

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:	<i>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.</i>	
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.			

