X-RAY DIFFRACTION APPLICATIONS FOR PETROLEUM GEOLOGY

Petroleum Geology MSc course

2020/21 1. Semester

COURSE COMMUNICATION FOLDER

University of Miskolc
Faculty of Earth Science and Engineering
Institute of Mineralogy and Geology

Course datasheet

Course Title: X-ray diffraction applications for petroleum geology (Optional courses II.)	**Credits: 4**

Type (lec. / sem. / lab. / consult.) and Number of Contact Hours per Week: **lec. 1, sem.1**

Neptun code: MFFAT730008

Type of Assessment (exam. / pr. mark. / other):**pr. mark**

Oral examination with practical exercises

Grading limits:

>90%: excellent,
76-90%: good,
60-76%: medium,
50-60%: satisfactory,
<50%: unsatisfactory.

Position in Curriculum (which semester): **third**

Pre-requisites *(if any)*:-

Course Description:

Acquired store of learning:

Study goals: this course will give the basic knowledge of XRD techniques used in petroleum geology research to support the planning and interpretations of petrology and petrography results. Meet and learn all the areas of X-ray diffraction which are routinely used and necessary in good quality petroleum geology research. The areas from sampling and specimen preparation to data evaluation and interpretation will be covered.

Course content: 1. Introduction to X-ray diffraction: crystallography review, X-rays and diffraction techniques, powder diffraction 2. Sample and specimen preparation for good diffraction practice, systematic aberrations, errors in obtained data, standards and calibration 3. Relations of crystal structures and XRD results, structure refinement 4. Interpretation of obtained data, mineral identification, proper use of databases, reference materials, integration of mineralogy knowledge into X-ray data evaluation 5. Quantitative evaluation, methods and practices, possibilities and limitations, software solutions 6. Mineral identification and quantification with solid solution species, use of mixtures from reference materials 7. Clay minerals, crystallography and mineralogy, properties, importance in petroleum geology, their investigation by XRD 8. Preparation of clay mineral samples and specimens, limitations, diagnostic chemical treatments 9. Diagnostic clay mineral investigation, detailed identification, data interpretation and integration into XRD mineralogy 10. Quantitative techniques for clay mixtures 11. Other analytical methods for XRD data validation, integration of chemical and petrology results 12. Preparing and selecting essential data for petrology report, documentation solutions 13. Testing the ability to apply XRD knowledge in petrology research planning.

Education method: lectures with .ppt presentation, laboratory exercises for sample and specimen preparation, data evaluation, interpretation of results, methods for data validation and documentation.

Competencies to evolve:

T1, T5, T7, T10, T12, K2, K7

The 3-5 most important compulsory, or recommended **literature**(textbook, book) **resources**:

- Bish D.L. & Post J.E. (eds.) (1981) Modern Powder Diffraction./Reviews in Mineralogy, **20**/. Mineralogical Society of America, Washington, D.C.
- Woolfson, M.M. (1997) An Introduction to X-ray Crystallography. 2nd ed. Cambridge University Press, Cambridge.

- Pecharsky, V.K. & Zavalij, P.Y. (2003) Fundamentals of Powder Diffraction and Structural Characterization of Materials. Kluwer, Dordrecht.
- Jenkins, R. & Snyder, R. (eds.) (2002) Introduction to X-ray Powder Diffractometry. Wiley, New York.
- Cullity, B.D. (1956) Elements of X-ray Diffraction. Addison-Wesley, Reading, Massachusetts.
- Guinier, A. (1952) X-ray Crystallographic Technology. Hilger and Watts, London.
- Dinnebier, R.E. & Billinge, S.J.L. (eds.) (2008) Powder Diffraction: Theory and Practice. Royal Society of Chemistry, Cambridge.
- Klug H. P. & Alexander L. E. (1974) X-Ray Diffraction Procedures: For Polycrystalline and Amorphous Materials. John Wiley & Sons, Inc., New York.

Responsible Instructor(*name, position, scientific degree):*

Ferenc Kristály Dr., senior research fellow, PhD

Syllabus of the semester

X-ray diffraction applications for petroleum geology

Monday, 09:00 – 11:00

Week	Thematics
2020.09.07.	Introduction to X-ray diffraction: crystallography review, X-rays and diffraction techniques, powder diffraction
2020.09.14.	Sample and specimen preparation for good diffraction practice, systematic aberrations, errors in obtained data, standards and calibration
2020.09.21.	Relations of crystal structures and XRD results, structure refinement
2020.09.28.	Interpretation of obtained data, mineral identification, proper use of databases, reference materials, integration of mineralogy knowledge into X-ray data evaluation
2020.10.05.	Quantitative evaluation, methods and practices, possibilities and limitations, software solutions
2020.10.12.	Mineral identification and quantification with solid solution species, use of mixtures from reference materials
2020.10.19.	Clay minerals, crystallography and mineralogy, properties
2020.10.26.	Clay minerals, importance in petroleum geology, their investigation by XRD
2020.11.02.	Preparation of clay mineral samples and specimens, limitations, diagnostic chemical treatments
2020.11.09.	Diagnostic clay mineral investigation, detailed identification, data interpretation and integration into XRD mineralogy
2020.11.16.	Quantitative techniques for clay mixtures
2020.11.23.	Other analytical methods for XRD data validation, integration of chemical and petrology results
2020.11.30.	Preparing and selecting essential data for petrology report, documentation solutions
2020.12.07.	Testing the ability to apply XRD knowledge in petrology research planning

Practical work examination:
- evaluation and interpretation of X-ray powder diffraction patterns
- preparing powder specimens for measurment
- creating report from evaluation and interpretation data