

## UČNI NAČRT PREDMETA / COURSE SYLLABUS

**Predmet:** SODOBNE DIFRAKCIJSKE TEHNIKE  
**Course Title:** MODERN DIFFRACTION TECHNIQUES

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
DR Kemijske znanosti, 3. stopnja	/	1.	1. in 2.
Doctoral programme in Chemical Sciences, 3 <sup>rd</sup> Cycle	/	1 <sup>st</sup>	1 <sup>st</sup> and 2 <sup>nd</sup>

**Vrsta predmeta / Course Type:** izbirni/Elective

**Univerzitetna koda predmeta / University Course Code:** KZ303

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
/	/	/	/	75	75	5

**Nosilec predmeta / Lecturer:** prof. dr. Anton Meden /Dr. Anton Meden, Full Professor

**Jeziki / Languages:** Predavanja / Lectures: slovenski / Slovenian  
 Vaje / Tutorial: slovenski / Slovenian

**Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:**

Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

Študent s soglasjem mentorja med spodaj navedenimi tehnikami v izbere tiste, ki so najtesneje povezane z njegovim raziskovalnim delom. Nosilec predmeta in vodja študija poskrbita, da obseg študentovega dela ustreza 5 KT.  
 Kratka osvežitev znanja o difrakciji rentgenskih žarkov, nevtronov in elektronov na trdnih snoveh.  
 Uporaba zahtevnejših tehnik na monokristalih (elektronska gostota, anomalna disperzija, absolutna konfiguracija, uporaba več valovnih dolžin v okolici absorpcijskega roba, strukturna analiza dvojčenih kristalov).

**Content (Syllabus outline):**

With mentor's agreement students chose among the techniques, which are closest to their respective research area. The course coordinator and the program coordinator make sure that the total workload of students does not exceed 5 ECTS.  
 Refreshing/revising student's knowledge of the diffraction of X-rays, neutrons and electrons on a solid state material.  
 Application of advanced single crystal techniques (electron density, anomalous dispersion, absolute configuration, use of a larger number of wavelengths in the vicinity of absorption edge, structure analysis of twinned crystals).

Uporaba zahtevnejših tehnik na polikristaliničnih in amorfni materialih (določevanje strukture, Rietveldova metoda za strukturno, mikrostrukturno in kvantitativno fazno analizo, kombinacija nevtronske in rentgenske difrakcije, totalno sipanje in porazdelitvena funkcija parov (lokalna urejenost kristaliničnih in amorfni snovi), difrakcija na nano-materialih

Application of advanced techniques on polycrystalline and amorphous materials (structure determination, Rietveld method for structure, microstructure and quantitative phase analysis, combination of neutron and X-ray diffraction, total scattering and pair-distribution-function (local order of crystalline and amorphous compounds), diffraction of nano-materials).

**Temeljna literatura in viri / Readings:**

Literaturo, ki jo mora študent preštudirati, s spodnjega seznama izbere nosilec predmeta po pogovoru s študentom in izbiri metod, ki jih študent izbere, izbrani obseg je v okviru 300-400 strani./The literature, that the student has to study, is chosen by the lecturer from the list below after the discussion with the student and the student's choice of methods, the selection will comprise between 300 and 400 pages.

- Giacovazzo, Carmelo, Fundamentals of Crystallography, International Union of Crystallography, Oxford: Oxford University Press, 2000, cop. 1992.
- Clegg, William, Crystal Structure Analysis: principles and practice, International Union of Crystallography, Oxford, New York : Oxford University Press, 2001.
- Christopher Hammond, The Basics of Crystallography and Diffraction International Union of Crystallography, Oxford University Press, 2001.
- Pecharsky, Vitalij K. Zavalij, Peter Y., Fundamentals of powder diffraction and structural characterization of materials, New York: Springer, 2005
- Young, Robert Alan, The rietveld method, Oxford International Union of Crystallography: Oxford University Press, 1995.
- Novejši metodološki članki iz znanstvenih revij/Newer methodological papers from scientific journals.

**Cilji in kompetence:**

Študenti spoznajo teoretične osnove in se naučijo praktično uporabljati nove zahtevne tehnike difrakcijske analize za različne vidike karakterizacije trdnih snovi.

**Objectives and Competences:**

Students acquire fundamentals in theory and practical applications of various novel advanced techniques of diffraction analysis for different aspects of characterization of solid state compounds.

**Predvideni študijski rezultati:**

Znanje in razumevanje  
Poglobljeno znanje o teoretičnih osnovah difrakcije in njenih različnih instrumentalnih izvedbah.

Uporaba  
Strukturna analiza vzorcev, primerjava struktur, kristalokemijska karakterizacija.

Refleksija  
Pomen strukturne informacije za razumevanje lastnosti materialov.

**Intended Learning Outcomes:**

Knowledge and Comprehension  
Advanced knowledge on theoretical background of diffraction and various instrumental applications thereof.

Application  
Structural analysis of samples, comparison of structures, crystallochemical characterization.

Analysis  
Importance of structural information for understanding of material's properties.

**Prenosljive spretnosti**

Uporaba instrumentov, uporaba zbirk podatkov in različnih računalniških programov za analizo in predstavitev struktur.

**Skill-transference Ability**

Use of instruments, use of databases and various computer programs for analysis and presentation of structures.

**Metode poučevanja in učenja:**

Praktično delo, po možnosti na lastnih vzorcih iz raziskovalnega dela študenta, izdelava seminarske naloge.

**Learning and Teaching Methods:**

Practical work, if possible with samples taken from students' research work, preparation of a seminar work.

Delež (v %) /

Weight (in %) **Assessment:****Načini ocenjevanja:**

Priprava in zagovor seminarske naloge, ustni izpit.

Sem. 40 %  
Izp. /Ex. 60 %

Preparation and defense of seminar work, oral exam.

**Reference nosilca / Lecturer's references:**

MAKAROVIČ, Kostja, MEDEN, Anton, HROVAT, Marko, HOLC, Janez, BENČAN, Andreja, DAKSKOBLER, Aleš, KOSEC, Marija. The effect of processing conditions on the properties of LTCC material. *Journal of the American Ceramic Society*, ISSN 0002-7820, 2012, vol. 95, issue 2, str. 760-767, doi: [10.1111/j.1551-2916.2011.05027.x](https://doi.org/10.1111/j.1551-2916.2011.05027.x). [COBISS.SI-ID [25443367](https://www.cobiss.si/id/25443367)]

KASUNIČ, Marta, MEDEN, Anton, ŠKAPIN, Srečo D., SUVOROV, Danilo, GOLOBIČ, Amalija. Structure of LaTi<sub>2</sub>Al<sub>9</sub>O<sub>19</sub> and reanalysis of the crystal structure of La<sub>3</sub>Ti<sub>5</sub>Al<sub>15</sub>O<sub>37</sub>. *Acta crystallographica. Section B, Structural science*, ISSN 0108-7681, 2011, vol. B67, no. 6, str. 455-460, doi: [10.1107/S0108768111039759](https://doi.org/10.1107/S0108768111039759). [COBISS.SI-ID [35540741](https://www.cobiss.si/id/35540741)]

MALI, Gregor, MEDEN, Anton, DOMINKO, Robert. <sup>6</sup>Li MAS NMR spectroscopy and first-principles calculations as a combined tool for the investigation of Li<sub>2</sub>MnSiO<sub>4</sub> polymorphs. *Chemical communications*, ISSN 1359-7345, 2010, issue 19, str.3306-8, doi: [10.1039/c003065a](https://doi.org/10.1039/c003065a). [COBISS.SI-ID [4386074](https://www.cobiss.si/id/4386074)]