Question 1 (10 marks)

Crystallographic phase transition

Upon changing temperature or pressure many materials undergo crystallographic phase transitions. Especially under the application of high hydrostatic pressure, the structural phase transition results in a lowering of the volume of the unit cell.

(a) Calculate the change in volume when the crystallographic structure is changed from body centered cubic (bcc) to face centered cubic (fcc). Assume that the ionic radius remains constant.

(b) Calculate the change in the next nearest neighbor distance for this phase transition.

(c) Is there a difference in a symmetry operation between bcc and fcc.

Question 2 (10 marks)

Explain the following, each in a few words

(a) Give the five different chemical bonds inside a solid sorted them by their strength.

(b) What are static and dynamic lattice defects? Give one example for each!

(c) Describe three different symmetry operations and give their proper symbol using either the Schönfliess or Hermann-Mauguin notation.

(d) Determine all symmetry operations of a H_2O and a CH_4 molecule.

(e) Explain the Piezoelectric effect. Do crystals with a center of inversion show piezoelectric properties? Use a sketch to answer this question.

Question 3 (10 marks)

Reciprocal Lattice

Consider a two-dimensional face centered-cubic, one-atomic lattice.

(a) Draw a sketch of this lattice and indicate the primitive unit cell and the Wigner-Seitz cell of this lattice.

(b) Determine the reciprocal lattice vectors.

(c) Prove that for the three-dimensional Volume in real and reciprocal space the following relation is valid: $V_R \cdot V_K = 1$.

(d) Demonstrate that a real space face centered cubic lattice has a body centered cubic reciprocal lattice.

Question 4 (10 marks)

Bragg's Law

(a) Give the definition of the reciprocal lattice vectors. What is the relation between a direct lattice vector and a reciprocal lattice vector, i.e. calculate $R_i \cdot G_j$.

(b) Derive Bragg's law. (c) Explain one example for the setup of one diffraction experiment (either single crystal or powder diffraction. Sketch the setup of this diffraction experiment.