NE 312 SIMULATION & MODELING OF MATERIALS

Course Code	Course Name	Semester	
NE 312	**Simulation & Modeling of Materials**	Fall ☐ Spring ☒ Summer ☐	
Hours		**Credit**	**ECTS**
Theory	**Practice** / **Lab**	4	5
3	-- / 2		

Course Details	
Department	Nanotechnology Engineering
Course Language	English
Course Level	Undergraduate ☒ Graduate ☐
Mode of Delivery	Face to Face ☒ Online ☐ Hybrid ☐
Course Type	Compulsory ☒ Technical Elective ☐
Course Objectives	■ The objective of this course is to introduce students to the fundamental principles and computational techniques used in the simulation and modeling of materials. It aims to provide an understanding of how different modeling approaches—such as atomistic, mesoscopic, and continuum-level simulations—are applied to study the structure, properties, and behavior of materials. Students will learn to use basic simulation tools and methods, such as molecular dynamics, Monte Carlo, finite element analysis, and phase field modeling, to analyze microstructural evolution, mechanical behavior, and thermodynamic stability. The course prepares students to apply modeling as a complementary tool to experiments in materials research and engineering design.
Course Content	■ **Simulation and Modeling of Materials** introduces the fundamental concepts and computational techniques used to analyze and predict material behavior across multiple length and time scales. The course begins with an overview of modeling approaches, including atomistic (molecular dynamics, Monte Carlo), mesoscopic (phase field, cellular automata), and continuum (finite element method) models. Students learn the principles of interatomic potentials, force fields, and statistical mechanics in the context of materials simulations. The course covers microstructure evolution, diffusion, phase transformations, mechanical deformation, and thermal properties. Emphasis is placed on interpreting simulation results, validating models with experimental data, and using software tools to simulate real-world materials problems. Practical sessions may involve using tools such as LAMMPS, COMSOL, ANSYS, or Python-based scripts for basic simulations.
Course Method/ Techniques	Lecture ☒ Question & Answer ☒ Presentation ☐ Discussion ☒

Prerequisites/ Corequisites	MATH 101-102, CENG 109, plus knowing Finite Element Analysis would be beneficial.
Work Placement(s)	No work placements.

Textbook/References/Materials

- Introduction to Computational Materials Science, Richard Lesar.
- Additional course notes.

Course Category				
Mathematics and Basic Sciences	☐		Education	☒
Engineering	☒		Science	☐
Engineering Design	☒		Health	☐
Social Sciences	☐		Profession	☒

Weekly Schedule

No	Topics	Materials/Notes
1	Introduction to Materials Modeling and Simulation	Lesar
2	Random walk model	Lesar
3	Random walk model	Lesar
4	Simulation of finite systems	Lesar
5	Electronic Structure Methods	Lesar
6	Interatomic Potentials	Lesar
7	Molecular Dynamics	Lesar
8	**MIDTERM**	
9	Monte Carlo Method	Lesar
10	Monte Carlo Method	Lesar
11	Molecular Macromolecular Systems	Lesar
12	Kinetic Monte Carlo	Lesar
13	Kinetic Monte Carlo	Lesar
14	Materials Selection and Design	Lesar
15	Linear, Non-linear Elasticity	Lesar
16	**FINAL**	

Assessment Methods and Criteria		
In-term studies	**Quantity**	**Percentage**
Attendance	14	--
Lab	14	--
Practice	--	--
Fieldwork	--	--
Course-specific internship	--	--
Quiz/Studio/Criticize	--	--
Homework	10	--
Presentation / Seminar	0	--
Project	1	**15 %**
Report	0	--
Seminar	--	--
Midterm Exam	1	**35 %**
Final Exam	1	**50 %**
	Total	**100%**
Contribution of Midterm Studies to Success Grade		50 %
Contribution of End of Semester Studies to Success Grade		50 %
	Total	**100%**

ECTS Allocated Based on Student Workload			
Activities	**Quantity**	**Duration (Hrs)**	**Total Workload**
Course Hours	14	3	42
Lab	0	0	0
Practice	0	0	0
Fieldwork	0	0	0
Course-specific Work Placement	0	0	0
Out-of-class study time	10	5	50
Quiz/Studio/Criticize	0	0	1
Homework	5	20	20
Presentation / Seminar	0	0	0
Project	0	0	0
Report	0	0	0
Midterm Exam and Preparation for Midterm	1	5	5
Final Exam and Preparation for Final Exam	1	10	10
Total Workload			**128**
Total Workload / 25			**128/25**

ECTS Credit	**5.12 ≅ 5**

Course Learning Outcomes	
No	**Outcome**
L1	**Apply fundamental simulation techniques** such as molecular dynamics, Monte Carlo methods, and finite element analysis to model the structure, properties, and behavior of materials.
L2	**Interpret and analyze simulation results** to understand material responses under various conditions, including mechanical, thermal, and phase transformation processes.
L3	**Design and evaluate materials systems** using computational tools by integrating structure–property relationships and applying simulations to guide materials selection and optimization.

Contribution of Course Learning Outcomes to Program Competencies/Outcomes

Contribution Level: 1: Very Slight, 2: Slight, 3: Moderate, 4: Significant, 5: Very Significant

	PO-1		PO-2		PO-3		PO-4		PO-5			PO-6			PO-7						PO-8		PO-9		PO-10			PO-11		Total
#	1.1	1.2	2.1	2.2	3.1	3.2	4.1	4.2	5.1	5.2	5.3	6.1	6.2	6.3	7.1	7.2	7.3	7.4	7.5	7.6	8.1	8.2	9.1	9.2	10.1	10.2	10.3	11.1	11.2	#
L1	5	5	5	5					4			4		3	5	5							5	5						48
L2	5	5	5	5	5	5	5	5	4			4		3	5	5							5	5						71
L3	5	5	5	5					4			4		3	5	5							5	5						51
																														Total= 170

#	**PROGRAM ÇIKTILARI ve ALT BİLEŞENLERİ**
1.1.	Matematik, fen bilimleri ve ilgili mühendislik disiplinine özgü konularda yeterli bilgi birikimi; Adequate knowledge in mathematics, science and subjects specific to the relevant engineering discipline;
1.2.	Bu alanlardaki kuramsal ve uygulamalı bilgileri, karmaşık mühendislik problemlerinin çözümünde kullanabilme becerisi. Ability to use theoretical and applied knowledge in these areas to solve complex engineering problems.
2.1.	Karmaşık mühendislik problemlerini tanımlama, formüle etme ve çözme becerisi; Ability to identify, formulate and solve complex engineering problems;
2.2.	Bu amaçla uygun analiz ve modelleme yöntemlerini seçme ve uygulama becerisi. Ability to select and apply appropriate analysis and modeling methods for this purpose.
3.1.	Karmaşık bir sistemi, süreci, cihazı veya ürünü gerçekçi kısıtlar ve koşullar altında, belirli gereksinimleri karşılayacak şekilde tasarlama becerisi; The ability to design a complex system, process, device or product under realistic constraints and conditions to meet specific requirements;
3.2.	Bu amaçla modern tasarım yöntemlerini uygulama becerisi. Ability to apply modern design methods for this purpose.
4.1.	Mühendislik uygulamalarında karşılaşılan karmaşık problemlerin analizi ve çözümü için gerekli olan modern teknik ve araçları seçme ve kullanma becerisi;

	Ability to select and use modern techniques and tools necessary for the analysis and solution of complex problems encountered in engineering practice;
4.2.	Bilişim teknolojilerini etkin bir şekilde kullanma becerisi. Ability to use information technologies effectively.
5.1.	Karmaşık mühendislik problemlerinin veya disipline özgü araştırma konularının incelenmesi için deney tasarlama, Design experiments to investigate complex engineering problems or discipline-specific research topics,
5.2.	Deney yapma, Experimentation
5.3.	Veri toplama, sonuçları analiz etme ve yorumlama becerisi. Ability to collect data, analyze and interpret results.
6.1.	Disiplin içi takımlarda etkin biçimde çalışabilme becerisi; Ability to work effectively in disciplinary teams;
6.2.	Çok disiplinli takımlarda etkin biçimde çalışabilme becerisi; Ability to work effectively in multidisciplinary teams;
6.3.	Bireysel çalışma becerisi. Ability to work individually.
7.1.	Sözlü ve yazılı etkin iletişim kurma becerisi; Ability to communicate effectively both orally and in writing;
7.2.	En az bir yabancı dil bilgisi; Knowledge of at least one foreign language;
7.3.	Etkin rapor yazma ve yazılı raporları anlama becerisi, Ability to write effective reports and understand written reports,
7.4.	Tasarım ve üretim raporları hazırlayabilme becerisi, Ability to prepare design and production reports,
7.5.	Etkin sunum yapabilme becerisi, Ability to make effective presentations,
7.6.	Açık ve anlaşılır talimat verme ve alma becerisi. Ability to give and receive clear and understandable instructions.
8.1.	Yaşam boyu öğrenmenin gerekliliği konusunda farkındalık; Awareness of the necessity of lifelong learning;
8.2.	Bilgiye erişebilme, bilim ve teknolojideki gelişmeleri izleme ve kendini sürekli yenileme becerisi. Ability to access information, to follow developments in science and technology and to continuously renew oneself.
9.1.	Etik ilkelerine uygun davranma, mesleki ve etik sorumluluk ve Acting in accordance with ethical principles, professional and ethical responsibility and
9.2.	Mühendislik uygulamalarında kullanılan standartlar hakkında bilgi. Information about standards used in engineering applications.
10.1.	Proje yönetimi, risk yönetimi ve değişiklik yönetimi gibi, iş hayatındaki uygulamalar hakkında bilgi; Knowledge of business practices such as project management, risk management and change management;

10.2.	Girişimcilik, yenilikçilik hakkında farkındalık; Awareness about entrepreneurship and innovation;
10.3.	Sürdürülebilir kalkınma hakkında bilgi. Knowledge about sustainable development.
11.1.	Mühendislik uygulamalarının evrensel ve toplumsal boyutlarda sağlık, çevre ve güvenlik üzerindeki etkileri ve çağın mühendislik alanına yansıyan sorunları hakkında bilgi; Knowledge about the effects of engineering applications on health, environment and safety in universal and social dimensions and the problems of the era reflected in the field of engineering;
11.2.	Mühendislik çözümlerinin hukuksal sonuçları konusunda farkındalık. Awareness of the legal implications of engineering solutions.