List of topics for the lesson „Diffraction methods in materials science I."

1. Basic concepts of crystallography. Primitive translation vectors. Primitive (unit) cell. Bravais-lattice, basis. Reciprocal lattice. Simple cubic, face-centered cubic, body-centered cubic and diamond cubic structures. Hexagonal close-packed structure. Crystallographic directions and planes. Miller indices. Correlation between the reciprocal lattice vectors and the crystallographic planes.
2. The kinematical theory of diffraction. Correlation between the scattering center density and the diffracted intensity. Structure factor. Atomic scattering factor (formfactor). Laue-conditions. Ewald-contruction. Bragg equation. Systematic extinction.
3. Production of X-rays. Interaction between X-ray photons and materials. X-ray detectors. Absorption of X-rays. Diffraction methods. Debye-Scherrer camera. Powder diffractometer. Evaluation of powder diffractograms. Phase identification using database. Indexing of cubic structures. Determination of lattice parameter. Single crystal diffraction. Laue-method. Zone-axis.
4. Crystallite size broadening of X-ray line profiles. Convolution. Form function. Correlation between the volume of the common and the intensity profile. Column-length distribution. Bertaut-theorem. Determination of the volume-weighted and area-weighted mean column length from the peak profile. Determination of the column-length distribution. Dependence of the shape of line profile on the median and the variance of crystallite size distribution. Effect of anisotropic crystallite shape on line profiles. Meaning of coherently scattering domain (crystallite) size.
5. Strain broadening of X-ray diffraction peaks. General effect of lattice distortions on line profiles. Mean-square strain. Strain broadening caused by dislocations. Strain anisotropy. Contrast (orientation) factor. Dislocation arrangement parameter. Average contrast factors for cubic and hexagonal crystals. Asymptotic shape of the line profile caused by dislocations.
6. Evaluation methods of diffraction line profiles. Warren-Averbach method. Modified Warren-Averbach procedure. Multiple Whole Profile (MWP) fitting method. Evaluation of breadth of line profiles. Scherrer-equation. Conventional Williamson-Hall plot. Modified Williamson-Hall method. The difference between the order dependence of diffraction peak broadening caused by crystallite size, dislocations and planar faults. Variance methods. Intensity profile fitting methods. Convolutional Multiple Whole Profile fitting (CMWP). Determination of dislocation structure in hexagonal materials. Comparison between TEM and X-ray line profile analysis methods for studying the microstructure.