

Structure Analysis by X-ray Diffraction (C004152)

Due to Covid 19, the education and evaluation methods may vary from the information displayed in the schedules and course details. Any changes will be communicated on Ufora.

Course size (nominal values; actual values may depend on programme)
Credits 4.0 Study time 120 h Contact hrs 37.5 h

Course offerings and teaching methods in academic year 2020-2021

A (semester 2)	English	Gent	teaching methods	hours
			seminar: coached exercises	8.75 h
			online lecture	0.0 h
			online seminar: coached exercises	0.0 h
			lecture	15.0 h

Lecturers in academic year 2020-2021

Depla, Diederik	WE04	lecturer-in-charge
De Buysser, Klaartje	WE06	co-lecturer
Dendooven, Jolien	WE04	co-lecturer

Offered in the following programmes in 2020-2021

programme	crdts	offering
Master of Science in Teaching in Science and Technology (main subject Chemistry)	4	A
Master of Science in Chemistry (main subject Analytical and Environmental Chemistry)	4	A
Master of Science in Chemistry (main subject Materials and Nano Chemistry)	4	A
Exchange Programme in Chemistry (master's level)	4	A

Teaching languages

English

Keywords

Powder diffraction, Rietveld refinement, Crystal structures, phase identification, analysis techniques, texture analysis.

Position of the course

Structure determination by X-ray diffraction and structure solving/refining is the main goal of this course. A practical oriented course will be provided in which students learn how to understand, evaluate and extract all possible structural information from a diffraction pattern. Indexation, crystal parameters, powder diffraction, quantitative analysis, single crystal X-ray diffraction and texture analysis of thin films will be covered.

Contents

1. Powder diffraction
 - data collection : Sample preparation, Diffractometer settings
 - Structure refinement from powder diffraction : Indexing, cell parameters, qualitative and quantitative analysis
 - Refinement evaluation
2. Advanced X-ray techniques: pair-distribution function, GISAXS, WAXS, SAXS
3. Texture analysis of thin films
 - Definitions related to X-ray diffraction of thin layers and thin film technology: Texture, Epitaxy, Substrate, Roughness, Microstructure
 - X-ray diffraction techniques : Bragg-Brentano, rocking curves, glancing angle, grazing incidence, texture analysis (Pole figures)
 - X-ray reflectometry

- Electron diffraction techniques : EBSD, RHEED, LEED
- X-ray diffraction for stress analysis

Initial competences

De students should have obtained credits for the following curriculum courses: 'Wiskunde I', 'Fysica I: mechanica', 'Algemene chemie', 'Wiskunde II', 'Fysica II', 'Elektromagnetisme'

Final competences

- 1 The students must be able to analyze in detail and discuss an X-ray diffraction pattern - manually and using databases and software packages.
- 2 Students are capable of selecting a suitable technique for the analysis of texture of a thin film.
- 3 Students are acquainted with advanced analysis techniques using X-rays.

Conditions for credit contract

Access to this course unit via a credit contract is determined after successful competences assessment

Conditions for exam contract

This course unit cannot be taken via an exam contract

Teaching methods

Lecture, seminar: coached exercises, online lecture, online seminar: coached exercises

Extra information on the teaching methods

Due to COVID19 alternative work forms can be rolled out.

- Lecture : 22.5 h
- Seminars: 6 (2 lecture hours) sessions organized by the 3 lecturers: participation in these seminars is obliged!

Learning materials and price

The slides will be posted via Ufora + references to English handbooks.

References

- Crystallography made Crystal Clear (Gale Rhodes)
- Crystal structure determination (William Clegg)
- Powder Diffraction: Theory and Practice (Robert Ernst Dinnebier, Simon J. L. Billinge)
- Fundamentals of Powder Diffraction and Structural Characterization of Materials (Vitalij Pecharsky)

Course content-related study coaching

Interactive support by means of Ufora. Possibility for questions and discussions following each classroom lecture.

Evaluation methods

end-of-term evaluation and continuous assessment

Examination methods in case of periodic evaluation during the first examination period

Written examination with open questions, oral examination

Examination methods in case of periodic evaluation during the second examination period

Written examination with open questions, oral examination

Examination methods in case of permanent evaluation

Participation, assignment

Possibilities of retake in case of permanent evaluation

examination during the second examination period is possible in modified form

Extra information on the examination methods

- Non-periodic evaluation: seminar sessions plus quoted exercises.
 - Periodic evaluation: theory and exercises.
- Examination during the second examination period is not possible for the non-periodic evaluation.

Calculation of the examination mark

- Periodical evaluation (80%)
- Permanent evaluation (20%)