17, 19

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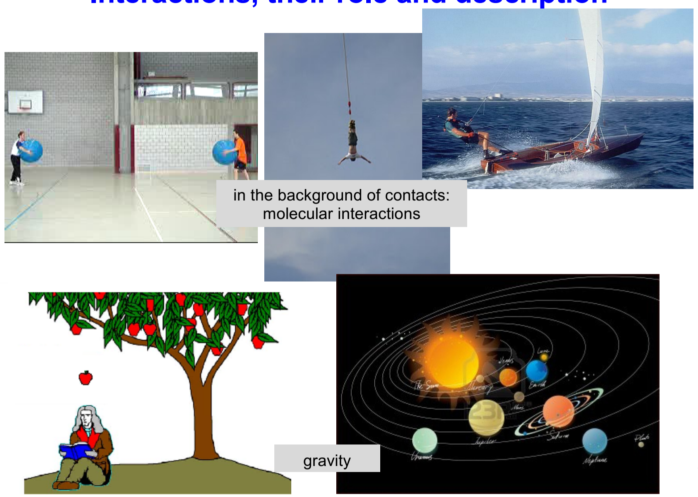
Interactions, their role and description



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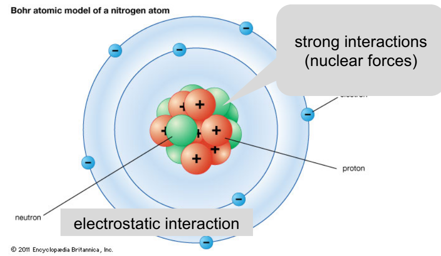

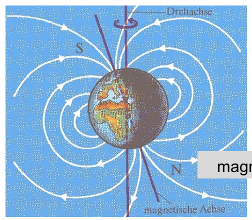

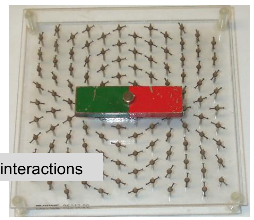

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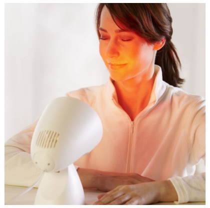
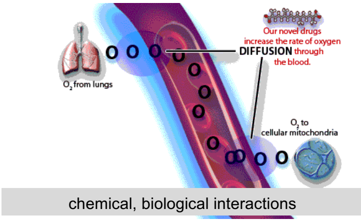
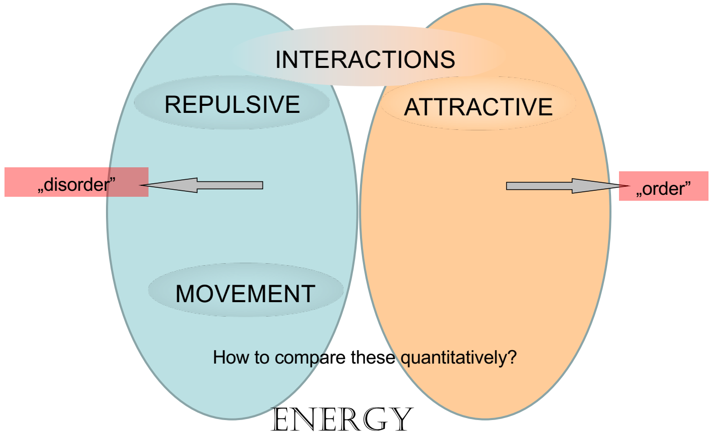
thermal interaction (heat)





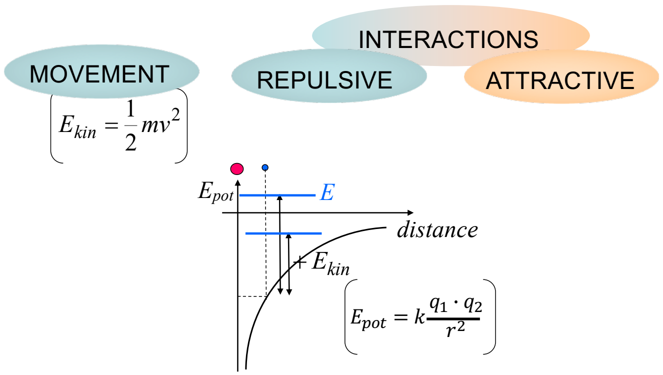
chemical, biological interactions

How bodies are formed in general:



ENERGY

Energy of an interaction (potential energy), kinetic energy

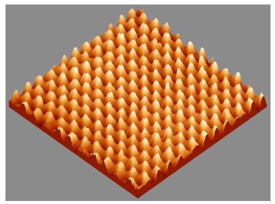


$E = E_{pot} + E_{kin} < 0$ ⟹ bound e$^-$

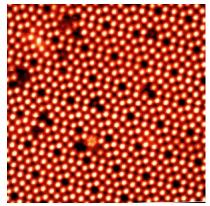
$E = E_{pot} + E_{kin} > 0$ ⟹ free e$^-$

All matter is composed of atoms

- Democritus B.C. 5th century
- Dalton's atomic theory 1803
- Rutherford 1911
- Bohr 1913



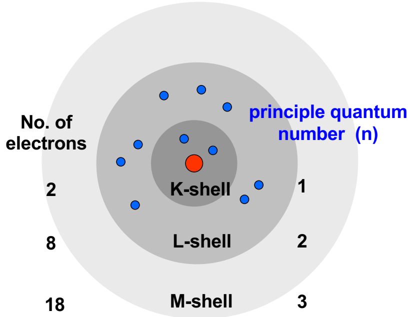
C atoms in crystal lattice
no vacancies

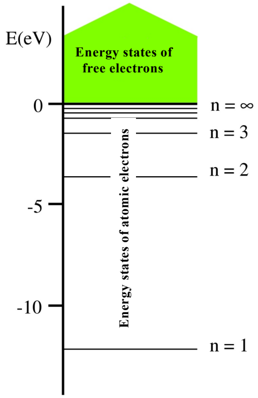


Si crystal with
vacancies

Structure of the atom

- Rutherford experiment, Spectroscopy (Bohr)
- Discrete energy levels
- Energy minimum
- Pauli-principle

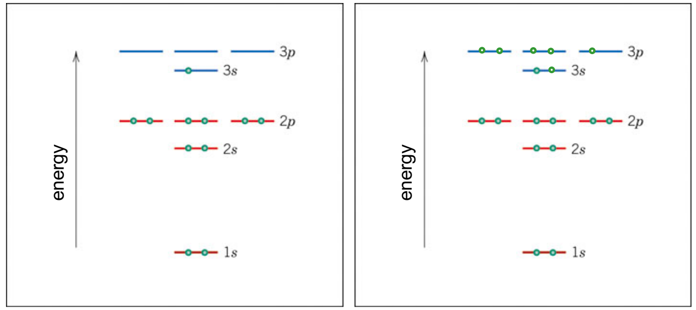




Energy unit:
elektronvolt (eV),
1 eV = $1{,}6 \cdot 10^{-19}$ J

Electron configuration:

i.e. $_{11}$Na atom | i.e. $_{17}$Cl atom

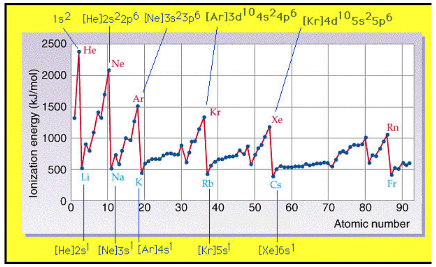


$1s^2 2s^2 2p^6 3s^1$ | $1s^2 2s^2 2p^6 3s^2 3p^5$

Electronegativity

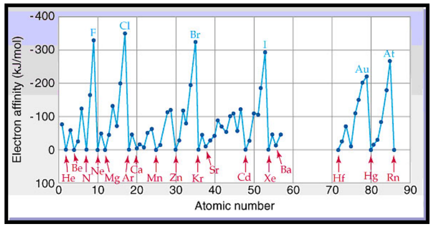
Ionization energy(*I*):

The amount of energy that is necessary to remove the most loosely bound electron from an atom **(eV/atom; kJ/mol)**



Electronaffinity (*A*):

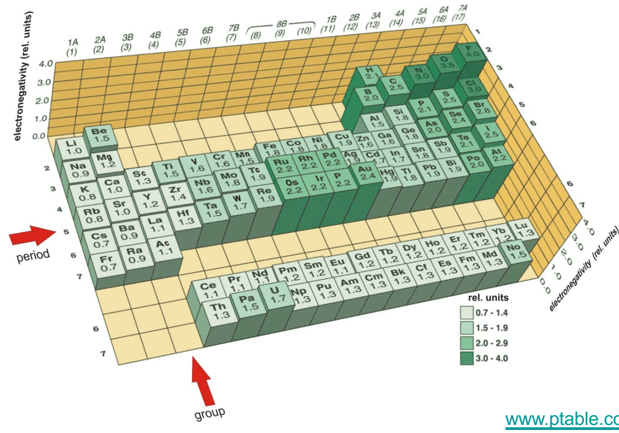
The amount of energy released when an electron is added to an atom **(eV/atom; kJ/mol)**



Electronegativity (EN):

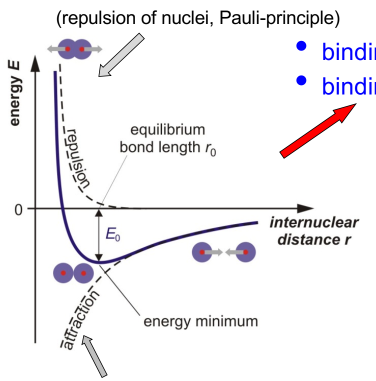
$$EN = I + |A|$$

Pauling-scale:

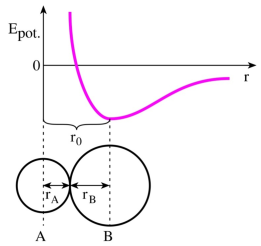


www.ptable.com

Atomic interactions



- binding distance (r_0) ≈ 0,1 nm (1Å)
- binding energy (E_0) ≈ 2-1000 kJ/mol



- shared electron orbitals
- electrostatic interactions (ion-ion, ion-dipole, dipole-dipole)

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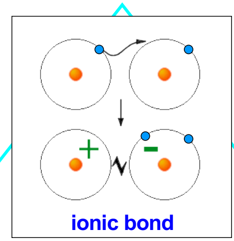
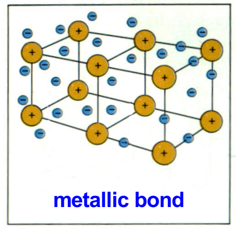
Bond types

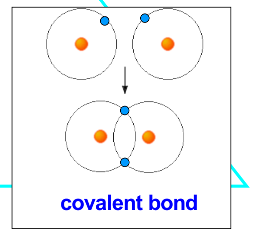
- primary (strong) ≈100 kJ/mol
  - covalent
  - metallic
  - ionic



NaCl



pl. Na



H_2

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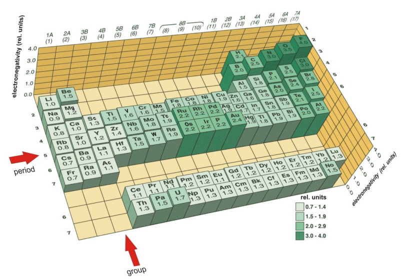

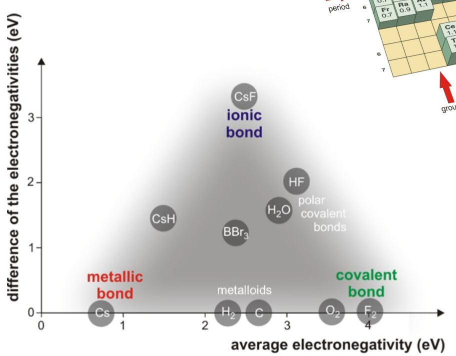

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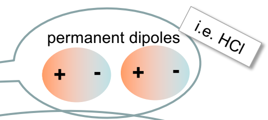
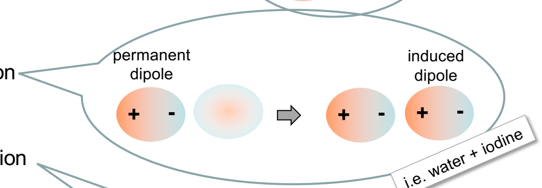
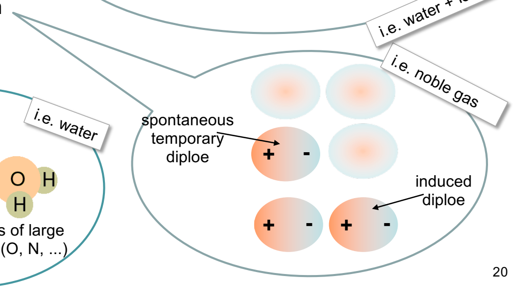
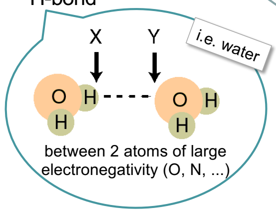
- secondary (weak) ≈ 10 kJ/mol
  - van der Waals - between diploes
    - orientation
    - induction
    - dispersion
  - H-bond









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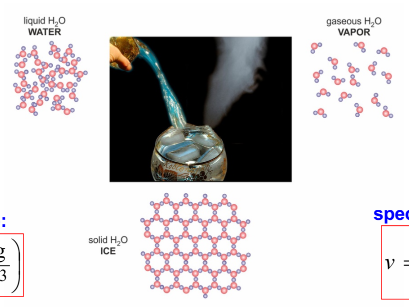
States of matter - Phases

T

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



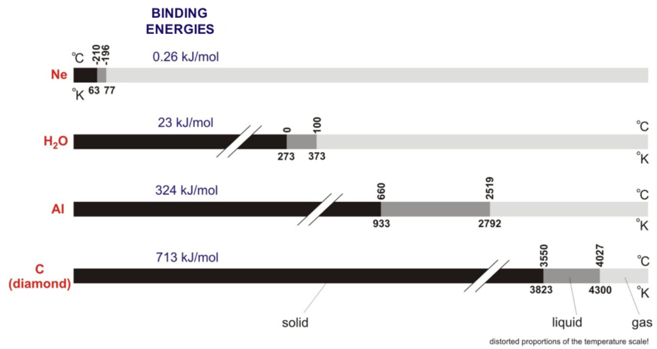
density (ρ):

$$\rho = \frac{m}{V} \left(\frac{\text{kg}}{\text{m}^3}\right)$$

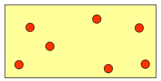
specific volume (v):

$$v = \frac{1}{\rho} \left(\frac{\text{m}^3}{\text{kg}}\right)$$

attraction ⟺ repulsion + movement *T*



Gases



Macroscopic description:

- No definite volume or shape
- isotropic

$p,\ V,\ n,\ T$

$$pV = nRT$$

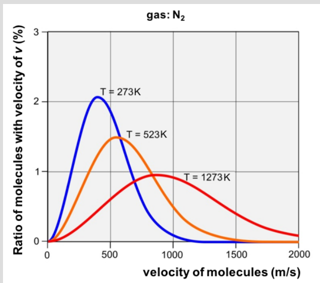
(ideal gas)

Microscopic description:

- random
- movement in many degrees of freedom

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

Maxwell-Boltzmann- distribution

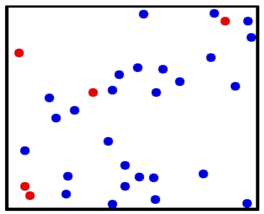


Temperature

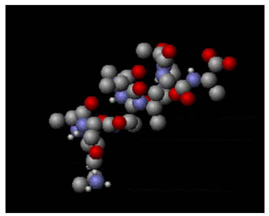
Temperature is a parameter proportional to the average kinetic energy available for each degree of freedom.

$$T(K) = t(°C) + 273$$

hot and cold gas particles

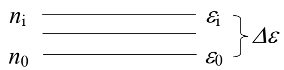


macromolecule

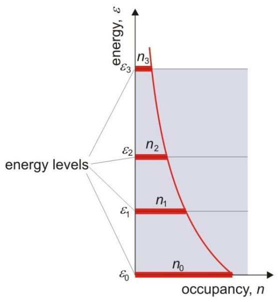


Boltzmann-distribution

The Boltzmann distribution describes the distribution of the particles between energy levels in a force field in case of thermal equilibrium.



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



$$n_i = n_0 \cdot e^{-\frac{\Delta\varepsilon}{kT}} = n_0 \cdot e^{-\frac{\Delta E}{RT}}$$

$$\Delta E = \Delta\varepsilon \cdot N_A$$

$$R = k \cdot N_A$$

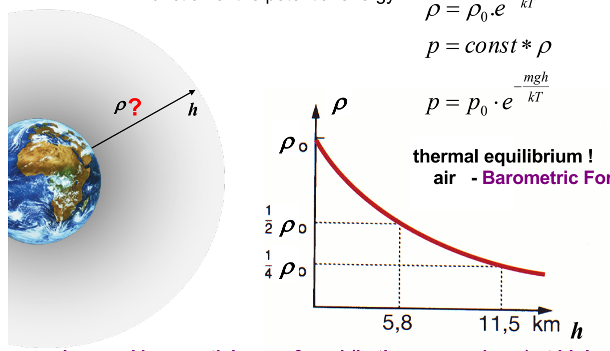
Gas in a force field – gravitation

Example: density (ρ) of air ***changes*** in function of the potential energy

$$\rho = \rho_0 . e^{-\frac{mgh}{kT}}$$

$$p = const * \rho$$

$$p = p_0 \cdot e^{-\frac{mgh}{kT}}$$



thermal equilibrium !
air - Barometric Formula

less and less particles are found (in the same volume) at higher potential energy (at higher altitudes)

Examples for Boltzmann-distribution:

- barometric formula
- thermal emission of electrons from metals
- Nernst-equation
- rate of chemical reactions
- conductivity of semiconductors
- number of vacancies in a metal
- ...