X-Ray Scattering:  
Introduction and Applications in Materials Science

PD Dr. Martin Schmidbauer  
Leibniz-Institut für Kristallzüchtung, Max-Born-Str.2, 12489 Berlin 
Tel: 6392-3097, Email: martin.schmidbauer@ikz-berlin.de

1. Introduction, Historical Review, X-Ray Sources  
History of X-rays, history of X-ray diffraction, origin of X-rays, bremsstrahlung, characteristic radiation, fine structure, other properties; standing anodes, rotating anodes, synchrotron radiation, properties of SR

2. Overview of the 'Kinematical' Diffraction Theory  
Bragg equation; introduction of reciprocal space, kinematic description of intensities: scattering amplitude; structure factor; extinction rules, lattice factor, atomic form factor, absorption of X-rays

3. Crystal Structure Determination  
Basic presentation of methods (Laue geometry, rotating crystal method, Weißenberg geometry, diffractometry), phase problem, calculations (Patterson method; limits: light atom structures), direct methods

4. Phase Analysis, Powder Diffraction, Analysis of Polycrystals  
Powder diffractometry: methods, techniques, evaluation, database, shear formula

5. Dynamical diffraction theory  
Brief repetition of the kinematic equation(s), discussion of the approximations contained therein, presentation of phenomena which cannot be explained by kinematic theory; brief outline of the dynamical theory

6. X-Ray Topography  
Lang method, Berg-Barrett method, Double-Crystal Topography, 2D detectors

7. Analysis of Epitaxial Layer Systems: High Resolution diffractometry  
Experimental basics, Ewald construction, double-crystal, triple-crystal arrangement, Du-Mond diagram, dispersion effects, applications to layer systems (layer thicknesses, stress, strain, plastic relaxation)

8. Analysis of Epitaxial Layer Systems: Reflectometry  
Fresnel equations, dispersion and absorption, evanescent effects, roughness

9. Analysis of Epitaxial Layer Systems: Diffuse scattering from Interfacial Roughness  
1st Born approximation, self-affined models for roughness, DWBA, GID

10. Small Angle X-Ray Scattering  
Shape and Correlation Function, Guinier Approximation, Contrasts, Experimental Realization, GISAXS

11. Analysis of Epitaxial Layer Systems: Diffuse Scattering from Misfit Dislocations  
Formation of misfit dislocations, dependence of diffuse scattering on dislocation density
12. **Diffuse Scattering from Phonons, Point Defects and Clusters**
Thermal and static Debye Waller factor, thermal diffuse scattering, Huang scattering, Stokes-Wilson scattering

13. **Spectroscopic Methods**
X-ray fluorescence analysis, absorption spectroscopy EXAFS/XANES, DAFS, standing waves

**Location:** IKZ, Max-Born-Str.2., 12489 Berlin; 19.31 R322

**Time:**
- Lectures: **Monday** 13:15-14:45
- Exercises Monday 17:15-18:45 (every two weeks)

**Suggestion:** Instead of the exercises, a 1-2 day laboratory internship is also possible by arrangement (crystal orientation using the Laue method, topography, high-resolution diffractometry, reflectometry, diffuse scattering).

**Amount, Credit Points; Exam / major course assessment**
3 SWS, 6 SP/ECTS

**Assigned Modules**
P25.2.c, P35.4

**Scripts:** [http://lehre.ikz-berlin.de/physhu/](http://lehre.ikz-berlin.de/physhu/)

**Literature:**
- W. Massa: Kristallstrukturbestimmung, Teubner, 3. Auflage, 2002