Level: PhD

Course title: The study of materials by radiation scattering

Status: elective

ECTS: 15

Requirements: master studies

Learning objectives

Introducing students into the material characterization using diffraction methods.

Learning outcomes

Students should develop:

- General abilities: knowledge of the techniques of studying materials by radiation.
- Specific abilities: some techniques will be elaborated in detail and therefore the knowledge could be later applied in practice.

Syllabus

Theoretical instruction

Phenomenon of the diffraction. The relation between the diffraction picture and the molecular arrangement. Diffraction and the equation of Braggs. Reciprocal lattice. Determination of the crystal system, parameters of the crystal unit cell, number of stoichiometric units, space group. Experimental methods of the crystal structure analysis (rotating monocrystal method, Weissenberg method, powder method). Experimental foundations of diffraction (X – rays, electrons, neutrons, synchrotron radiation): radiation monochromatization, recording of scattered radiation, correction for polarization and absorption, intensity normalization. Experimental techniques for diffraction measurements: monocrystal diffraction, diffraction on powdered sample, measurement at high and low temperatures. Scattering of an atom and atom groups. Structural factor. The relation between the intensity of scattered radiation and the structural factor. Phase problem. The relation between the electron density and the structural factor (Fourier transform). Trial structure and R-factor. Methods for solving the phase problem (heavy atom method, method of isomorphous substitution, direct method). Structure refinement (Fourier method, least square method, method of differential Fourier synthesis). Application of the diffraction of X-rays, neutrons and synchrotron radiation for the analysis of polycrystalline materials. Qualitative and quantitative analysis of the crystal components. Analysis of the crystallites size. Analysis of polymer materials and liquid crystals by small angle scattering. The study of the structure of nanocrystals and amorphous materials and liquids. The determination of the distribution function of electron density. Radial distribution function of intermolecular electron density.

Practical instruction

The application of the selected diffraction methods for the characterization of matter structure. Preparation and public defence of the seminar following and broadening the curriculum.

Weekly teaching load				Other:
Lectures: 4	Exercises:	Other forms of teaching:	Student research: 6	