UNIVERSITÄT SIEGEN

FESTKÖRPERPHYSIK

CRYSTALLOGRPAHY (*winter term 2015-2016*)

Lecturer: **Dr Semën Gorfman (ENC B-011)**

Exercise tutor: **Hyeokmin Choe (ENC B-015)**

1. Introduction: Historical development of the ideas about crystals. Transparent ice and natural minerals. Crystalline and amorphous solids. Accumulation of first scientific knowledge about crystals: Steno's law of constancy of interfacial angles; Haüy's law of rational indices. Anisotropy of physical properties of crystals. The hypothesis about periodicity of crystal structures. Experimental proof of periodic structure of crystals: Laue experiment. Modern definition of a crystal. The concepts of a short-range order and a long-range order.

2. Unit cell and crystal lattice: Definition of crystal lattice and unit cell. Basis vectors and lattice parameters in 1D, 2D and 3D spaces. Atomic positions and fractional atomic coordinates. Crystallographic unit cell. Matrix of dot products. Reciprocal lattice: definition and relationship between direct and reciprocal basis vectors. Mathematical reason to introduce reciprocal basis vectors. Calculation of distances, angles and plane normals in a crystal space. The theorem about the choice of lattice basis vectors.

3. Miller planes and crystal morphologies: Separation of a crystal lattice into the set of parallel lattice planes. 2D lattice planes (rows) and 3D lattice planes. Appropriate choices of basis vectors for a given set of planes. Interplanar distances. The equation of planes. Miller indices and their mutually prime character. Calculation of Miller indices for given lattice planes and, conversely, drawing lattice planes with predefined Miller indices. The role of reciprocal lattice in the description of Miller planes. Properties of lattice planes. The relationship between interplanar distance and the length of the reciprocal lattice vector. Description of crystal polyhedral shapes by Miller planes. Indexing of crystal faces and calculating of interfacial angles. Gibbs-Wulff theorem.

4. Symmetry: Definition of symmetry. Symmetry operations and symmetry elements. Crystal lattice as a symmetry operation. Point symmetry operations: rotation axes and the order of rotation axis, mirror plane, inversion centre, rotoinversion. Mathematical presentation of a symmetry operation: rotation matrix. Combination of symmetry operations. Space symmetry operations: screw axes and glide planes. Graphical symbols for symmetry operations. Mathematical presentation of space symmetry operation by rotation matrix and displacement vector.

5. Crystal systems and Bravais types of lattice: Symmetry of a crystal and symmetry of a crystal lattice. The main theorem of crystallography: which symmetry operations are compatible with lattice periodicity? Definition of a crystal system. 2D crystal systems. Bravais types of lattices. Why are there more Bravais types of lattices than crystal systems? 3D crystal systems and 3D Bravais lattices. Conventional choice of lattice basis vectors in different crystal systems. Primitive and non-primitive unit cells. The reason to introduce of non-primitive unit cells. Body-centred, face-centred, base-centred and R-centered unit cells.

6. Point symmetry groups: Assembling symmetry operations into a group. Mathematical concept of a group: closure, identity elements, associativity and invertibility of elements. Construction of 32 point symmetry groups. Holohedry groups. International (Hermam-Mauguin) point group symbols.

7. Space symmetry groups: The concept of a group for space symmetry operation. Matrix / vector representation of a space symmetry operations and their combinations. CIF (xyz) -format of symmetry operations. The total number of 2D and 3D space groups. International space group symbols. International Tables for Crystallography, Volume A. Bilbao Crystallographic Server. Wyckoff positions. Special and general positions.

8. The simplest structural types: BCC, FCC, Rock Salt, Diamond, Sphalerite, Perovskite and HCP structural types. Their crystal systems, Bravais types of lattices and space groups. The number and the positions of symmetry independent atoms. The number and the positions of all atoms in a unit cell.

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9. Introduction to X-ray crystallography: Physical principles behind the experimental methods for the determination of crystal structures. Interference of electromagnetic waves. Amplitude, wavelength, wave vector and a phase. Phase difference and path difference. Constructive and destructive interference. Discovery of X-ray diffraction by crystals. Laue experiment. Bragg's interpretation of X-ray diffraction by crystals. Reflection of X-rays from Miller planes and Bragg's equation. Bragg angle and the order of the reflections. Laue equation and the role of reciprocal lattice.

10. Diffraction experiments and reciprocal space: Scattering vector. Ewald sphere. Experiments with monochromatic and polychromatic X-rays. Rotation photographs and rocking curves. Single-crystal X-ray diffractometry. Laue diffraction experiments. Organization of Laue patterns. Zone planes / axis and their appearences in Laue patterns. Electron diffraction. Approximation of Ewald sphere by a plane. The role of zone axis for the description of electron diffraction. Structure factor and systematic absences.