MASTERS COURSE
"MATERIALS SCIENCE AND SIMULATION"

MODULE DESCRIPTIONS

July 2025

COURSE SCHEDULE

Module	Module description	Semester					
		WH	CP	1st sem. L E	2nd sem. L E	3rd sem. L E	4th sem. L E
	Compulsory modules						
1	Fundamental Materials Physics	**4**	**5**	2 2			
2	Thermodynamics and Statistical Mechanics	**3**	**4**	2 1			
3	Elements of Microstructure	**4**	**6**	3 1			
4	Programming Concepts in Materials Science	**4**	**6**	2 2			
5	Numerical Methods in Materials Science	**4**	**6**		3 1		
6	**Fundamental option modules**						
	Fundamental Option Module 1	**4**	**6**		3 1		
	Fundamental Option Module 2	**4**	**6**		3 1		
	Fundamental Option Module 3	**4**	**6**			3 1	
7	**Advanced option module**						
	Advanced Option 1	**4**	**6**		2 2		
	Advanced Option 2	**4**	**6**			2 2	
	Advanced Option 3	**4**	**6**			2 2	
	General option module						
8	General Option Module	**4**	**6**			2 2	
	Key qualifications (* module 9 is compulsory)						
9 *	Documenting and Communicating Science	**4**	**6**				
9a	*Documenting and Communicating Science 1*	*2*	*3*	x			
9b	*Documenting and Communicating Science 2*	*2*	*3*		x		
10	Non-technical elective or language course	**2**	**3**		x		
	Practical modules						
11	Materials Modelling Lab	**4**	**6**	x			
	Research project and master thesis						
12	Research Project (180 h)		**6**			x	
13	Master Thesis and Seminar (900 h)		**30**				x

	Sum semester weekly hours	**80**		**20**	**20**	**20**	**20**
	Sum workload	**3600**		**900**	**900**	**900**	**900**
	Sum of credit points		**120**	**30**	**30**	**30**	**30**

Note: The title of lectures (submodules) referring to one module are typed in italic. The according weekly hours (WH) and credit points (CP) are summed in the title line of the module.

EXPLANATIONS

Compulsory Modules

1-5 The compulsory modules comprise the scientific focus of the programme and are therefore mandatory for every student.

- Fundamental Materials Physics (1)
- Thermodynamics and Statistical Mechanics (2)
- Elements of Microstructure (3)
- Programming Concepts in Materials Science (4)
- Numerical Methods in Materials Science (5)

Fundamental Option Modules in Materials Science

6 Three elective modules can be chosen freely from:

2nd semester/summer term

- Quantum Mechanics in Materials Science (6.1)
- Microstructure and Mechanical Properties (6.2)
- Advanced Characterization Methods (6.3)
- Materials Informatics (6.4)
- Microstructure Evolution during Materials Processing (6.5)

3rd semester/winter term

- Atomistic Simulation Methods (6.6)
- Advanced Programming for Materials Science (6.7)
- Functional Materials: Properties and Modelling (6.8)

Advanced Option Modules in Materials Science

7 Three optional modules can be chosen freely from the modules listed below (but also from the fundamental option modules listed above, see 6):

2nd semester/summer term

- Interfaces and Surfaces (7.1)
- Data-driven Materials Science – Hands on (7.2)
- Introduction to Parallel- and Scientific Computing (7.3)
- Physics of Complex Phase Transitions in Solids (7.4)
- The CALPHAD Method in Thermodynamics and Diffusion (7.5)
- Fundamental Aspects of Materials Science and Engineering (7.6)
- Polymers and Shape Memory Alloys (7.7)
- Computational Plasticity (7.8)
- Engineering Ceramics and Coating Technology (7.9)
- Theory of Electronic Excitations in Materials (7.10)
- Mathematics for Materials Modelling (7.11)

3rd semester/winter term

- Phase-field Theory and Application (7.12)
- Multiscale Mechanics of Materials (7.13)
- Advanced Atomistic Simulation Methods (7.14)

- Computational Fracture Mechanics (7.15)
- Advanced Statistical Methods in Materials Science (7.16)
- Surface Science and Corrosion (7.17)
- Materials for Aerospace Applications (7.18)
- Introduction to 3-Dimensional Materials Characterization Techniques (7.19)
- Application and Implementation of Electronic Structure Methods (7.20)
- Lattice Boltzmann Modelling: From Simple Flows to Interface Driven Phenomena (7.21)
- Interatomic Potentials (7.22)
- Atomistic Theory of Defects in Materials

General Option Module

8	Any module from any of RUB's master's programmes will be recognized. A selection of courses offered is listed under points 6 and 7 (Elective and Specialization Modules in MS). Courses from the RUB's main course catalogue and from the international course catalogue can be taken into account. It is also possible to take a six-week industrial internship (8.1).

Key Qualifications (* Module 9 is compulsory)

9 *	The Key Qualification module 9 is divided into two parts, Documenting and Communicating Science 1 (1st semester) and Documenting and Communicating Science 2 (2nd semester).
10	This non-technical elective module should be chosen from the key qualifications offers like German language for foreigners, Project and Quality Management, Business Skills, Intercultural Competence etc.

Practical Module

11	Materials Modelling Lab: 4-5 block lectures, introduction of methods, including practical demonstration, followed by hands-on blocks.

Scientific Theses

12, 13	The research project and the master thesis with seminar represent practical self-guided research and make up 30% of all credit points.

EXAMINATIONS, CREDITS AND GRADES

Each module is usually assessed by one final examination, which defines the grade for this module and is the prerequisite for credit point allocation. Module 9 spans over two semesters with two examinations, each at the end of the corresponding term.

Credit points are allocated in accordance with the students' work load comprising classes and preparation time for classes and assignments. The work load makes up the double or triple amount of the instructional contact time, depending on the degree of difficulty of the class. Together with the results of written and oral examinations as well as of practical exercises (if applicable) they form the basis for the final module grade. Since the Master's course puts an emphasis on practical research in the project report and the Master's thesis the results of these two assignments count for 30% of the total grade. The total grade is derived according to the average of all allocated module credits.

CREDIT ALLOCATION

Semester	**1**	**2**	**3**	**4**	**Σ**
Compulsory modules: 1, 2, 3, 4, 5, 11	27	6	0		33
Option modules: 6, 7, 8	0	18	24		42
Key qualifications: modules 9, 10	3	6			9
Research project: module 12			6		6
Master's thesis: module 13				30	30
Σ	**30**	**30**	**30**	**30**	**120**

Credits are allocated according the the following scheme:

- Compulsory 33 CP = 28%
- Option 42 CP = 35%
- Key qualifications 9 CP = 7%
- Research project and Master's thesis 36 CP = 30%

DE-REGISTRATION FROM EXAMS

The current examination regulations allow to withdraw from examination registrations.

In the case of compulsory modules (1-5, 9, 11), the withdrawal must be made in written form, stating valid reasons. Deregistration from elective and compulsory elective modules must also be made in written form, but without giving reasons, up to 1 week before the examination date.

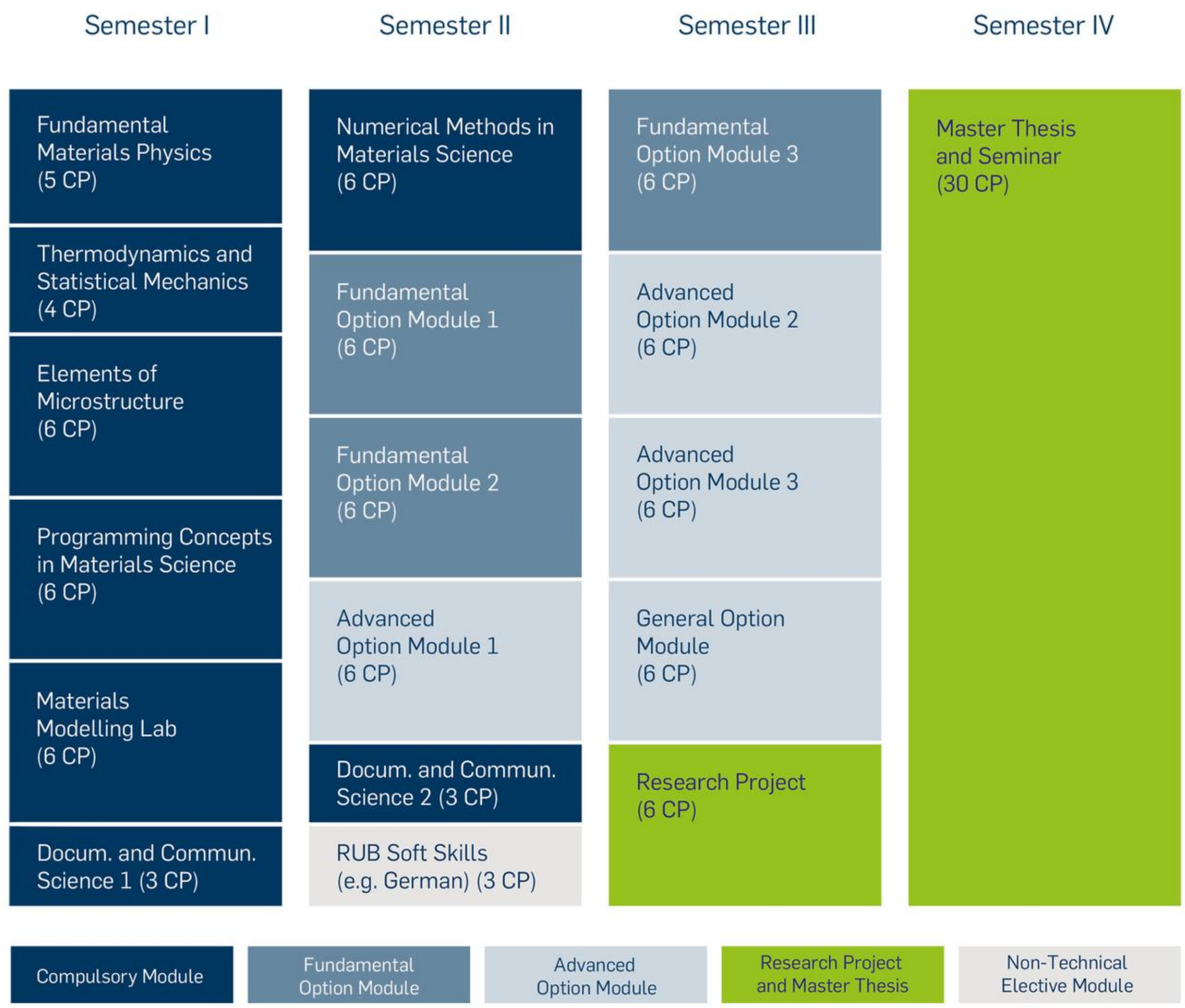
Valid reasons include, for example:

• Illness of the candidate. In this case, a doctor's certificate and, in cases of doubt, a certificate from a medical officer of the RUB must also be submitted.

• The illness of a child or person to be cared for mainly alone is equivalent to the illness of the candidate.

• The examination board decides on further valid reasons.

MODULE SCHEME AND CREDITS



Course scheme: the size of the fields represents the allocated credit points.

ALL MODULES

FUNDAMENTAL MATERIALS PHYSICS

Module code	Student work-load	Credits	Semester	Frequency	Duration
1	150 hours	5 ECTS	1st	winter term	1 semester

1	**Types of courses** a) lecture b) class	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 90 hours	**Class size** 30 students

2	**Learning outcomes** On successful completion of this module, students recall the connections between electronic structure, atomic bonds and macroscopic physical and mechanical properties of solids. The students can classify materials according to their phenotypical properties and atomic structures. They can analyze simple tasks on material behavior under applied electric, magnetic, electromagnetic, thermal and mechanical fields and create solutions based on their understanding of the relations between atomic interactions and macroscopic behavior.
3	**Subject aims** • Introduction to quantum mechanics and wave functions, many-electron systems • Atomic orbitals, covalent and ionic bonds, electron gas and metallic bonds • Band structure, conductors, semi-conductors, insulators, electronic transport • Electrical and optical properties • Magnetism, electron spin, elementary magnetic moments • Stress and strain tensors, Hooke's law and atomic interaction, mechanical equilibrium • Metals: crystal structure, strength, equivalent stress • Polymers: molecular structure, mechanical and physical properties • Ceramics and glasses, including semi-conductors: atomic structure, mechanical and physical properties
4	**Teaching methods** lecture, including classes with practical application of theoretical content
5	**Prerequisites for participation** None
6	**Assessment methods** Written examination (2 hours). Bonus points can be gained by providing solutions to the problem sheets in classes.
7	**Prerequisites for the assignment of credit points** Passing the written examination (bonus points will be taken into account)
8	**This module is used in the following degree programmes as well** None
9	**Impact of grade on total grade** 5/117
10	**Responsibility for module** Prof. Dr. Alexander Hartmaier
11	**Other information** Moodle course with lecture notes and additional materials

THERMODYNAMICS AND STATISTICAL MECHANICS					
Module code 2	**Student workload** 120 hours	**Credits** 4 ECTS	**Semester** 1st	**Frequency** winter term	**Duration** 1 semester

1	**Types of courses:** a) lecture b) class	**Contact hours** a) 30 hrs (2 SWS) b) 15 hrs (1 SWS)	**Independent study** 75 hours	**Class size** 30 students
2	**Learning outcomes** Students remember the basic laws of thermodynamics, thermodynamic potentials and concepts such as phase coexistence, phase transitions and phase diagrams. They combine this knowledge with the variational principle to construct simple models of the temporal and spatial evolution of thermodynamic properties of solids, e.g., alloys and magnetic materials. Moreover, the students apply fundamental concepts of statistical mechanics to put such basic models on a microscopic footing. They discuss approximations involved in these models and systematically propose improvements for the individual steps.			
3	**Subject aims** • Basic principles of thermodynamics, phase coexistence, Gibbs phase rule and phase diagrams • Equation of state of ideal gases and extension towards the van-der-Waals theory • Landau theory and variational principle (Ginzbourg-Landau) • Statistical theory of ideal gases, lattice gases and the regular solution theory for thermodynamic properties of gases and solid alloys • Statistical mechanics of stress tensor: The Virial formula • Statistics of quantum harmonic oscillator and specific heat of solids • Spin statistics: Para and ferromagnetism, mean field approximation for ferro-magnetism			
4	**Teaching methods** lecture, group work			
5	**Prerequisites for participation** None			
6	**Assessment methods** written examination (1.5 hours), bonus points can be gained by providing solutions to the problem sheets in class.			
7	**Prerequisites for the assignment of credit points** passing the exam			
8	**This module is used in the following degree programs as well** None			
9	**Impact of grade on total grade** 4/117			
10	**Responsibility for module** Prof. Dr. Fathollah Varnik			
11	**Other information** Literature: McQuarrie: Statistical Mechanics, C. Garrod: Statistical mechanics and thermodynamics, D.R. Gaskell; Introduction to the thermodynamics of materials, D.A. Porter & K.E. Easterling; Phase transformation in metals and alloys.			

ELEMENTS OF MICROSTRUCTURE: AN INTRODUCTION TO MATERIALS SCIENCE

Module code	Student work-load	Credits	Semester	Frequency	Duration
3	180 hours	6 ECTS	1st	winter term	1 semester

	Types of courses	Contact hours	Independent study	Class size
1	a) lecture b) class	a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	120 hours	30 students 15 students

2	**Learning outcomes** Students acquire the basic concepts required to understand microstructures of materials, and to appreciate their role in governing many important materials properties. They learn to combine knowledge from different fields (chemistry, solid state physics, crystallography, physical chemistry and physical metallurgy) which allows them to understand microstructural evolution during processing and heat treatments of materials. They also learn to apply this knowledge to interpret materials properties.
3	**Subject aims** • Basics of crystallography, waves, scattering and diffraction • Chemical bond, elasticity and thermal expansion • Defects and interfaces • Diffusion phenomenology and physics • Basics of thermodynamics and phase transformations • Phase diagram • Solidification and time-temperature-transformation (TTT) diagrams • Precipitation strengthening • Order and disorder transformation • Martensite, pearlite, bainite in steels • Shape memory alloys • Brittle and ductile materials behavior
4	**Teaching methods** lecture, class
5	**Prerequisites for participation** None
6	**Assessment methods** Written examination (2 hours).
7	**Prerequisites for the assignment of credit points** Passing the written examination.
8	**This module is used in the following degree programmes as well** none
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** Prof. Dr. Alexander Kauffmann, Prof. Dr. Tong Li
11	**Other information** Literature, lecture script, Moodle course, etc.

PROGRAMMING CONCEPTS IN MATERIALS SCIENCE					
Module code 4	**Student work-load** 180 hours	**Credits** 6 ECTS	**Semester** 1st	**Frequency** winter term	**Duration** 1 semester

1	**Types of courses** Lecture with integrated practical hands-on	**Contact hours** 60 hrs (4 SWS)	**Independent study** 120 hours	**Class size** 30 students

2	**Learning outcomes** On successful completion of this module the students recall the basic concepts of computers, operating systems. They analyse, write and test Python language programs of moderate complexity. Furthermore, they have the ability to work with code editors and programming tools and to program and to solve basic numerical problems in the context of other modules, in particular project work and Master thesis. The students will transfer materials science problems into an abstract algorithm and implement this algorithm into the taught structured programming language.

3	**Subject aims**
	• Introduction to principles of computers and operating systems (Linux)
	• Introduction to a modern programming language (Python)
	• Introduction to relevant mathematical and graphical software
	• Examples that will gain an overview of modern programming approaches and tools will comprise:
	  • data interpolation and fitting
	  • linear algebra
	  • numerical integration
	  • numerical solution of ordinary and partial differential equations

4	**Teaching methods** Lecture with integrated hands-on computer exercises with Python and Jupyter notebook
5	**Prerequisites for participation** None
6	**Assessment methods** Written examination (3 hours).
7	**Prerequisites for the assignment of credit points** Passing the written examination
8	**This module is used in the following degree programmes as well** none
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** PD Dr. habil. Thomas Hammerschmidt, Prof. Dr. Godehard Sutmann
11	**Other information** An online repository provides Lecture notes (lecture files and video material), source code of programs which are discussed and developed during the class and exercises with solutions. The book “A primer on scientific programming with Python” by Hans Petter Langtangen will be covered.

NUMERICAL METHODS IN MATERIALS SCIENCE					
Module code 5	**Student work-load** 180 hours	**Credits** 6 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses** a) lecture b) class	**Contact hours** a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	**Independent study** 120 hours	**Class size** a) 30 students b) 30 students
2	**Learning outcomes** Students will remember the basic principles of solving numerical problems in materials science. They memorize the numerical solution strategies for different problems and are able to analyse, select and apply appropriate numerical strategies for a wide variety of numerical modelling tasks in materials science, from the electronic structure to continua. The students appraise the unified, holistic approach to materials simulation which is not centered on or limited to a particular length scale. Furthermore, the students assess and evaluate given numerical problems in materials science and devise and implement optimal solutions.			
3	**Subject aims** Numerical methods are the foundation of materials simulation and necessary for the implementation of materials theory and its application to practical problems. The principles of numerical methods are independent of length scale, i.e. the solutions of electronic, atomistic, microstructural and continuum problems often follow closely related strategies. In this course the focus is on numerical problems and challenges in materials science. Applications to different length scales are introduced by way of example. • Basics: Differentiation and integration, vectors and tensors, products and norms, series expansions • Partial differential equations: Numerical integration for electrons, atoms and continuum models • Variational calculus: Functional derivatives and derivation of partial differential equations • Optimization: Optimization/root finding algorithms, methods for eigenvalue problems • Regression and statistical analysis: Data analysis, error estimates, machine learning			
4	**Teaching methods** Lectures, classes			
5	**Prerequisites for participation** None			
6	**Assessment methods** Written examination (2 hours). Bonus points can be gained by presenting solutions to the worksheets in class.			
7	**Prerequisites for the assignment of credit points** Passing the written examination			
8	**This module is used in the following degree programmes as well** none			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Ralf Drautz			
11	**Other information** Recommended literature will be announced in class.			

QUANTUM MECHANICS IN MATERIALS SCIENCE					
Module code 6.1	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses:** a) lecture b) class	**Contact hours** a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	**Independent study** 120 hours	**Class size** a) 30 students b) 10-15 students
2	**Learning outcomes** Students are able to classify the fundamentals and the application of quantum mechanics in materials science. They are able to understand textbooks and the research literature in the field. They understand the principles of electronic structure calculations in materials science, in particular density functional theory, and their limitations, and also gain insight into the numerical implementation of electronic structure methods. The students can relate electronic structure properties to the crystal structure and other properties of materials.			
3	**Subject aims** • Schrödinger equation • Many-electron problem • Hartree/Hartree-Fock • Density-functional theory • Overview of basis sets, plane waves vs local orbitals, pseudopotentials • Band structure, symmetry groups, density of states • Magnetism • Tight-binding approximation • Selected applications for molecules and solids, including semiconductors and metals			
4	**Teaching methods** lecture, class			
5	**Prerequisites for participation** None			
6	**Assessment methods** written examination (2 hours).			
7	**Prerequisites for the assignment of credit points** Passing the written examination			
8	**This module is used in the following degree programmes as well** None			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Ralf Drautz			
11	**Other information** Lecture notes will be provided. Relevant literature will be discussed in the first lecture.			

MICROSTRUCTURE AND MECHANICAL PROPERTIES					
Module code 6.2	**Student work-load** 180 hours	**Credits** 6 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses** a) lecture b) class	**Contact hours** a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	**Independent study** 120 hours	**Class size** a) 30 students b) 15 students
2	**Learning outcomes** The students memorize the definitions of mechanical equilibrium and discuss their different mathematical formulations and solution strategies. They recall the basics ideas of the concept of strength for different materials. The students discuss microstructural principles of elastic-plastic deformation and their relation to atomic bonds and crystal structures. They describe the definition of an equivalent stress and apply it to solve simple problem for the deformation of elastic-plastic materials. They classify the basic hardening mechanisms of materials and apply theoretical models to predict material strength of different materials as function of their microstructural parameters. They analyze simple problems in mechanics of materials and solve the resulting boundary value problems by using different finite element solvers.			
3	**Subject aims** • Definitions and mathematical formulations of mechanical equilibrium • Theory and application of finite element analysis as numerical tool to analyze the deformation of elastic-plastic materials under given boundary conditions • Concepts of strength and equivalent stress in continuum plasticity • Relations between atomic bonds and crystal structures to the elastic-plastic behavior of materials • Phenomenology and microscopic origin of hardening mechanisms, including grain boundaries, dislocations, solid solutions and precipitation hardening • Micromechanical modelling of material properties			
4	**Teaching methods** lecture, classes			
5	**Prerequisites for participation** None			
6	**Assessment methods** Written examination (2 hours). Bonus points can be gained by providing solutions to the problem sheets in classes.			
7	**Prerequisites for the assignment of credit points** Passing the written examination (bonus points will be taken into account)			
8	**This module is used in the following degree programmes as well** none			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Alexander Hartmaier			
11	**Other information** Lecture notes are provided online via Moodle course. Literature: T.H. Courtney: Mechanical behavior of materials, (2nd edition) McGraw-Hill International Editions, Boston/USA (2000) G. Gottstein: Physical foundations of materials science, Springer-Verlag (2004)			

ADVANCED CHARACTERIZATION METHODS

Module code	Student work-load	Credits	Semester	Frequency	Duration
6.3	180 hours	6 ECTS	2nd	summer term	1 semester

1	**Types of courses** a) lecture b) class	**Contact hours** a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	**Independent study** 120 hours	**Class size** a) 30 students b) 30 students

2 Learning outcomes

Students understand the basic description of the structure of solids. They recall advanced crystallographic concepts and have acquired fundamental knowledge of scattering and diffraction of electron, X-ray, synchrotron and neutron waves. They know how to apply the Bragg equation and the Ewald construction to understand diffraction data of different origines. They will apply basic concepts to two of the most important characterization techniques in materials science, SEM and TEM. For both methods the mechanisms which are responsible for different types of image contrast will be appreciated. The students will also develop an appreciation of advanced in situ methods. After this course the students are able to fully appreciate the scientific literature on advanced characterization methods. They are able to judge the usefulness of specific methods with respect to their potential to progress materials technology.

3 Subject aims

- Introduction to crystalline and amorphous solids
- Learn basic crystallographic concepts
- Scattering and diffraction of particle waves (X-rays, synchrotron radiation, neutrons and electrons)
- Learn basic interpretation of diffraction results (applying Bragg equation, Ewald construction, structure factor; interpreting diffracted intensities, extra spots ...)
- Learn advanced scanning electron microscopy (introduction, secondary and back scattered electrons, energy dispersive and wave length dispersive chemical analysis, indexing of Kikuchi lines as a basis of orientation imaging SEM, in-situ experiments in the SEM)
- Learn advanced transmission electron microscopy (introduction, differences between conventional and advanced methods – field emission guns [FEG], high angular dark field detectors [HAAD]), chemical analysis by EDX and EELS, using Kikuchi lines as maps for tilting experiments, apply tilting experiments to identify crystal defects [focus: dislocations], in-situ experiments in the SEM)
- Learn to appreciate other important advanced characterization methods (brief introduction to atom probe analysis and high resolution transmission electron microscopy)

4 Teaching methods

lecture, class, lab

5 Prerequisites for participation

successful completion of "Elements of Microstructure" (2) or equivalent

6 Assessment methods

written examination (2 hours)

7 Prerequisites for the assignment of credit points

passing the written examination

8 This module is used in the following degree programmes as well

Master of Science in Mechanical Engineering: Werkstoff- and Microengineering

9 Impact of grade on total grade

6/117

10 Responsibility for module

Prof. Dr.-Ing. Jan Frenzel, Prof. Dr. Tong Li

11 Other information

A list with recommended literature and class notes is available online.

MATERIALS INFORMATICS					
Module code 6.4	**Student work-load** 180 hours	**Credits** 6 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses** a) lecture b) class	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** a) 30 students b) 15 students
2	**Learning outcomes** After successful completion of the module students are able to explain the impact of *informatics* in materials science. They can assess quality and dimensions of materials data and metadata. Successful students are able to judge the applicability and choose an appropriate data science / machine learning method to solve a problem in materials science. They are able to solve a "data problem" in materials science by implementation in Python code and can document, visualize and present a "workflow" in written and presentation form.			

3	**Subject aims**
	• From data to data science to materials informatics
	• Data sources: materials data bases and how to organize data
	• Combinatorics, probabilities, and statistics
	• Descriptors and representations for materials: dimensions of data
	• Machine learning
	  o Classification and regression
	  o Supervised and unsupervised learning
	  o Dimensionality reduction
	  o Clustering
	  o Deep learning and artificial neural networks
	• End-to-end workflows: data, features, model, validation, application			

4	**Teaching methods** lecture, assisted tutorials in CIP-pool			
5	**Prerequisites for participation** None			
6	**Assessment methods** Written exam (2 hours)			
7	**Prerequisites for the assignment of credit points** Passing the module examination			
8	**This module is used in the following degree programmes as well** None			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Markus Stricker			
11	**Other information** Suggested literature: Materials Data Science – An Introduction to Data Mining, Machine Learning, and Data-Driven Predictions for Materials Scientists; Stefan Sandfeld, Springer (2024)			

MICROSTRUCTURE EVOLUTION DURING MATERIALS PROCESSING

Module code	Student workload	Credits	Semester	Frequency	Duration
6.5	180 hours	6 ECTS	3rd	summer term	1 semester

	Types of courses:	Contact hours	Independent study	Class size
1	a) lecture b) numerical exercises	a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	120 hours	a) 30 students b) 15 students

2	**Learning outcomes** Students can explain the underlying principles of the finite element/finite volume method to solve problems in continuum mechanics including phase transformations. They recall mean-field models and rate equation solutions. With the phase-field method they are able to solve free boundary problems coupled to a thermodynamic material description. With the help of these widely used numerical methods in industrial and academic materials science the students can model and solve materials science problems and they can describe the limitations of these methods.
3	**Subject aims** • Introduction into Partial Differential Equation and Boundary Value Problems (BVP) • Principles of thermodynamics of multi-phase systems • CALPHAD thermodynamics and kinetics of multicomponent diffusion • Mean field models of microstructure evolution • Rate equations for precipitation including numerical integration • Concepts of non-equilibrium phase transformations • Introduction to free boundary problems • Thermodynamic concept of the Phase-field method and practical applications
4	**Teaching methods** lecture, numerical exercises
5	**Prerequisites for participation** background in mechanical engineering, physics or related discipline
6	**Assessment methods** written examination (2 hours). Bonus points can be gained by providing solutions to the problem sheets in class.
7	**Prerequisites for the assignment of credit points** passing the written examination (bonus points will be taken into account)
8	**This module is used in the following degree programmes as well** none
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** Prof. Dr. Ingo Steinbach
11	**Other information** Lecture notes are provided online.

ATOMISTIC SIMULATION METHODS					
Module code 6.6	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 3rd	**Frequency** winter term	**Duration** 1 semester

1	**Types of courses:** a) lecture b) class	**Contact hours** a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	**Independent study** 120 hours	**Class size** a) 30 students b) 10-15 students
2	**Learning outcomes** Students recall models for the interatomic interaction and can explain how these interactions can be represented by potentials. They are able to apply methods such as molecular dynamics and kinetic Monte Carlo simulations to calculate the evolution of the atomic structure of materials and the resulting material properties. They can discuss the importance of the time and length scales in atomic modelling. The successful participants will be able to apply atomistic simulation methods to solve problems in materials science.			
3	**Subject aims** • Empirical and semi-empirical potentials for ionic, covalent and metallic materials • Atomic dynamics • Statistics of atomic ensembles • Observables in atomistic simulations (MSD, RDF, specific heat and free energy) • Monte Carlo (kinetic, Metropolis) and Transition-state theory • Lattice-gas-Hamiltonian (Ising-model, cluster expansion) • Magnetism (Heisenberg-model) • Linking atomistic simulations to the electronic, microstructural and macroscopic models			
4	**Teaching methods** lecture, class, problem sheets			
5	**Prerequisites for participation** successful completion of “Quantum Mechanics in Materials Science”(Module 6.1) is recommended			
6	**Assessment methods** written examination (2 hours). Bonus points can be gained by providing solutions to the problem sheets in class.			
7	**Prerequisites for the assignment of credit points** passing the written examination (bonus points will be taken into account)			
8	**This module is used in the following degree programmes as well** none			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Ralf Drautz			
11	**Other information** Lecture notes will be provided. Relevant literature will be discussed in the first lecture.			

ADVANCED PROGRAMMING FOR MATERIALS SCIENCE

Module code	Student workload	Credits	Semester	Frequency	Duration
6.7	180 hours	6 ECTS	2nd	winter term	1 semester

	Types of courses	Contact hours	Independent study	Class size
1	a) lecture b) class	a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	120 hours	a) 30 students b) 15 students

2 Learning outcomes

The students recognize the advanced programming techniques that are relevant for materials science. They can classify different programming languages and are able to generate computer code for compiled languages to solve basic mathematical and physical problems. They use tools that facilitate code development and employ best programming practices. The students apply these concepts to create advanced algorithms that solve complex problems in materials science.

3 Subject aims

- Compiled languages (Fortran, C)
- Object-oriented programming (python, C++)
- Parallel programming
- Best practices (testing, documentation, version control)
- Advanced algorithms
  - Variational basis set methods for PDEs
  - Stochastic Monte-Carlo methods
  - Time-propagation

4 Teaching methods

lecture, assisted tutorials in CIP-pool, mini-project

5 Prerequisites for participation

None

6 Assessment methods

Portfolio exam including mini-project, seminar, and report

7 Prerequisites for the assignment of credit points

Passing the module examination

8 This module is used in the following degree programmes as well

None

9 Impact of grade on total grade

6/117

10 Responsibility for module

Prof. Dr. Miguel Marques

11 Other information

-

FUNCTIONAL MATERIALS: PROPERTIES AND MODELLING					
Module code 6.8	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 3rd	**Frequency** winter term	**Duration** 1 semester

1	**Types of courses** a) lecture b) class	**Contact hours** a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	**Independent study** 120 hours	**Class size** a) 30 students b) 15 students
2	**Learning outcomes** After participation in this module, students memorize the discussed functional properties of materials. They recall and understand the underlying physical concepts. Furthermore, they can outline the challenges for materials science, and suggest proper simulation methods to address these on the relevant scales. They are able to analyse, compare and apply these concepts and methods to current problems in materials science.			
3	**Subject aims** This course focuses on functional materials, their relevance for application, and the interplay of electronic, atomistic, microstructural and functional properties. The objectives are the fundamental understanding of functional responses and their degeneration through functional fatigue as well as routes to optimize functional properties. The main focus is on materials for energy conversion and storage, e.g. • Battery materials • Materials for capacitors • Permanent magnets • Materials for solar cells • Magnetic, ferroelectric, multiferroic phases and phase transitions • Superconducting materials In addition to physical concepts, the lecture focuses on the modelling of the material properties across the relevant scales. We will discuss, compare and apply simulations using e.g. • Spin models • Density functional theory • Molecular Dynamics • Landau theory			
4	**Teaching methods** lecture, class			
5	**Prerequisites for participation** Basic knowledge on quantum mechanics / solid state physics is of advantage			
6	**Assessment methods** Written exam (2 hours); if less than 10 students: oral exam (20 minutes)			
7	**Prerequisites for the assignment of credit points** Passed examination			
8	**This module is used in the following degree programmes as well** -			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Anna Grünebohm			
11	**Other information** Lecture notes will be provided.			

INTERFACES AND SURFACES

Module code	Student workload	Credits	Semester	Frequency	Duration
7.1	180 hours	6 ECTS	2nd	summer term	1 semester

1	**Types of courses:** a) lecture b) class	**Contact hours** a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	**Independent study** 120 hours	**Class size** a) 20 students b) 10 students

2	**Learning outcomes** Students will understand the relevance of surfaces and interfaces in materials science and gain basic knowledge of experimental and computational techniques to characterize them. They understand the relationship between atomistic descriptions of interfaces/surfaces and macroscopic materials properties, especially thermodynamic and mechanical properties. They will develop the skills to read and understand the relevant literature, to choose the most suited experimental or modelling approaches for specific tasks and to applythem to material science problems.
3	**Subject aims** • Introduction to surfaces and interfaces for optical, electronic, magnetic and mechanical properties and their importance for materials design including metals, semiconductor, oxides • Principles of interface/surface crystallography and indexing geometries in atomistic models. Introducing classification and nomenclature of surfaces and grain boundaries • Mechanisms and importance of surface relaxation/reconstruction and optimization of solid-solid interface degrees of freedom • Empirical and thermodynamic models of interface/surface properties, for pure interfaces/surfaces as well as for interactions with adsorbates, vacancies, impurities, and dislocations • Experimental characterization of interface/surface structures (diffraction, scanning, microscopy, spectroscopy methods), planning specific experiments and relate experimental and theoretical results • Methods for computational determination of atomistic interface/surface structures and properties. Possibilities and limitations of atomistic models
4	**Teaching methods** lecture, computer exercises
5	**Prerequisites for participation** background in physics, chemistry or related discipline
6	**Assessment methods** written (2 hours) or oral examination (0.5 hours) depending on size of the class. Bonus points can be gained by complementary tasks distributed in the lecture.
7	**Prerequisites for the assignment of credit points** passing the examination (bonus points will be taken into account)
8	**This module is used in the following degree programmes as well** none
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** PD Dr. habil. Thomas Hammerschmidt, PD Dr. habil. Rebecca Janisch
11	**Other information** Lecture notes will be provided. Recommended Literature: J. M. Howe: Interfaces in materials, Wiley Interscience (1997); A. Gross: Theoretical surface science: A microscopic perspective, Springer (2009).

DATA-DRIVEN MATERIALS SCIENCE – HANDS ON

Module code	Student workload	Credits	Semester	Frequency	Duration
7.2	180 hours	6 ECTS	2nd	summer term	1 semester

	Types of courses:	Contact hours	Independent study	Class size
1	a) lectures b) hands-on practical studies	a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	120 hours	a) 20 students b) 20 students

2	**Learning outcomes** After participating in the module students • Remember the basic concepts of data-driven material science • apply common data-driven methods of supervised and unsupervised learning, deep learning to describe and analyze given data sets • discuss limitations and applicability of these methods in the context of materials science and select the proper methods for particular applications. • create Python code to implement and apply these methods to simple problems • apply the methods to organize and manipulate data efficiently
3	**Subject aims** • Data manipulation with Python • Data visualization and reporting • Supervised learning: regression and classification • Unsupervised learning: clustering, dimensionality reduction • Deep learning • Data storage and organization, databases of relevance in materials science • Design and management of databases
4	**Teaching methods** hands-on lectures and mini project
5	**Prerequisites for participation** Completion of the modules “Programming Concepts in Materials Science” and “Materials Informatics” is recommended
6	**Assessment methods** Completion of mini project with written project report
7	**Prerequisites for the assignment of credit points** Accepted project report
8	**This module is used in the following degree programmes as well** none
9	**Impact on total grade** 6/117
10	**Responsibility for module** Prof. Dr. Drautz, Dr. Yury Lysogorskiy
11	**Other information** Literature: Literature: W. McKinney: Python for Data Analysis: Data Wrangling with pandas, NumPy, and Jupyter, O'Reilly (2022); J. VanderPlas: Python Data Science Handbook: Essential Tools for Working with Data, O'Reilly (2016); J. Grus:Data Science from Scratch: First Principles with Python, O'Reilly (2015).

INTRODUCTION TO PARALLEL- & SCIENTIFIC-COMPUTING					
Module code 7.3	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses:** a) lectures b) exercises	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** 20 students
2	**Learning outcomes** After successful completion of the module the students have gained knowledge about parallel programming concepts. They can translate a serial algorithm into its parallel version and can apply parallel concepts to applications of scientific computing. The students have learned and applied the main important data communication concepts in shared memory and distributed memory programming via OpenMP and MPI. The students will have gained practical programming experience with specific problem oriented examples which support the experience in applying parallel computing methods. The students have worked on different numerical applications for which parallel algorithms are introduced, compared and assessed. They have learned how to analyze the potential of a serial program for its parallelization. The students will gain practical experience with numerical methods in computational projects that will be presented by the students in short talks and a final report.			
3	**Subject aims** • Parallel communication libraries MPI and OpenMP • Parallel algorithms for particle methods, linear algebra • Performance evaluation • Numerical optimisation • Application of numerical libraries			
4	**Teaching methods** lecture, class-room exercises, project work			
5	**Prerequisites for participation** basic knowledge in a higher programming language			
6	**Assessment methods** project work on a given topic of scientific computing Translation of a problem into an OpenP or MPI version. Seminar talk and written report on the project topic			
7	**Prerequisites for the assignment of credit points** submission of report and presentation of project work			
8	**This module is used in the following degree programmes as well** none			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Godehard Sutmann			
11	**Other information** An online repository provides lecture notes (lecture files and video material), source code of programs discussed and developed during the class, and exercises with solutions.			

PHYSICS OF COMPLEX PHASE TRANSITIONS IN SOLIDS					
Module code 7.4	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses** a) lecture b) seminar	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** 20 students
2	**Learning outcomes** After participation in this module, students are able to characterize and classify phase transitions in solid state materials. For the discussed examples (e.g. superconducting and ferroic phases) they know the underlying physical concepts and scale-bridging methods to address these. They are able to judge, compare and utilize these concepts and methods.			
3	**Subject aims** • Introduction to complex phase transitions in solid state materials (e.g. magnetic, ferroelectric and superconducting phases) • Classification of phase transitions and critical phenomena (e.g. order of phase transitions, critical exponents, displacive transitions) • Models and simulation methods (e.g. spin models, Landau theory, molecular dynamics simulations)			
4	**Teaching methods** lecture, seminar/project			
5	**Prerequisites for participation** basic knowledge on quantum mechanics / solid state physics and thermodynamics / statistical physics			
6	**Assessment methods** Written and oral presentation of project work and short oral examination related to project			
7	**Prerequisites for the assignment of credit points** taking part in the seminar / project work			
8	**This module is used in the following degree programmes as well** Physics			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Anna Grünebohm, Prof. Dr. Michael Scheren			
11	**Other information** Lecture notes will be provided.			

THE CALPHAD METHOD IN THERMODYNAMICS AND DIFFUSION					
Module code 7.5	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses:** a) lecture b) class	**Contact hours** a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	**Independent study** 120 hours	**Class size** 15 students

2	**Learning outcomes** Students understand the concept of phase equilibrium, learn how to model Gibbs energy and its derivatives using fundamental theories and the connection to experimental determined thermodynamic properties. They learn to handle thermodynamic and diffusion databases. After a successful participation of the course students know the mathematical models of diffusion and numerical methods as well as diffusion processes. They will be able to understand physical relationships in the diffusion process and the connection to the thermodynamic properties. They learn to select a suitable model according to a requirement profile and are able to carry out simple material-specific simulations of diffusion processes in materials.
3	**Subject aims** • Thermodynamic functions and calculation of phase diagrams. • Constructions of the CALPHAD-type computational thermodynamic databases after critical evaluation of experimental information as well first- principles calculated data. • Microstructure simulations using thermodynamic quantities • Mathematical basics of the diffusion equation, diffusivity, mobility coefficients • Diffusion as a coupling of mobility and thermodynamics • Multicomponent Diffusion • Introduction to DICTRA • Mobility databases
4	**Teaching methods** lecture, exercises, individual project, case studies, discussions, presentation of modeling results
5	**Prerequisites for participation** basic knowledge in thermodynamics and statistical physics, basic knowledge of structure and properties of materials, ordinary differential equations.
6	**Assessment methods** written report (10 to 15 pages) of individual project
7	**Prerequisites for the assignment of credit points** positively evaluated written report
8	**This module is used in the following degree programmes as well** none
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** Prof. Dr. Ingo Steinbach, Dr. Julia Kundin
11	**Other information** Literature: H.L. Lukas, S.G. Fries, B. Sundman: Computational thermodynamics, the Calphad method, Cambridge University Press (2007). A. Paul, T. Laurila, V. Vuorinen, S.V. Divinski: Thermodynamics, Diffusion and the Kirkendall Effect in Solids, Springer, Cham, (2014).

<table>
<tr><td colspan="7">FUNDAMENTAL ASPECTS OF MATERIALS SCIENCE AND ENGINEERING (FAMSE)</td></tr>
<tr><td colspan="2">Module code
7.6</td><td>Student workload
180 hours</td><td>Credits
6 ECTS</td><td>Semester
2nd</td><td>Frequency
summer term</td><td>Duration
1 semester</td></tr>
<tr><td>1</td><td colspan="2">Types of courses:
a) lecture
b) class</td><td colspan="2">Contact hours
a) 45 hrs (3 SWS)
b) 15 hrs (1 SWS)</td><td>Independent study
120 hours</td><td>Class size
a) 10 students
b) 10 students</td></tr>
<tr><td>2</td><td colspan="6">Learning outcomes
Students will be able to apply elements from the materials science curriculum to actual engineering problems in advanced materials technology. They are aware of the strong link between elementary atomistic, crystallographic, thermodynamic/kinetic and microstructural processes and the behaviour of materials/components on the macro scale. They will be able to use the understanding of basic processes to develop new and improve classical materials, to assess the mechanical and functional properties of materials and to understand kinetic processes in solids and at surfaces. In addition to an increased familiarity with advanced basic concepts, the students will be able to apply materials science theory to four fascinating material classes: High entropy alloys, intermetallic phases, single crystal Ni-base superalloys and shape memory alloys.</td></tr>
<tr><td>3</td><td colspan="6">Subject aims
Importance of atoms and electrons in materials engineering and the transition from atoms to alloys and from alloys to components
Thermodynamic concepts in materials engineering and fundamentals of alloy design (with a special focus on ternary phase diagrams)
Kinetic concepts in materials science and engineering (especially precipitation processes)
Basic concepts of solid state phase transformations
Understanding and application of knowledge to four materials classes: high entropy alloys, intermetallic phases, single crystal superalloys and shape memory alloys
Acquisition of knowledge about high temperature strength (example: superalloys)
Acquisition of knowledge about fracture mechanics and fatigue (example: shape memory alloys)</td></tr>
<tr><td>4</td><td colspan="6">Teaching methods
lecture, class</td></tr>
<tr><td>5</td><td colspan="6">Prerequisites for participation
successful completion of “Elements of Microstructure” (3) and “Statistical Mechanics and Fundamental Materials Physics” (1, 2) recommended</td></tr>
<tr><td>6</td><td colspan="6">Assessment methods
oral examination (0.5 hours)</td></tr>
<tr><td>7</td><td colspan="6">Prerequisites for the assignment of credit points
passing the exam</td></tr>
<tr><td>8</td><td colspan="6">This module is used in the following degree programmes as well
Master of Science in Mechanical Engineering: Werkstoff- und Microengineering</td></tr>
<tr><td>9</td><td colspan="6">Impact of grade on total grade
6/117</td></tr>
<tr><td>10</td><td colspan="6">Responsibility for module
Prof. Dr.-Ing. Gunther Eggeler</td></tr>
<tr><td>11</td><td colspan="6">Other information
A list with recommended literature and class notes will be available online.</td></tr>
</table>

POLYMERS AND SHAPE MEMORY ALLOYS					
Module code 7.7	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses:** a) lecture b) class	**Contact hours** a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	**Independent study** 120 hours	**Class size** a) 10 students b) 10 students
2	**Learning outcomes** Students will be familiar with the morphology/microstructure of polymers and shape memory alloys and know how to process these materials. They will understand the basic mechanical and functional properties of these two materials classes with a special focus on engineering applications and be familiar with scale bridging concepts, i.e. they can discuss macroscopic properties in view of atomistic interactions and morphological/microstructural features. Most importantly, they will understand the relation between morphology/microstructure and mechanical and functional properties.			
3	**Subject aims** • Processing and morphology of polymers • Characterization of polymers • Physical and thermodynamic aspects of polymer materials science • Mechanical and functional properties of polymers and engineering applications • Introduction of the shape memory effects in crystalline materials • Characterization of shape memory alloys • Role of the martensitic transformation in shape memory technology • Mechanical and functional properties of shape memory alloys			
4	**Teaching methods** lecture, class			
5	**Prerequisites for participation** successful completion of “Elements of Microstructure” (3) or equivalent recommended			
6	**Assessment methods** written examination (2 hours)			
7	**Prerequisites for the assignment of credit points** passing the written examination			
8	**This module is used in the following degree programmes as well** Master of Science in Mechanical Engineering: Werkstoff-Engineering			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Dr. Klaus Neuking, Prof. Dr.-Ing. Jan Frenzel			
11	**Other information** Lecture notes will be provided.			

COMPUTATIONAL PLASTICITY					
Module code 7.8	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses** lecture and class	**Contact hours** 60 hrs (4 SWS)	**Independent study** 120 hours	**Class size** no restrictions
2	**Learning outcomes** After successfully completing the module, the students recall the definitions of different types of mechanical behavior into which materials can be classified. They understand the phenomenology and mechanisms of elastic and plastic behavior of crystalline materials and can outline the different types of plasticity models in solid mechanics. Furthermore, they can explain the basic concepts and the mathematical formulation of continuum plasticity and crystal plasticity. They discuss the basic concepts of the numerical implementation of plasticity models and identify the method which is most suited to solve a given mechanical problem. Students can implement and apply a numerical scheme for the solution of elasto-plastic problems within the finite element method.			
3	**Subject aims** • Basics of continuum mechanics and Finite Element Analysis • Phenomenology and atomistic origin of elastic and plastic deformation • Concepts of continuum plasticity (yield criterion, flow rule, isotropic and kinematic hardening) • Rate dependent and rate-independent formulations of continuum plasticity • Numerical solution schemes for elasto-plasticity (operator split, return mapping, consistent tangent modulus) • Computational aspects of small and large strain formulations • Concepts of crystal plasticity (dislocation slip, flow rule, hardening models, consistent tangent modulus) • Structure, implementation and application of an Abaqus UMAT			
4	**Teaching methods** lecture, hands-on classes, mini project incl. seminar talk, assignments			
5	**Prerequisites for participation** none			
6	**Assessment methods** Portfolio exam including reports on assignments, seminar and self-evaluation report			
7	**Prerequisites for the assignment of credit points** passed final module examination			
8	**This module is used in the following degree programmes as well** Master of Science Computational Engineering, Master of Science Maschinenbau			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Alexander Hartmaier			
11	**Other information** Lecture notes will be provided.			

ENGINEERING CERAMICS & COATING TECHNOLOGY					
Module code 7.9	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses:** a) lecture b) class	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 135 hours	**Class size** a) 10 students b) 10 students
2	**Learning outcomes** The students obtain a profound knowledge of engineering ceramics and their technical applications. By examples, they learn and understand the major processing steps in manufacturing engineering ceramics and in manufacturing routes for fibre-reinforced ceramic matrix composites. They become familiar with the typical thermo-mechanical and functional properties of ceramics. This knowledge enables the students to select ceramics for specific needs. In addition, the students gain basic knowledge on coating technologies for thick layers of ceramic materials, including thermal spray and sintering technologies, which enables the students to select suitable coating methods for wear, corrosion, functional and high temperature applications.			
3	**Subject aims** • Powder synthesis & conditioning, shaping, sintering of ceramic materials • Characterisation of ceramics with different methods • Properties and applications of engineering ceramics • Basic knowledge on different thick film deposition technologies (thermal spray processes and sintering techniques) • Demonstration how coatings can improve the functionality of components			
4	**Teaching methods** lecture, class, assignment			
5	**Prerequisites for participation** knowledge in materials properties is recommended.			
6	**Assessment methods** written report on assignment (weight for final grade: 30%); oral examination (20 minutes) or written examination (90 minutes) (weight for final grade: 70%)			
7	**Prerequisites for the assignment of credit points** passing the exam			
8	**This module is used in the following degree programmes as well** Master of Science in Mechanical Engineering: Werkstoff-Engineering			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Robert Vaßen			
11	**Other information** Literature: Ceramic Materials, Science and Engineering, C. Barry Carter, M. Grant Norton, Springer 2013; Handbook of Properties of Technical & Engineering Ceramics, R. Morrell, HMSO 1989; Ceramics, D. Munz, T. Fett, Springer, 1999; The Mechanics and Reliability of Films, Multilayers and Coatings, M.R. Begley, J.W. Hutchinson, Cambridge University Press, 2017; Plasma Spray Coating, Robert B. Heiman, Wiley, 2008. Slides will be available online.			

THEORY OF ELECTRONIC EXCITATIONS IN MATERIALS

Module code	Student workload	Credits	Semester	Frequency	Duration
7.10	180 hours	6 ECTS	2nd	summer term	1 semester

1	**Types of courses** a) lecture b) hands-on	**Contact hours** a) 30 hrs (2 SWS b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** 20 students

2	**Learning outcomes** Electronic Structure Theory is a successful and growing area of materials science, taking advantage of the increasing availability of high performance computers. Starting only from the knowledge of the types of atoms that make up the system (molecule, crystal, nanostructure, ...), students will learn how to accurately calculate the response properties of materials without any further experimental input, i.e. using only the fundamental laws of electrodynamics and quantum physics. Students get familiar with state-of-the-art theoretical and computational approaches to electronic excitations and theoretical spectroscopy (density functional theory, time-dependent density functional theory, Green's function methods). In practical classes, students gain hands-on experience in the use of various software packages for electronic structure simulations beyond the ground state. In the final weeks, they undertake a small simulation project in which they learn how to carry out simulations and analyse and present the numerical results.
3	**Subject aims** • Foundations of theory for interacting electrons: mean fields and auxiliary systems, particles and quasiparticles, functionals in many-particle physics • Electronic excitations: particle-hole excitations, collective excitations, excitations in 2D, 1D, 0D nanostructures • Linear response and excitation energies • Modeling neutral excitations by time-dependent density functional theory • Modeling charged and neutral excitations by Green's function methods • Applications to spectroscopy
4	**Teaching methods** Lectures, hands-on computer classes, individual project
5	**Prerequisites for participation** Knowledge of linux/unix environment, completion of "Fundamental MaterialsPhysics" or equivalent courses is recommended
6	**Assessment methods** Oral examination (0.5 h) on the content of the lecture, including a short presentation (<10 minutes) on the computational project. Bonus points can be gained by presenting solutions to the worksheets in class.
7	**Prerequisites for the assignment of credit points** Passing the oral examination
8	**This module is used in the following degree programmes as well** Physics
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** Prof. Dr. Silvana Botti
11	**Other information** Recommended literature: Richard M. Martin, "Electronic Structure" Cambridge University Press; Richard M. Martin, Lucia Reining, David M. Ceperley, "Interacting Electrons" Cambridge University Press.

MATHEMATICS FOR MATERIALS MODELLING					
Module code 7.11	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses:** a) lectures b) exercises	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** a) 10 students b) 10 students
2	**Learning outcomes** After participating in the module, students are able to understand fundamental mathematical concepts encountered in quantum mechanics, statistical mechanics, thermodynamics and transport phenomena. They can solve and analyze specific problems in integral and differential calculus and linear algebra that appear in physics and materials science, including Fourier integrals, Fourier and Laplace integral transforms and convolution, wave and diffusion differential equations, vector and tensor calculus, eigenvalue problems, and linear operators.			
3	**Subject aims** • Complex analysis (functions of complex variable, Cauchy's and residue theorem) • Analytic functions and their use in evaluation of definite integrals • Vectors and matrices • Linear transformations and tensors • Fourier series • Dirac's delta function • Integral transforms (Fourier, Laplace, convolution theorem) • Sturm-Liouville theory of linear differential operators • Partial differential equations			
4	**Teaching methods** lectures and exercises			
5	**Prerequisites for participation** undergraduate level of mathematics for materials science and engineering			
6	**Assessment methods** Homework assignment, written final examination (120 min.)			
7	**Prerequisites for the assignment of credit points** none			
8	**This module is used in the following degree programmes as well** none			
9	**Impact on total grade** 6/117			
10	**Responsibility for module** Dr. Matous Mrovec			
11	**Other information** Literature: Erwin Kreyszig: Advanced Engineering Mathematics; George Arfken: Mathematical Methods for Physicists; Mary L. Boas: Mathematical Methods in Physical Sciences.			

PHASE-FIELD THEORY AND APPLICATION

Module code	Student workload	Credits	Semester	Frequency	Duration
7.12	180 hours	6 ECTS	2nd	winter term	1 semester

1	**Types of courses:** a) lecture b) exercises	**Contact hours** a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	**Independent study** 120 hours	**Class size** a) 30 students b) 10-15 students

2	**Learning outcomes** The students understand the principles of mesoscopic structure formation in condensed matter as the basis of the phase-field theory. They are able to derive the basic relations of this theory and relate the parameters to measurable physical quantities. They are able to use theoretical methods to investigate scale separation in condensed matter. The students are skilled in the application of the phase-field theory in numerical simulations. In the practical exercises, they developed a simple software code to simulate dendritic growth in 3D, thus being able to independently formulate new branches of the simulation software developed at ICAMS.
3	**Subject aims** Dendric solidification, scale invariant solution and microscopic solvability Traveling wave solution of a phase front, sharp and thin interface limit Anisotropy and the ξ-vector approach Coupling to outer fields, elasticity Coupling to multiphase flow via the Lattice Boltzmann method Microscopic variables and fluctuations, extension to critical phenomena Miscellaneous applications in materials science
4	**Teaching methods** lecture, exercises
5	**Prerequisites for participation** Students must have good knowledge in statistical and condensed matter physics. Programming skills in C++ are of advantage.
6	**Assessment methods** written exam (2 hours)
7	**Prerequisites for the assignment of credit points** passing the written examination
8	**This module is used in the following degree programmes as well** none
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** Prof. Dr. Ingo Steinbach, Prof. Dr. Fathollah Varnik, Dr. Oleg Shchyglo
11	**Other information** Lecture notes will be provided online.

MULTISCALE MECHANICS OF MATERIALS					
Module code 7.13	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 3rd	**Frequency** winter term	**Duration** 1 semester

1	**Types of courses** a) lecture b) class	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** a) 20 students b) 10 students
2	**Learning outcomes** Students understand the multiscale nature of the mechanical behaviour of materials and of the different approaches to take this into account in mechanical modelling of microstructures. They can identify the relevant length- and timescales of the microscopic processes that lead to meso-/macroscopic structure-property relationships. The students understand the principles of effective theory construction, coarse graining and homogenisation methods, and they can apply them to identify, analyse and model multiscale problems, such as plastic deformation, hardening behaviour, and fracture of microstructures. They are able to use state of the art numerical and theoretical scale-bridging modelling methods. They can apply numerical tools on different length scales, and understand the underlying principles (atomistic modelling, discrete dislocation dynamics, continuum plasticity).			
3	**Subject aims** • State of the art in bridging length-scales in modeling of elasticity, plasticity, and fracture • Principles and concepts of concurrent and hierarchical multiscale modeling of materials • Basics of atomistic modeling: from density functional theory to large scale molecular dynamics • Defect identification in atomistic simulations • Discrete dislocation dynamics • Crystal plasticity: phenomenological and density based methods • Homogenization methods			
4	**Teaching methods** lecture, computer exercises, and seminar			
5	**Prerequisites for participation** successful completion of “Basics in Materials Science” (module 2) or equivalent			
6	**Assessment methods** oral (0.5 hours) or written (2 hours) examination, depending on size of the class			
7	**Prerequisites for the assignment of credit points** taking part in the hands-on exercises and submitting a report, passing the examination.			
8	**This module is used in the following degree programmes as well** None			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** PD Dr. habil. Rebecca Janisch			
11	**Other information** Lecture notes will be provided.			

ADVANCED ATOMISTIC SIMULATION METHODS

Module code	Student workload	Credits	Semester	Frequency	Duration
7.14	180 hours	6 ECTS	3rd	winter term	1 semester

1	**Types of courses:** a) lecture b) classes focusing on hands-on computational tasks	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** 20 students

2	**Learning outcomes** The students gain fundamental knowledge of techniques and methods used in advanced atomistic simulations that address large system sizes, long-time scales, and long-range interactions. They can classify simulation methods including molecular statics, molecular dynamics and Monte Carlo simulations, and apply appropriate models of interatomic interactions (DFT, tight binding, empirical potentials). The students can evaluate the validity of the simulation outcomes and their relation to measurable material properties for several case studies. The students are able to plan, execute and monitor atomistic simulations.
3	**Subject aims** • Generation, analysis and optimization of atomic structures • Molecular statics and relaxation algorithms • Molecular dynamics in various ensembles, thermostats • Monte Carlo methods, spin lattice models, transition state theory • Accelerated techniques and hybrid approaches • Rigorous coarse-graining of atomic interaction models • Workflows for atomistic simulations • Case studies: e.g. elasticity and phonons, diffusion, ferroelectricity, melting
4	**Teaching methods** lecture, exercises
5	**Prerequisites for participation** background in physics, chemistry or related discipline, knowledge of linux/unix environment and Python/C/Fortran programming languages participation in “advanced numerical methods: atomistic simulation methods” or similar course.
6	**Assessment methods** oral (0.5 hours) or written (2 hours) examination. Bonus points can be gained by submitting solutions to the problem sheets that are distributed in class.
7	**Prerequisites for the assignment of credit points** passing the exam (bonus points will be taken into account)
8	**This module is used in the following degree programmes as well** none
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** Prof. Dr. Anna Grünebohm and Dr. Matous Mrovec
11	**Other information** -

COMPUTATIONAL FRACTURE MECHANICS					
Module code 7.15	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 3rd	**Frequency** winter term	Duration 1 semester

1	**Types of courses:** a) lecture b) class	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** a) 20 students b) 10 students
2	**Learning outcomes** The students attain the ability to independently simulate fracture including plasticity for a wide range of materials and geometries. Based on the acquired understanding of the different types of brittle fracture and ductile failure of materials, they are enabled to choose appropriate fracture models and to implement them in a finite element environment. They gain sufficient knowledge about the theoretical background of the different types of fracture models, to study the relevant literature independently. On an engineering level, the students discriminate between situations, where cracks in a structure or component can be tolerated or under which conditions cracks are not admissible, respectively.			
3	**Subject aims** • Phenomenology of fracture/Fracture on the atomic scale • Concepts of linear elastic fracture mechanics • Concepts of elastic-plastic fracture mechanics • R curve behavior of materials • Concepts of cohesive zones (CZ), extended finite elements (XFEM) and damage mechanics • Finite element modeling of fracture for static and dynamic cracks • Application to brittle fracture & ductile failure for different geometries and loading situations			
4	**Teaching methods** lecture, hands-on classes, mini-project incl. seminar talk, assignments			
5	**Prerequisites for participation** basic knowledge about solid mechanics and plasticity is recommended			
6	**Assessment methods** Portfolio exam including reports on assignments, seminar and self-evaluation report			
7	**Prerequisites for the assignment of credit points** passing final module examination			
8	**This module is used in the following degree programmes as well** Computational Engineering, Master course: Maschinenbau			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Alexander Hartmaier			
11	**Other information** Lecture notes will be provided.			

ADVANCED STATISTICAL METHODS IN MATERIALS SCIENCE

Module code	Student work-load	Credits	Semester	Frequency	Duration
7.16	180 hours	6 ECTS	3rd	winter term	1 semester

1	Types of courses	Contact hours	Independent study	Class size
	a) lecture b) class	a) 45 hrs (2 SWS) b) 15 hrs (1 SWS)	120 hours	a) 15 students b) 15 students

2 Learning outcomes

After participating in the module students

- remember a variety of uncertainty indication methods, their limitations and applicability
- apply active learning and Bayesian optimization methods to materials properties optimization problems
- construct deep generative models for materials properties generation
- assess limitations and applicability of these methods and select proper methods for particular tasks
- create Python code to implement and use above-mentioned methods to solve simple problems

3 Subject aims

- Probability distributions and Bayesian statistics
- Uncertainty indication and quantification
- Bayesian optimization
- Active learning
- Generative models (neural networks - auto-encoders, generative adversarial networks, etc.)

4 Teaching methods

lecture, classes including hands-on exercises with Python and Jupyter notebook, mini project

5 Prerequisites for participation

Successful completion of the modules “Materials Informatics” and “Data-driven materials science – hands on” course is recommended.

6 Assessment methods

Completion of mini project with written project report

7 Prerequisites for the assignment of credit points

Accepted project report

8 This module is used in the following degree programmes as well

None

9 Impact of grade on total grade

6/117

10 Responsibility for module

Prof. Dr. Drautz, Dr. Yury Lysogorskiy

11 Other information

Literature:

- T. Hastie, R. Tibshirani, J. Friedman: The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Springer (2009);
- A. Gelman, J. B. Carlin, H. S. Stern, D. B. Dunson, A. Vehtari, D. B. Rubin: Bayesian Data Analysis, Chapman and Hall/CRC (2013);
- Downey, Allen B. (2021). Think Bayes: Bayesian Statistics in Python (2nd ed.). O'Reilly.
- Foster D. Generative deep learning: teaching machines to paint, write, compose, and play. – O'Reilly Media, 2019.
- J. VanderPlas: Python Data Science Handbook: Essential Tools for Working with Data, O'Reilly (2016)

SURFACE SCIENCE AND CORROSION

Module code	Student workload	Credits	Semester	Frequency	Duration
7.17	180 hours	6 ECTS	3rd	winter term	1 semester

1	Types of courses:	Contact hours	Independent study	Class size
	a) lecture b) class	a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	120 hours	a) 25 students b) 25 students

2	**Learning outcomes** Students will gain a fundamental understanding of corrosion science, from basic electrochemistry of homogeneous metal corrosion to general aspects of localized corrosion, as well as of complex components and structures. They will memorize the basics of applied surface technologies providing corrosion protection, including an outlook of novel technological developments. Furthermore, the are able to relate their knowledge to engineering aspects of materials selection, analysing corrosion damage and measures for counteracting corrosion.
3	**Subject aims** • short introduction into surface science and electrochemistry • fundamental aspects of corrosion science: thermodynamics and kinetics (Pourbaix diagrams, Butler-Volmer equation etc. • passivity of materials • typical corrosion problems, such as atmospheric corrosion, bimetal corrosion, localised corrosion, corrosion under biofilms, basics of high temperature corrosion • materials choices based on application requirements (such as corrosiveness of the environment) • countermeasures against corrosion, such as by electrochemical corrosion protection, by improved construction, metallic, inorganic and organic coatings and related pre-treatments, inhibitors • evaluation of corrosion damage • counteracting methods best to use for different cases
4	**Teaching methods** lecture, class, including a short lab course
5	**Prerequisites for participation** successful completion of “Statistical Mechanics and Fundamental Materials Physics” (2c) and “Elements of Microstructure” (2a) recommended.
6	**Assessment methods** written examination (2 hours)
7	**Prerequisites for the assignment of credit points** passing the written examination
8	**This module is used in the following degree programmes as well** Master of Science in Mechanical Engineering: Werkstoff-Engineering
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** Prof. Dr. rer. nat. Martin Stratmann, Dr. rer. nat. Michael Rohwerder
11	**Other information** Lecture notes will be provided.

MATERIALS FOR AEROSPACE APPLICATIONS

Module code	Student workload	Credits	Semester	Frequency	Duration
7.18	180 hours	6 ECTS	3rd	winter term	1 semester

1	Types of courses:	Contact hours	Independent study	Class size
	a) lecture b) class	a) 45 hrs (3 SWS) b) 15 hrs (1 SWS)	120 hours	a) 25 students b) 25 students

2	**Learning outcomes** Students gain a comprehensive overview of high performance materials for aerospace applications, which includes the well-introduced materials and material systems as well as new developments and visionary concepts. They understand how materials and material systems are designed to be 'light and reliable' under extreme service conditions such as fatigue loading, high temperatures, and harsh environments. The students can categorize the degradation and damage mechanisms and learn how characterization and testing methods are used for qualifying materials and joints for aerospace applications. They are able to apply concepts and methods for lifetime assessment.
3	**Subject aims** • Loading conditions for components of air- and space crafts (structures and engines) • Development of materials and material systems for specific service conditions in aerospace applications (e.g. for aero-engines, rocket engines, thermal protection shields for re-entry vehicles, light weight structures for airframes, wings, and satellites) • Degradation and damage mechanisms of aerospace materials and material systems under service conditions • Characterization and testing methods for materials and joints for aerospace applications • Concepts and methods for lifetime assessment. Introduction to concepts of mechanical properties of materials (stress-strain curves, stiffness, strength, ductility)
4	**Teaching methods** lecture, class
5	**Prerequisites for participation** background in materials science, mechanical engineering, physics or related discipline
6	**Assessment methods** written (2 hours) or oral (0.5 hours) examination, depending on number of students
7	**Prerequisites for the assignment of credit points** passing the exam
8	**This module is used in the following degree programmes as well** Master of Science in Mechanical Engineering: Werkstoff-Engineering Master of Science in Computational Engineering
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** Prof. Dr.-Ing. Marion Bartsch
11	**Other information** Lecture notes will be provided online.

INTRODUCTION TO THREE-DIMENSIONAL MATERIALS CHARACTERIZATION TECHNIQUES					
Module code 7.19	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 3rd	**Frequency** winter term	**Duration** 1 semester

1	**Types of courses:** a) lecture b) exercises	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** a) 15 students b) 15 students
2	**Learning outcomes** By completing the course, students gain insight into a range of three-dimensional nanoscale and atomic scale material characterization techniques, e.g. 3D x-ray microscopy, electron tomography and atom probe tomography. They can describe the working principles of each technique in detail, summarize applications in a vast of applications, such as engineering alloys, catalyst materials, semiconductors, etc. and solve scientific questions related to material science by using three-dimensional material characterization techniques. Additionally, students will understand three-dimensional nanoscale and atomic scale material characterization methods, which are currently extremely important in both industry and academia, and achieve some basic hands-on experience on sample preparation and sample analysis on one of these techniques (depends on the availability of instrument).			
3	**Subject aims** • 3D Energy-dispersive X-ray spectroscopy • 3D-Field ion microscopy • Atom probe tomography • Electron tomography • X-ray tomography • Focused ion beam slicing/scanning electron microscopy			
4	**Teaching methods** lecture, exercises			
5	**Prerequisites for participation** none			
6	**Assessment methods** During the semester each student will be assigned a current topic on which the student has to write a five-page report and give a talk.			
7	**Prerequisites for the assignment of credit points** Submission of report and holding of seminar talk			
8	**This module is used in the following degree programmes as well** Masters Mechanical Engineering: Werkstoff-Engineering			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Tong Li			
11	**Other information** -			

APPLICATION AND IMPLEMENTATION OF ELECTRONIC STRUCTURE METHODS					
Module code 7.20	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 3rd	**Frequency** winter term	**Duration** 1 semester

1	**Types of courses:** a) lecture + group seminar b) practical studies	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** a) 10 students b) 10 students
2	**Learning outcomes** Students are able to formulate and describe the foundations of electronic structure calculations. This will include the translation of the quantum mechanical equations into pseudocode that may then be implemented in computer code. They will be able to use and implement the most common numerical solvers that are employed in quantum mechanical problems. In this way they will be able to appraise and implement quantum mechanical simulation codes. Students will also be enabled to choose the most appropriate electronic structure computational method and implementation for a given research project.			
3	**Subject aims** • Numerical implementation and solution of a single particle Schrödinger equation (electron in an effective potential) • Basis sets, representation of operators in a basis • Results, analysis and visualization of electronic structure calculations • Numerical convergence • Plane-wave pseudo-potential method (iterative diagonalization, self-consistency) • Tight binding Method • Bond-order potentials • Special topics and applications (structural stability, magnetism).			
4	**Teaching methods** lecture, practical studies and group seminars			
5	**Prerequisites for participation** successful completion of "Introduction to Quantum Mechanics in Solid State Physics" is recommended.			
6	**Assessment methods** written examination (1,5 hours)			
7	**Prerequisites for the assignment of credit points** positively evaluated written report and passing of exam			
8	**This module is used in the following degree programmes as well** None			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Ralf Drautz, Prof. Dr. Jörg Neugebauer			
11	**Other information** Lecture notes will be provided.			

LATTICE BOLTZMANN MODELLING: FROM SIMPLE FLOWS TO INTERFACE DRIVEN PHENOMENA					
Module code 7.21	**Student work-load** 180 hours	**Credits** 6 ECTS	**Semester** 3rd	**Frequency** winter term	**Duration** 1 semester

1	**Types of courses** a) lecture b) class	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** a) 10 students b) 10 students
2	**Learning outcomes** On successful completion of this module, students will recall equations of hydrodynamics and their solutions for simple cases such as hydrostatic pressure in an ideal gas (barometric formula), planar Couette flow and the Poiseuille flow. They can outline the lattice Boltzmann method (LBM) and apply a simple code for simulating flow via LBM. Using the above mentioned simple cases, the students will be able to examine the validity of the LBM code and also address a number of interesting problems such as Laplace law for pressure difference in drops and their environments and wetting of liquids on solid surfaces.			
3	**Subject aims** • Introduction to fluid dynamics on the continuum level (Euler and Navier-Stokes equations) • Basics of the lattice Boltzmann method (LBM) • Simulation of multiphase fluids: drops, bubbles • Wetting			
4	**Teaching methods** lecture, group work, case studies, discussions			
5	**Prerequisites for participation** familiarity with computer programming (C, Fortran, or equivalent)			
6	**Assessment methods** oral examination (0.5 hours)			
7	**Prerequisites for the assignment of credit points** passing the exam (for active participation in the lecture, bonus points will be considered)			
8	**This module is used in the following degree programmes as well** none			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Fathollah Varnik			
11	**Other information** Lecture notes will be provided.			

INTERATOMIC POTENTIALS					
Module code 7.22	**Student work-load** 180 hours	**Credits** 6 ECTS	**Semester** 3rd	**Frequency** winter term	**Duration** 1 semester

1	**Types of courses** a) lecture b) exercises	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** a) 10 students b) 10 students
2	**Learning outcomes** After participating in the module, students are able to understand fundamental concepts of interatomic potentials based on the electronic structure, on classical approaches and on machine-learning. They are able to carry out atomistic simulations for various materials using interatomic potentials and to analyze and interpret the outcomes.			
3	**Subject aims** • overview of interatomic interactions • electronic-structure approximations (tight-binding, bond-order potentials) • classical potentials (Lennard-Jones, embedded-atom/Finnis-Sinclair, Tersoff) • force fields (Amber, Charmm, ReaxFF) • many-atom expansions/cluster expansions • machine-learning potentials (neural networks, Gaussian-approximation potentials, moment-tensor potentials, atomic-cluster expansion, message-passing and graph representations) • magnetism, charge-transfer, polarization • parameterization and validation • simulation tools and applications			
d4	**Teaching methods** lecture, computer exercises			
5	**Prerequisites for participation** none			
6	**Assessment methods** individual project and/or oral examination (0.5 hours), depending on size of class			
7	**Prerequisites for the assignment of credit points** successful completion of project / passing of written examination			
8	**This module is used in the following degree programmes as well** none			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Dr. Matous Mrovec, PD Dr. habil. Thomas Hammerschmidt			
11	**Other information** Lecture notes will be provided.			

ATOMISTIC THEORY OF DEFECTS IN MATERIALS

Module code	Student work-load	Credits	Semester	Frequency	Duration
7.23	180 hours	6 ECTS	3rd	winter term	1 semester

1	**Types of courses** a) lecture b) exercises	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** a) 10 students b) 10 students

2	**Learning outcomes** Students understand the atomistic theory of crystal defects in materials, their thermodynamic and kinetic characteristics. They classify the geometry, structure and behaviour of point and spatial defects in pure materials, alloys and compounds. They are able to apply atomistic theory to interpret material behaviour and evaluate how defects govern key properties such as strength, ductility, diffusion, and phase stability. They know how temperature, composition and deformation affect the properties of defects. They can solve basic problems in materials science using atomistic simulation methods.
3	**Subject aims** • Principles of crystallography. Crystal structure of pure materials and compounds. Hierarchy of crystal defects. • Point defects in pure materials: bcc, fcc, hcp, diamond lattice. Equilibrium concentration. Point defects in compounds and alloys. Migration of point defects. Relationship with diffusion, creep and phase transitions. • Dislocations. Geometry of dislocations in various crystals. Dislocation core. Jogs and kinks of dislocation. Dislocation mobility. Link with plasticity and diffusion. Interaction of dislocation with point defects. • 2D spatial defects: GB, interface, surface. Grain boundary migration. Defects within defects. Defects in 2D crystals. Complexion transitions of spatial defects. • Atomistic mechanisms of defect migration. Correlation Effects. Chemical Diffusion. Impurity diffusion. Diffusion along the spatial defects. Ionic diffusion in Nonmetals. • Atomistic simulation methods for study of defect properties. Basic modelling tasks in materials science with focus on defect behaviour.
d4	**Teaching methods** lecture, computer exercises
5	**Prerequisites for participation** none
6	**Assessment methods** individual project and/or oral examination (0.5 hours), depending on size of class
7	**Prerequisites for the assignment of credit points** successful completion of project / passing of written examination
8	**This module is used in the following degree programmes as well** none
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** Dr. Sergei Starikov
11	**Other information** Lecture notes will be provided. Literature: G. Gottstein: Physical foundations of materials science, Springer-Verlag (2004). P.M. Anderson, J.P. Hirth and J. Lothe: Theory of dislocations, Cambridge University Press (2017).

GENERAL OPTION MODULE					
Module code 8	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 1st	**Frequency** free choice of available modules	**Duration** 1 semester

1	**Types of courses:** lecture and class	**Contact hours** 60 hrs	**Independent study** 120 hours	**Class size**
2	**Learning outcomes** By freely choosing lectures, the students can widen their skill and method spectrum according to their personal interests.			
3	**Subject aims** • Develop knowledge and skills in fields beyond engineering and science • Deepen knowledge about specific topics in Materials Science and Simulation according to own interests • Any module from a Master´s course at RUB will be recognized. Some suggested courses are listed under points 6 and 7 (Elective and Specialization Modules in MS). Courses from the RUB's main course catalogue and from the international course catalogue can be taken into account.			
4	**Teaching methods** see specific module description			
5	**Prerequisites for participation** none			
6	**Assessment methods** written or oral examination as given in specific module description			
7	**Prerequisites for the assignment of credit points** passing the examination			
8	**This module is used in the following degree programmes as well** see specific module description			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** Prof. Dr. Alexander Hartmaier			
11	**Other information** -			

INDUSTRIAL INTERNSHIP

Module code	Student workload	Credits	Semester	Frequency	Duration
8.1	180 hours	6 ECTS	3rd	Summer and winter term	1 semester

1	**Types of courses:** practical work	**Contact hours** 20 hours	**Independent study** 160 hours	**Class size** 1 student

2	**Learning outcomes** The students gain an initial insight into industrial practice, enabling them to apply the skills they have learned thus far to real-world problems. They learn about various areas of activity within a company, which allows them to assess the requirements of different tasks and use this knowledge for their own purposes, particularly in making informed career choices in a targeted manner.
3	**Subject aims** During the six week internship in a research and development department, activities must be related to one or more of the following fields: • materials design or development • materials synthesis • materials testing • materials selection in the product development process • materials processing • materials characterisation • materials simulation • materials related data science • other materials related areas
4	**Teaching methods** 6 week internship in research and development department of a materials science related company
5	**Prerequisites for participation** none
6	**Assessment methods** Written report (12-20 pages) in the common scientific format, to be handed in two weeks after the end of the six week internship
7	**Prerequisites for the assignment of credit points** Positive evaluation of the written report, internship confirmation or reference letter of employer
8	**This module is used in the following degree programmes as well** none
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** Prof. Dr. Alexander Hartmaier
11	**Other information** A workplan must be coordinated with the corresponding supervisor at RUB in advance.

DOCUMENTING AND COMMUNICATING SCIENCE 1

Module code	Student workload	Credits	Semester	Frequency	Duration
9a	90 hours	3 ECTS	1st	winter term	1 semester

1	**Types of courses:** a) lecture b) class	**Contact hours** a) 15 hrs (1 SWS) b) 15 hrs (1 SWS)	**Independent study** 60 hours	**Class size** 30 students
2	**Learning outcomes** Participants will learn how to prepare different types of scientific documents. Structural elements of different formats will be discussed. An introduction to scientific typesetting, plotting and graphic tools will be given. After successful participation, students know the basics about scientific writing and can independently • choose an appropriate format for presenting numerical data • create appealing, publication-ready graphics, figures, and tables • create structured documents using LaTeX for typesetting			
3	**Subject aims** • Structures, style, and types of scientific documents • LaTeX • Graphics and images • Assessment, structuring, and visualization scientific data			
4	**Teaching methods** Lecture and hands-on tutorials in CIP-pool			
5	**Prerequisites for participation** none			
6	**Assessment methods** Hands-on assessment in CIP pool: visualizing given scientific data and embedding, description in a LaTeX document template			
7	**Prerequisites for the assignment of credit points** Positive evaluation of the hands-on assessment			
8	**This module is used in the following degree programmes as well** none			
9	**Impact of grade on total grade** 3/117			
10	**Responsibility for module** Prof. Dr. Anna Grünebohm, Prof. Dr. Markus Stricker			
11	**Other information** -			

DOCUMENTING AND COMMUNICATING SCIENCE 2					
Module code 9b	**Student workload** 90 hours	**Credits** 3 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses:** a) lecture b) class	**Contact hours** a) 15 hrs (1 SWS) b) 15 hrs (1 SWS)	**Independent study** 60 hours	**Class size** 30 students

2	**Learning outcomes** After successful participation, students can independently • perform literature research • evaluate text from scientific journal publications w.r.t. formal scientific writing criteria, style, and information content • prepare a short written report on a scientific topic in materials science • present (oral & slides) a literature survey on a current topic in materials science.
3	**Subject aims** • Literature research, citations, quotations, copyright issues, plagiarism • Presenting and structuring a scientific topic • Oral presentation tools
4	**Teaching methods** Lecture and hands-on tutorials in CIP-pool, literature-review as independent study
5	**Prerequisites for participation** none
6	**Assessment methods** Short written report, short oral presentation
7	**Prerequisites for the assignment of credit points** Positive evaluation of the written report (literature research on an individual topic) and successful presentation of the topic during a mini symposium.
8	**This module is used in the following degree programmes as well** none
9	**Impact of grade on total grade** 3/117
10	**Responsibility for module** Prof. Dr. Anna Grünebohm, Prof. Dr. Markus Stricker
11	**Other information** -

NON-TECHNICAL ELECTIVE MODULE - RUB SOFT SKILLS/LANGUAGE COURSE					
Module code 10	**Student workload** 120 hours	**Credits** 3 ECTS	**Semester** 2nd	**Frequency** summer term free choice of available modules	**Duration** 1 semester

1	**Types of courses:** lecture and class	**Contact hours** 45 hrs	**Independent study** 75 hours	**Class size**
2	**Learning outcomes** Students broaden their knowledge base, skills, or method spectrum according to their personal interests.			
3	**Subject aims** • Develop knowledge and skills in fields beyond engineering and science • Gain and develop knowledge in non-technical subjects, related to materials engineering, like business administration according to own interests • Develop and practice communication skills			
4	**Teaching methods** see specific module descriptions			
5	**Prerequisites for participation** none			
6	**Assessment methods** written or oral examination as given in specific module description			
7	**Prerequisites for the assignment of credit points** passing the examination			
8	**This module is used in the following degree programmes as well** none			
9	**Impact of grade on total grade** ---			
10	**Responsibility for module** see specific module description			
11	**Other information** -			

MATERIALS MODELLING LAB

Module code	Student work-load	Credits	Semester	Frequency	Duration
11	180 hours	6 ECTS	1st	Winter term	1 semester

1	**Types of courses** class	**Contact hours** 45 hrs (3 SWS)	**Independent study** 135 hours	**Class size** 30 students

2	**Learning outcomes** Students are able to perform materials related computer simulations on different time and length scales. They can critically analyze the simulation results and summarize and discuss them in short written reports. They learn self-organization and time management by planning, performing and evaluating simulations along the standards of good research practice.
3	**Subject aims** The following methods will be introduced and applied for computer simulations of material behavior at various length and time scales: • Electronic structure calculations (Density Functional Theory) • Molecular Dynamics • Phasefield • Calculation of Phase Diagrams (CalPhaD) • Micromechanical simulations with the Finite Element Method • Artificial Intelligence and machine learning
4	**Teaching methods** class with practical course (computer experiments) as teamwork in teams of 2-3 students
5	**Prerequisites for participation** None
6	**Assessment methods** Oral exam (20 minutes) Group work for each experiment: entrance exam (5-10 minutes), written report (3-5 pages) and oral discussion of results (5-10 minutes) for each team
7	**Prerequisites for the assignment of credit points** Passing of oral exam and accepted written reports of all experiments; up to two experiments can be repeated.
8	**This module is used in the following degree programmes as well** none
9	**Impact of grade on total grade** 6/117
10	**Responsibility for module** Prof. Dr. Alexander Hartmaier, Dr. Oleg Shchyglo
11	**Other information** A lecture script, including instructions to the individual experiments is provided. Each experiment consists of a short introduction lecture by the supervisor, an entry exam, the computer simulation, analysis of the results, a written report and the discussion of the report with the supervisor.

RESEARCH PROJECT					
Module code 12	**Student workload** 180 hours (4 months)	**Credits** 6 ECTS	**Semester** 3rd	**Frequency** continuous offers of topics	**Duration** 1 semester

1	**Types of courses:** practical work	**Contact hours** 20 hrs	**Independent study** 160 hours	**Class size** 1-3 students
2	**Learning outcomes** The students can structure a complex research task into sub-tasks and work packages. They develop individual problem solution strategies to tackle different tasks by applying scientific methods. Students are able to report and present scientific projects.			
3	**Subject aims** Treatment of a scientific subject in a given time Scientific solution for a given practical problem Application of learned techniques from previous modules Teamwork Written presentation of the results			
4	**Teaching methods** continuous contact periods to advice the student, presentation of progress during group seminars and discussions			
5	**Prerequisites for participation** successful completion of all compulsory modules of first and second semester			
6	**Assessment methods** written report (20 to 50 pages)			
7	**Prerequisites for the assignment of credit points** positively evaluated written report			
8	**This module is used in the following degree programmes as well** none			
9	**Impact of grade on total grade** 6/117			
10	**Responsibility for module** all lecturers of the Master course			
11	**Other information** -			

MASTER THESIS									
Module code 13		**Student workload** 900 hours		**Credits** 30 ECTS	**Semester** 4th		**Frequency** continuous offers of topics		**Duration** 1 semester
1	**Types of courses:** practical work			**Contact hours** 100 hrs		**Independent study** 800 hours		**Class size** 1 student	
2	**Learning outcomes** After successful completion of the master thesis students are in a position to independently process research tasks by applying scientific methods within a predefined period of time. In particular, they are able to independently plan, organize, develop, operate and present research tasks from the field of materials science. They develop advanced problem solution strategies to tackle different tasks by applying the theoretical knowledge gained in the Master course. Students are able to report and present the progress scientific projects, to summarize their results in an oral presentation, and to write a scientific project documentation.								
3	**Subject aims** • Independent scientific project • Application of learned techniques from previous modules • Independent identification and solution of scientific problems • Literature survey • Written and oral presentation of the results								
4	**Teaching methods** continuous contact to advice the student, presentation of progress during group seminars and discussions								
5	**Prerequisites for participation** successful completion of project work (module 12) and a total of at least 80 ECTS from all modules								
6	**Assessment methods** written thesis (40 to 150 pages) 80%, assessed oral presentation 20%								
7	**Prerequisites for the assignment of credit points** positively evaluated thesis and presentation								
8	**This module is used in the following degree programmes as well** none								
9	**Impact of grade on total grade** 30/117								
10	**Responsibility for module** all lecturers of the Master course								
11	**Other information** -								