Computational material science and metallurgy		
Faculty:	Faculty of Geosciences	
Name of study program:	**Materials and Metallurgy**	
Department:	**Materials and Metallurgy**	
Level:	Master	
The code of subject:	2	
Subject:	**Computational material science and metallurgy**	
Subject Status:	Compulsory /Winter	(Winter / Summer)
Semester:	I	(According to approved programe)
Total hours:	2+2	(According to approved programe)
ECTS:	4	(According to approved programe)
Schedule / Hall		
Academic year:		
Professor:		
Assistants:	Lecturer:Muharrem Zabeli	Assistant
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Course description:	Computer modeling of materials is an increasingly important branch of materials science due to the evolution of modeling frameworks, the invention of new numerical algorithms, and the increase in computing capabilities. As a consequence, modeling and simulation are emerging as powerful complementary approaches to experiment with traditional theory and develop materials to another level of modeling and use.
Course objectives:	*The goals of this course are: (i) to introduce students to modeling and simulation techniques of materials covering a wide time and length scale; (ii) show how these modeling methods can be used to understand fundamental material structure, material defects, and the relationship between material structure and material behavior; and (iii) develop an understanding of the assumptions and approximations that are involved in modeling frameworks at different temporal and longitudinal scales.*
Learning outcomes:	1.Computational basis of materials science 2. Simulation techniques, 3. Calculation modeling, 4. Presentation and interpretation of simulation results. 5. Students will work with simulation modules to reinforce concepts learned in lectures.

Designed study plan:	Week	Lectures which will be held
	First week:	Introduction and summary in computational material science and metallurgy
	Second week:	Presentation and summary of calculations of computer materials
	Third week:	Introduction to the modeling of structures
	Fourth week:	Calculations based on phases and structures
	Fifth week:	Equilibrium properties and surfaces from phase calculations
	Sixth week:	Atomistic modeling of defects in materials
	Seventh week:	Methods of structural models
	Eighth week:	Atomic simulation projects
	Ninth week:	Introduction to continuum mechanics and elasticity

	Tenth week:	Introduction to dislocation dynamics modeling
	Eleventh week:	Dislocation Dynamics Project
	Twelfth week:	Continuous mechanics and methods of determining mechanical models
	Thirteenth week:	Mechanical properties simulation project
	Fourteenth week:	Course project presentations
	Fifteenth week:	Course project presentations

Literature	Basic	1. Computational Materials Science: An Introduction, Second Edition; Lee, June Gunn; 2017 Taylor & Francis Group, LLC. 2. Computational Materials Science; Kaoru Ohno, Keivan Esfarjani, Yoshiyuki Kawazoe; 2018 Springer Berlin Heidelberg
	Additional	1. C. Ricbard Brundle, Charles A. Evans, Jr.& Sbaun Wihon, "Encyclopedia of Mlaterials Characterization-Surfaces, Interfaces, Thin Films", Copyright by Butxetworch-Heinemann, a division of Reed Publishing CUSA) Inc

Teaching methods	Interactive lectures, numerical and exercises. Tests during lectures

Contribution on student load

Activity	Hours	Days/week	Total
Lectures	3	15	45
Exercise theoretical/laboratory	2	15	30
Practice work			
Contact with lecturer/consultations	2		2
Field exercises	-	-	-
Mid-terms, seminars	2	2	4
Homework	2	3	6
Individual time spent studying (at the library or home)	5	15	75
Final preparation for the exam	7	1	7
Time spent in evaluation (tests, quiz, final exam)	2	3	6
Projects, presentations, etc.	1	1	1
Total			176

Evaluation methods

Tests / Colloquia	2x15 (%)
Practical test during exercises	10 (%)
Seminar paper	10 (%)
Homework during the semester	10 (%)
Final exam 40 (%)	40 (%)

Academic policies and rules of conduct:	Regular attendance is required of students in lectures and exercises. Rules of conduct as quieting learning, access to the hall of learning time, turn off cell phones, etc. are also mandatory.