

## SYLLABUS

### 1. Informations on the study program

1.1. Higher education institution	WEST UNIVERSITY OF TIMISOARA
1.2. Faculty	FACULTY OF PHYSICS
1.3. Department	PHYSICS DEPARTMENT
1.4. Study program field	EXCACT SCIENCE
1.5. Study cycle	MASTER
1.6. Study programme / Qualification	ADVANCED RESEARCH METHODS IN PHYSICS / according to COR: physicist (211101); gymnasium teacher (232201 -according to the law); research assistant (248102); referent specialist in education (235204); analyst (213101).

### 2. Informations on the course

2.1. Course title		X-ray characterization of materials					
2.2. Lecturer instructor		Conf. univ. dr. Marius Ștef					
2.3. Seminar / Laboratory instructor		CS II. dr. Maria Poienar					
2.4. Study year	1	2.5. Semester	2	2.6. Examination type	E	2.7. Course type	DS ARMP1203

### 3. Estimated study time (number of hours per semester)

3.1. Attendance hours per week	4	out of which:	2	3.3. seminar / laboratory	2
		3.2. lecture			
3.4. Attendance hours per semester	56	out of which:	28	3.6. seminar / laboratory	28
		3.5. lecture			
<b>Distribution of the allocated amount of time*</b>					<b>hours</b>
Study of literature, course handbook and personal notes					35
Supplementary documentation at library or using electronic repositories					20
Preparing for laboratories, homework, reports etc.					20
Exams					4
Tutoring					15
Other activities.....					
3.7. Total number of hours of individual study	94				
3.8. Total number of hours on semester	150				
3.9. Number of credits (ECTS)	6				

#### 4. Prerequisites (if it is the case)

4.1. curriculum	<ul style="list-style-type: none"> <li>• Complements of Theoretical Physics</li> <li>• Complements of Solid State Physic</li> <li>• Complements of Atom and Molecule Physics</li> </ul>
4.2. competences	<ul style="list-style-type: none"> <li>• Creative application of research methods and problem solving; Elaborating studies and reports; Capacity to manage working groups and to communicate in different situations.</li> <li>• Skills in problems solving; Skill in using laboratory equipment; Skills in using computers and software for numerical simulation of physical phenomena.</li> </ul>

#### 5. Requirements (if it is the case)

5.1. for the lecture	<ul style="list-style-type: none"> <li>• laptop</li> <li>• projector</li> </ul>
5.2. for the seminar / laboratory	<ul style="list-style-type: none"> <li>• PCs with database for phases identification, Crystallography Open Database</li> <li>• software FullProf Suite, VESTA, OrientExpress</li> <li>• X-Ray diffractometer.</li> </ul>

#### 6. Specific acquired ompetences

Professional competences	<p><b>1. Knowledge and understanding:</b></p> <ul style="list-style-type: none"> <li>• Capacity of analyze and synthesize (adaptability to new situation, realization of synthesis and comparisons, correlations and propinquity).</li> <li>• Basic knowledge</li> <li>• Basic knowledge necessary to profess (presentation, dialog)</li> <li>• Knowledge of foreign languages (English)</li> </ul> <p><b>2. Technical skills:</b></p> <ul style="list-style-type: none"> <li>• Theoretical understanding</li> <li>• Deep understanding (of basic notions, of physical parameters)</li> <li>• Experimental skills (the understanding of experiments)</li> <li>• Computational skills (PC uses for research, data acquisition)</li> <li>• Culture in Physics domain</li> <li>• Bibliography investigation</li> <li>• Learning skills</li> <li>• Skills for team working</li> <li>• The capacity to transfer the acquired knowledge in practical applications</li> <li>• Capacity to plan and organize experimental or theoretical applications</li> </ul> <p><b>3. Practical skills:</b></p> <ul style="list-style-type: none"> <li>• Capacity of solving characteristic problems for real physical systems.</li> <li>• Capacity of real mechanical systems idealization by building up models.</li> </ul> <p><b>4. Attitude:</b></p> <ul style="list-style-type: none"> <li>• Capacity of critical evaluations and auto evaluation.</li> <li>• Capacity of communication inside a group</li> <li>• Concern for a permanent improvement of quality</li> </ul>
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Transversal competences	<ul style="list-style-type: none"> <li>• Effective use of information sources, communication resources and training assistance (Internet portals, specialized software, data bases, online courses, etc..) both in romanian and in a foreign language (english)</li> <li>• Creativeness and initiative in solving complex problems</li> </ul>
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## 7. Course objectives

7.1. General objective	Students to identify the specific concepts and phenomena in a given context and to apply these knowledge in the analysis and interpretation of experimental data.
7.2. Specific objectives	<ul style="list-style-type: none"> <li>• Students to define the specific notions of this discipline and to describe the phenomena</li> <li>• Students to use correct laboratory equipment to perform measurements.</li> <li>• Students to process experimental data using software packages and correctly interpret the experimental results.</li> <li>• Students to develop their organizational capacity</li> <li>• Students to develop their spirit of teamwork.</li> <li>• Students to appreciate and cultivate a scientific environment based on values and quality</li> </ul>

## 8. Contents

8.1. Lecture	Teaching methods	Remarks, details
1. Properties and nature of X-rays. Sources of X-rays (2h)	Lecture, introductory conversation, heuristic conversation, illustration, use of analogies and algorithms, learning retention and deepening conversation.	<ul style="list-style-type: none"> <li>• The lecture will be interactive, conducting learning being facilitated by engaging students in conversation episodes - to catching the attention, for updating of some knowledge acquired at university courses and systematization / fixing the new knowledge.</li> <li>• Students will develop their ability in of analysis and synthesis.</li> <li>• Students will use correctly the terminology in physics in writing and oral communication.</li> <li>• Students will become familiar with a scientific environment based on values and quality.</li> </ul>
2. Interaction of X-rays with matter (2h)		
3. Kinematical theory of X-ray diffraction. Laue and Bragg equations. (2h)		
4. Scattering by a free electron. Scattering by an atom (2h)		
5. Scattering from several atoms (2h)		
6. Diffraction by a small crystal. The unit cell structure factor (2h)		
7. Width of diffraction maxima (2h)		
8. The integrating intensity from a small crystal and the Lorentz factor (2h)		
9. Lattice vibrations and the Debye-Waller factor (2h)		
10. The integrating intensity from a powder sample (2h)		
11. Scattering of X-rays on disordered and amorphous materials (2h)		

12. Snell's law and the Fresnel equations in the X-ray region. (2h)		
13. Specular reflection from multilayers (2h)		
14. X-ray spectroscopies (XAFS, XRF, XPS) (2h)		
<p><b>Recommended literature</b></p> <p>1. J. Als-Nielsen, D. McMorrow, “<i>Elements of modern x-ray physics</i>”, 2<sup>nd</sup> edition, A John Wiley &amp; Sons, Ltd Publication, 2011.</p> <p>2. B. D. Cullity, “<i>Elements of x-ray diffraction</i>”, Addison-Wesley Publishing Company Inc. 1978.</p> <p>3. V. Pecharsky, P. Zavalij, “<i>Fundamentals of powder diffraction and structural characterization of material</i>”, Springer, Berlin, 2005</p> <p>4. E. Lifshin (Editor), „<i>X-ray characterization of materials</i>”, Wiley-VCH, New York 1999</p>		
<b>8.2. Seminar / Laboratory</b>	<b>Teaching methods</b>	<b>Remarks, details</b>
1. Production and properties of X-rays	Introductory conversation, heuristic conversation, problematization, learning-retention conversation, case studies, numerical simulation, problem solving.	<p>-The students will be asked to answer questions meant to help them update, deepen and systematize their knowledge, then we will apply this knowledge for solving specific problems.</p> <p>-The students will describe physical phenomena and systems using specific theories and instruments – experimental and theoretical models, algorithms, diagrams, etc.</p> <p>- The students will form / practice / develop their:</p> <ul style="list-style-type: none"> <li>- Data processing abilities and the ability to interpret experimental results</li> <li>- Team work abilities</li> <li>- Organization and investigation abilities</li> </ul> <p>-The students will use appropriate programs when analyzing and processing X-ray diffraction data.</p>
2. The X-Ray Diffraction: Equipment and radiologic security		
3. Phase analysis and the use of PDF database: single and multiple phases		
4. Elements of crystallography		
5. Crystal structure analysis		
6. Interpretation of Powder Diffraction Patterns		
7. Rietveld method- Theoretical background		
8. Rietveld refinement- FullProf program		
9. Exercises: determination of unit cell parameters for different materials.		
10. Study of micro-structural effects		
11. The determination of crystal structure from powder diffraction data		
12. Laue crystal orientation		
13. X-Ray diffraction on thin films		
14. Studies from research scientific articles: examples.		
<p><b>Recommended literature:</b></p> <p>1. C. Whiston, <i>X-Ray Methods</i>, John Wiley and Sons, 1996</p> <p>2. R. A. Young, <i>The Rietveld Method</i>, Oxford University Press, 1993</p> <p>3. B. D. Cullity, <i>Elements of X-Ray Diffraction</i>, 2<sup>nd</sup> edition. (Addison-Wesley, Reading, Mass., 1978)</p> <p>4. V. Pecharsky, P. Zavalij: <i>Fundamentals of Powder Diffraction and Structural Characterization of Materials</i> (Springer, Berlin, 2005)</p> <p>5. J. Rodriguez-Carvajal, <i>Recent advances in magnetic structure determination by neutron powder diffraction + FullProf</i>, Physica B: Condensed Matter 192 (1–2), Pages 55–6</p> <p>6. P. W. Stephens, <i>Phenomenological Model of Anisotropic Peak Broadening in Powder Diffraction</i> J.</p>		

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### 9. Evaluation

Activity	9.1. Assessment criteria	9.2. Assessment methods	9.3. Weight in the final mark
9.4. Course	Students to choose the correct answers to the grid test  (final evaluation)	Summative assessment: Grid test	100%
9.5. Seminar / Laboratory			
9.6. Minimum needed performance for passing			
Knowing the basic terminology. They don't make major mistakes.			

Date of completion:  
11 January 2024

Signature (lecture instructor):  
Conf. univ. dr. Marius ȘTEF

Signature (seminar instructor):  
CS.II dr. Maria Poienar

Signature (director of the department)  
Conf. univ. dr. Nicoleta ȘTEFU