Exercises Basics of Material Science

1) Please define the following terms!

a. Metal
b. Semiconductor
c. Ceramic
d. Alloy
e. Polymer
f. Composite
g. Phase
h. Phase transition
i. Polymorphism
j. Real crystal
k. Ideal crystal
l. Intercalation mixed crystal
m. Substitutional mixed crystal
n. Isotropy
o. Anisotropy
p. Unit cell
q. Single crystal
r. Structural disorder

2) Which technique can one use to distinguish an amorphous solid from a crystalline solid? Please also name two examples for amorphous solids!

3) The following table shows different material classes. Complete the table with self-chosen compounds!

	Halides	Oxides	Nitrides	Sulphides
Binary	MX MX_2 MX_3 MX_4	M_2O MO M_2O_3 MO_2 M_2O_5 MO_3 M_2O_7 MO_4	M_3N M_3N_2 MN M_3N_4	M_2S MS M_2S_3 MS_2 M_2S_5
Ternary	$M^1M^2X_3$ $M^1M^2X_4$ $M^1M^2X_5$ $M^1M^2X_6$	$M^1{}_2M^2O_2$ $M^1M^2O_3$ $M^1M^2{}_2O_4$ $M^1M^2{}_4O_7$	$M^1M^2N_2$ $M^1M^2{}_2N_5$ $M^1M^2{}_7N_{10}$ $M^1{}_2M^2{}_5N_8$	$M^1{}_2M^2S_2$ $M^1M^2S_3$ $M^1M^2{}_2S_4$ $M^1{}_2M^2{}_4S_6$
Quaternary	$M^1M^2M^3X_6$	$M^1M^2{}_2M^3O_6$ $M^1M^2M^3{}_5O_{10}$ $M^1M^2M^3{}_{10}O_{17}$ $M^1M^2M^3{}_{11}O_{19}$	$M^1M^2M^3N_3$ $M^1M^2M^3{}_4N_7$ $M^1{}_3M^2M^3{}_6N_{11}$ $M^1{}_5M^2{}_5M^3{}_{11}N_{23}$	$M^1{}_2M^2M^3S_4$ $M^1M^2{}_3M^3{}_2S_5$

4) Please give two compounds which form a solid solution without a miscibility gap with the following compounds under consideration of the ionic radii!

a. Al_2O_3
b. GaN
c. $LaPO_4$
d. YBO_3
e. $Y_3Al_5O_{12}$
f. $SrWO_4$

5) Please name the general formula for the resulting compounds with substituted ions. You have to consider the ionic radii and that the resulting charge is compensated!

a. $Y_3Al_5O_{12}$ Ca^{2+} and Si^{4+}
b. Sr_2SiO_4 Pr^{3+} and K^+
c. $CaAlSiN_3$ Ce^{3+} and Na^+
d. TiO_2 Cr^{3+} and Nb^{5+}

6) Calculate the spatial occupation in a lattice with a cubic primitive packing (Z = 1)!

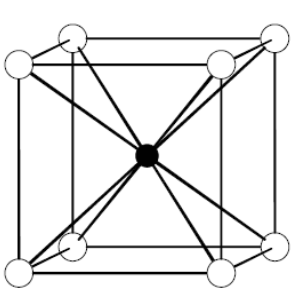
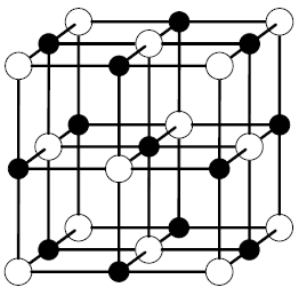
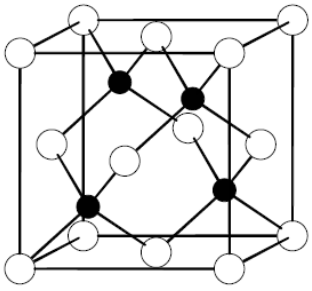
7) Calculate the spatial occupation in a lattice with a face-centred packing (Z = 4) and a cubic body-centred packing (Z=2)!

8) The density of a metal emerges of the structure type, the molar mass M and the lattices constant a. Calculate the density of strontium (M = 87.62 g/mol, a = 608.49 pm, Z = 4).

$$\rho = \frac{m}{V} = \frac{Z * M}{N_A * a^3}$$

9) Calculate the number of formula units per unit cell Z for the three compounds!

a) CsCl b) NaCl c) ZnS

10) There are 14 Braivais lattices in three dimensions. How many 2-dimensional lattices could exist? Please draw these lattices!

11) Which Bravais lattices are feasible for the following crystal systems?

a. Orthorhombic
b. Cubic
c. Monoclinic
d. Tetragonal

12) Please name the crystal system for the following lattice constants of compounds!
a. $a = b \neq c$ $\alpha = 90°, \gamma = 120°$
b. $a = b = c$ $\alpha = \beta = \gamma = 90°$
c. $a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$
d. $a \neq b = c$ $\alpha = \beta = \gamma = 90°$

13) Name the symmetry elements for the following molecules!
a. H_2O
b. CH_4
c. NH_3
d. BCl_3
e. WF_6
f. BrF_5
g. ClF_3
h. PCl_5
i. SF_4

14) Calculate the number of unit cells in a crystal (1 cm^3) of cubic NaCl (a = 563.1 pm) with the density of $\rho = 2170\ kg/m^3$!

15) Diffraction of x-rays is caused in the interaction between the electrons of the atom. Which problem can occur at the determination of atom sites in structure of specific compounds e.g. NaCl or KCl?

16) Calcium oxide crystallises in a cubic-face centred lattice with a = 481 pm and a density of $\rho = 3350\ kg/m^3$. Calculate the number of formula units Z per unit cell!

17) Thorium selenide $ThSe_2$ crystallises in an orthorhombic system with lattice constants a = 442.0 pm, b = 761.0 pm, c = 906.4 pm and a density of $\rho = 8500\ kg/m^3$. Calculate the number of formula unit Z per unit cell!

18) Order the following elements by their scattering power for x-rays!

Na, Co, Cd, H, Tl, Pt, Cl, F, O

19) Palladium has a cubic-face centred structure. The density is $\rho = 12.0\ g/cm^3$. Calculate the lattice constant a_0 for Pd! Assumption: No free lattice position, $N_A = 6.022*10^{23}\ mol^{-1}$, $M_{Pd} = 106.42\ g/mol$

20) Which types of n-dimension defects do you know?
a. 0-dim
b. 1-dim

c. 2-dim
d. 3-dim

21) How does the concentration of vacancies change in an ideal mixed crystal if the temperature increases?

22) Which atomic effects emerge because of atomic vacancies?

23) Explain the formation of defects in an ionic crystal with an energy diagram. How could you explain the mathematic dependence between the defect density N and the temperature?

24) Define the following terms!
a. Elastic deformation
b. Plastic ductility

25) Which types of atomic defects do you expect in oxides like FeO or MnO?

26) How could the ionic conductivity of a crystal increase?

27) Name the defect equation for the incorporation of $MnCl_2$ into NaCl!

28) Name the defect equation for the incorporation of AlF_3 into Al_2O_3!

29) Could a perfect single crystal present area defects?

30) What is the meaning of spatial defects? Name two examples for this defect type!

31) How do precipitations emerge?

32) Define the terms phase boundaries, grain boundaries and stacking faults!