

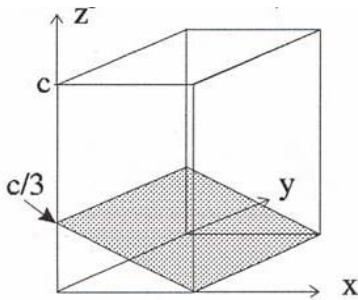
Exercises 1 WS 2011/12

*We wish you
a Merry Christmas*



Problem 1:

- (a) In the following sketch an orthorhombic unitcell is presented with lengths (a,b,c) along (x,y,z) -directions, respectively. Give the Miller indices for the shadowed plane.



- (b) Find a general expression for the minimum distance d_{hkl} between two (hkl) -planes in the orthorhombic structure for any given (hkl) .

Problem 2:

Aluminum is a metal with fcc structure.

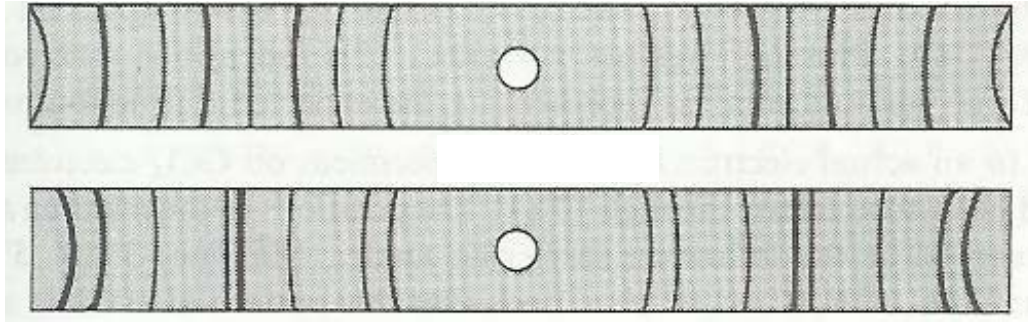
- How many atoms are positioned within the conventional non-primitive unit cell and what is the value of the related coordination number?
- Give the base vectors of a primitive unit cell.
- Calculate the volume of this primitive unit cell.

Problem 3:

Determine the elements of symmetry for H_2O and CH_4 molecules.

Problem 4:

The following diffraction patterns were taken on Tungsten (W, bcc) and Copper (Cu, fcc) powders. Indicate, which pattern is related to W and which to Co. Additionally, assign to the first three lines from the center the corresponding Miller indices.



Problem 5:

We are interested in the binding energies of ionic crystals. The Madelung constant of the sodium chloride structure is $\alpha = 1.7476$. Calculate for LiCl ($a=0.514$ nm), NaCl ($a=0.564$ nm), and RbF ($a=0.563$ nm) the Coulomb energy per pair of ions.

The total potential energy of the ions in a crystal is composed of the Coulomb energy U_C and a repulsive term. Assume for the repulsive term the so-called Born-Mayer ansatz:

$$U_{BM}(r_{ij}) = B \cdot \exp\left(-\frac{r_{ij}}{\rho}\right)$$

with r_{ij} being the distance of the ions i and j . B and ρ are material parameters. Experimentally one finds for the binding energies LiCl: $E_B = 8.93$ eV, NaCl: $E_B = 8.23$ eV, and RbF: $E_B = 8.17$ eV. Estimate typical values of the parameter ρ by using the above binding energies and the previously calculated Coulomb energies. Hint: As a result of the short range of the repulsive term only next neighbors have to be taken into account.

Problem 6:

- Assuming W-atoms and Al-atoms can be modelled by spheres of radius R_W and R_{Al} , respectively. W forms a bcc and Al a fcc lattice. Give relations between the length of the conventional cubic unit cells a_W and a_{Al} and the related radii.
- In the bcc case, is the center atom contained in the (111)plane?
- Analyzing W-powder by the Debye-Scherrer method: Give the value of the I_{100} Bragg reflex.
- Same question as in c), but now for CsCl powder

Problem 7:

Prove:

\underline{G}_{hkl} always perpendicular to (hkl)

$$|\underline{G}_{hkl}| = 2\pi/d_{hkl}$$