MASTERS COURSE
"MATERIALS SCIENCE AND SIMULATION"

MODULE DESCRIPTIONS

June 2023

COURSE SCHEDULE

Code	Module name	Semester					
		WH	CP	1. Sem. V Ü	2. Sem. V Ü	3. Sem. V Ü	4. Sem. V Ü
	Basic modules						
1	**Programming Concepts in Materials Science**	**4**	**6**	**2 2**			
2	**Basics in Materials Science**	**10**	**15**	**6 4**			
2a	*Elements of Microstructure*	*2*	*3*	*2*			
2b	*Introduction to Quantum Mechanics in Solid-State Physics*	*4*	*6*	*2 2*			
2c	*Statistical Mechanics and Fundamental Materials Physics*	*4*	*6*	*2 2*			
	Compulsory modules						
3	**Theoretical and Applied Materials Science**	**6**	**8**		**4 2**		
3a	*Quantum Mechanics in Materials Science*	*3*	*4*		*2 1*		
3b	*Microstructure and Mechanical Properties*	*3*	*4*		*2 1*		
4	**Advanced Characterization Methods**	**4**	**6**		**3 1**		
4a	*Advanced Characterization Methods*						
5	**Advanced Numerical Methods**	**6**	**8**			**4 2**	
5a	*Continuum Methods in Materials Science*	*3*	*4*			*2 1*	
5b	*Atomistic Simulation Methods*	*3*	*4*			*2 1*	
	Profile modules						
6	Profile module (Modelling & Simulation)	4	6		2 2		
7	Profile module (Processing & Characterization)	4	6		3 1		
8	Profile module (free choice)	4	6			2 2	
9	Profile module (free choice)	4	6			3 1	
	Optional modules						
10	General optional subject	4	6	3 1			
11	Optional scientific or engineering subject	3	4			2 1	
12	**Non-technical/non-scientific optional module**		7				
12a	*Key qualification*		*3*	x			
12b	*Key qualification*		*4*		x		
	Scientific Theses						
13	Project work (180 h)		6			x	
14	Master thesis (900 h)		30				x

	Sum Weekly Hours	**84**		**21**	**22**	**21**	**20**
	Sum Workload	**3600**		**900**	**900**	**900**	**900**
	Sum 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

Basic Modules

1 Compulsory module in numerical methods
2 Compulsory modules in materials science

Compulsory Modules

3 - 5 The compulsory modules comprise the scientific focus of the programme and are therefore mandatory for every student.

Profile Modules in Materials Science

6 Profile module 6 (MS) has to be chosen from:

- Interfaces and Surfaces (6-MS1)
- Data-driven Materials Science (6-MS2)
- Phase-field Theory and Application (6-MS3)
- Introduction to Parallel- and Scientific Computing (6-MS4)
- Continuum Mechanics (6-MS5)
- Physics of Complex Phase Transitions in Solids (6-MS6)
- The CALPHAD Method in Thermodynamics and Diffusion (6-MS7)

7 Profile module 7 (PC) has to be chosen from:

- Modern Coating Technologies (7-PC1)
- Fundamental Aspects of Materials Science and Engineering (7-PC2)
- MEMS and Nanotechnology (7-PC3)
- Polymers and Shape Memory Alloys (7-PC4)

8 - 9 Profile modules 8 and 9 can be chosen freely from:

- Multiscale Mechanics of Materials (8-MS1)
- Advanced Atomistic Simulation Methods (8-MS2)
- Computational Fracture Mechanics (8-MS3)
- Mechanical Modelling of Materials (8-MS4)
- Advanced Statistical Methods in Materials Science (8-MS5)
- Solidification Processing (9-PC1)
- Advanced Materials Processing and Microfabrication (9-PC2)
- Surface Science and Corrosion (9-PC3)
- Materials for Aerospace Applications (9-PC4)
- Introduction to 3-Dimensional Materials Characterization Techniques (9-PC5)

Optional Modules

10, 11 Module 10: Any module from any of RUB's master's programmes will be recognized.
Module 11: Any module from any of RUB's science or engineering master's programmes will be recognized.
A selection of courses offered is listed below:

- Application and Implementation of Electronic Structure Methods (10-1)
- Lattice Boltzmann Modeling: From Simple Flows to Interface Driven Phenomena (10-2)
- Theory and Application of Bond Order Potentials (10-3)
- Computational Plasticity (10-4)

- Advanced Finite Elemente Methods (10-5)
- Finite Element Methods in Linear Structural Mechanics (10-6)

- Mathematics for Materials Modelling (11-1)
- Engineering Ceramics and Coating Technology (11-2)
- Materials Informatics (11-3)

Non-technical/Non-scientific optional Module

12 These modules should be chosen from the key qualifications offers like Scientific Writing, German language for foreigners, Presentation techniques, Project and Quality Management, Business Skills, Intercultural Competence etc.

Scientific Theses

13, 14 The project work and the Master thesis represent practical self-guided research and make up 30% of all credit points.

EXAMINATIONS, CREDITS AND GRADES

Each module is assessed by one final examination, which defines the grade for this module and is the prerequisite for credit point allocation (except module 2, which consists of 3 examination elements).

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	21	14	8		43
Optional modules: 6, 7, 8, 9, 10, 11	6	12	16		34
Key qualifications: module 12	3	4			7
Project work: module 13			6		6
Master's thesis: module 14				30	30
Σ	**30**	**30**	**30**	**30**	**120**

Credits are allocated according the the following scheme:

- Compulsory 43 CP = 36%
- Optional 34 CP = 28%
- Key qualifications 7 CP = 6%
- Project report 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), 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:

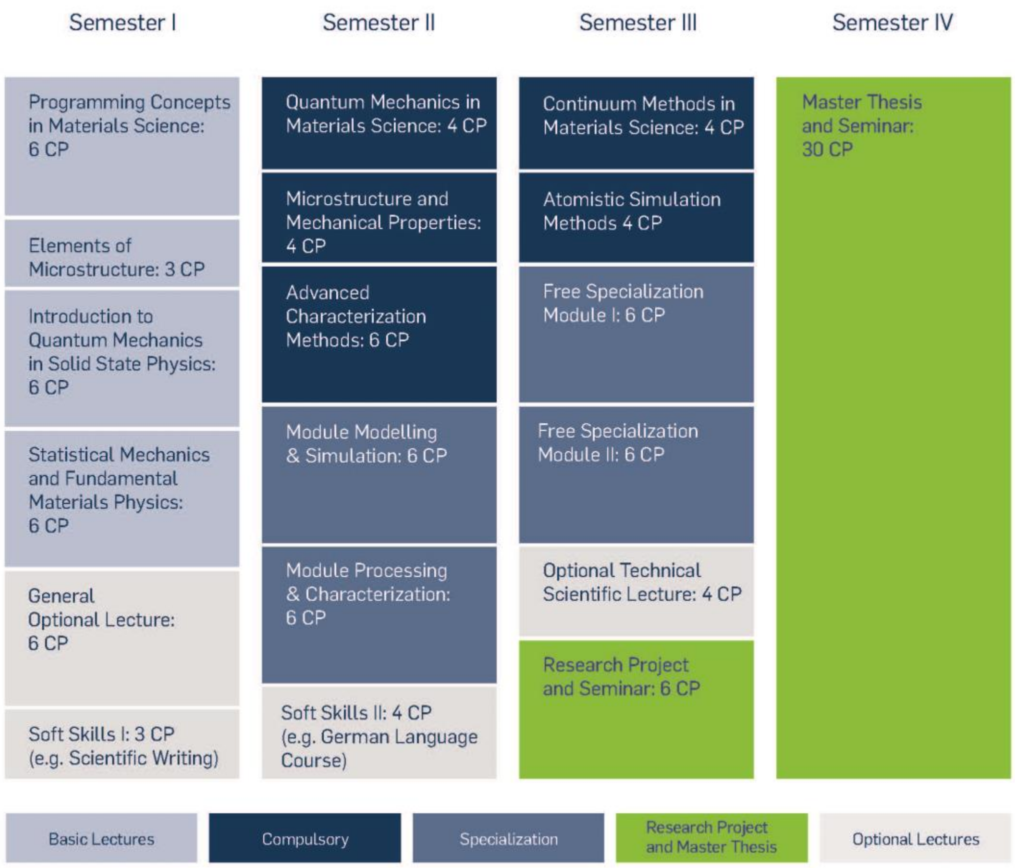
• Illness of the candidate. In this case, a doctor's certificate and, in cases of doubt, a certificate from a medical officer of the RUB must also be submitted.

• 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.

Note: If the examination for Module 2B "Introduction to Quantum Mechanics in Solid State Physics" has not yet been completed, this is considered a valid reason for deregistering from the examination for Module 3 "Theoretical and applied materials science".

MODULE SCHEME AND CREDITS



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

ALL MODULES

<table>
<tr><th colspan="9">PROGRAMMING CONCEPTS IN MATERIALS SCIENCE</th></tr>
<tr><td colspan="2">**Module code**
1</td><td>**Student workload**
180 hours</td><td>**Credits**
6 ECTS</td><td colspan="2">**Semester**
1st</td><td colspan="2">**Frequency**
winter 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) 30 hrs (2 SWS)
b) 30 hrs (2 SWS)</td><td colspan="2">**Independent study**
120 hours</td><td colspan="2">**Class size**
a) 30 students
b) 10 students</td></tr>
<tr><td>2</td><td colspan="8">**Learning outcomes**
On successful completion of this module the students recall the basic concepts of operating systems and analyse, write and test Python and Fortran90/C++ language programs of moderate complexity. Furthermore, they have the ability 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 one of the taught structured programming languages.</td></tr>
<tr><td>3</td><td colspan="8">**Subject aims**
• Introduction to operating systems (Linux and Unix)
• Introduction to modern programming languages (Python, Fortran90/C++)
• Introduction to relevant mathematical and graphical software
• Examples that will give an overview of modern programming approaches and tools will comprise:
o data interpolation and fitting
o linear algebra
o numerical integration
o theory and numerical solution of ordinary and partial differential equations
o fundamental solutions of boundary value problems</td></tr>
<tr><td>4</td><td colspan="8">**Teaching methods**
lectures, numerical exercises (class- and homework)</td></tr>
<tr><td>5</td><td colspan="8">**Prerequisites for participation**
none</td></tr>
<tr><td>6</td><td colspan="8">**Assessment methods**
final exam consists of numerical exercises (20%) and written examination (3 hours) (80%)</td></tr>
<tr><td>7</td><td colspan="8">**Prerequisites for the assignment of credit points**
passing the written examination (bonus points will be taken into account)</td></tr>
<tr><td>8</td><td colspan="8">**This module is used in the following degree programmes as well**
none</td></tr>
<tr><td>9</td><td colspan="8">**Impact of grade on total grade**
6/113</td></tr>
<tr><td>10</td><td colspan="8">**Responsibility for module**
PD Dr. habil. Thomas Hammerschmidt, Prof. Dr. Godehard Sutmann</td></tr>
<tr><td>11</td><td colspan="8">**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 Langentangen will be covered.</td></tr>
</table>

BASICS IN MATERIALS SCIENCE: ELEMENTS OF MICROSTRUCTURE

Module code	Student workload	Credits	Semester	Frequency	Duration
2a	90 hours	3 ECTS	1st	winter term	1 semester

1	**Types of courses:** Lecture	**Contact hours** 30 hrs (2 SWS)	**Independent study** 60 hours	**Class size** 30 students

2	**Learning outcomes** Students recall the basic elements of materials science and engineering in a qualitative and comprehensive way. This enables them to understand the evolution of materials microstructure during processing and service. They memorize basic facts about the solid state, about crystal defects, about thermodynamic stability, about materials kinetics and about phase transformation. They also acquire basic knowledge about materials characterization. With these basics about microstructures and their characterisation they are enabled to study and understand advanced textbooks on materials science independently.
3	**Subject aims** • Introduction to amorphous and crystalline solids • Introduction to nano, micro, and macro structures • Basics of diffraction and materials microscopy • Introduction to crystal defects (vacancies, other point defects, dislocations, interfaces) • Appreciation of precipitates, foreign phases (like oxide particles in metals or fibers in metallic or ceramic matrices), inclusions and voids • Introduction to the relation between phase diagrams and microstructures • Introduction to the relation between diffusion processes and microstructures • Introduction to the basic principles of phase transformations (solidification processes and transformations in the solid state)
4	**Teaching methods** lecture, group work
5	**Prerequisites for participation** None
6	**Assessment methods** written examination for submodule 2a (1,5 hours)
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** 3/113
10	**Responsibility for module** Prof. Dr.-Ing. Gunther Eggeler
11	**Other information** A list with recommended literature and class notes will be available online.

BASICS IN MATERIALS SCIENCE: INTRODUCTION TO QUANTUM MECHANICS IN SOLID-STATE PHYSICS

Module code	Student workload	Credits	Semester	Frequency	Duration
2b	180 hours	6 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** 120 hours	**Class size** a) 20 students b) 10 students

2	**Learning outcomes** Students will acquire a basic understanding of quantum mechanics and the necessary conceptual and mathematical background. This will enable the students to transfer knowledge gained in this course to applications in chemistry, materials science and solid-state physics. They will be able to independently analyse problems of systems in which descriptions of both particles as well as waves are relevant and they will understand the relation between the electronic structure and the properties of materials.
3	**Subject aims** • Fundamental quantum mechanics (history and Heisenberg relation) • Schrödinger equation and interpretation of wave functions • Stationary solutions (quantum wells, tunneling) • The hydrogen atom and the periodic system of elements • Electrons in a periodic potential and band formation • Harmonic oscillator and lattice vibrations • Crystallography in solid-state physics • Fundamentals of magnetism
4	**Teaching methods** lecture, class
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 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** 6/113
10	**Responsibility for module** Prof. Dr. Ralf Drautz
11	**Other information** Lecture notes will be provided.

BASICS IN MATERIALS SCIENCE: STATISTICAL MECHANICS AND FUNDAMENTAL MATERIALS PHYSICS

Module code	Student workload	Credits	Semester	Frequency	Duration
2c	180 hours	6 ECTS	1st	winter 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) 20 students
2	**Learning outcomes** Students are able to describe the basic concepts of mechanical behaviour of materials. They gain an overview on the different mechanical properties and their assessment methods, including the microstructural strengthening mechanisms of materials. They understand the definition of mechanical equilibrium and are able to apply it to solve simple problems. They also memorize basic thermodynamic concepts for phase stability and liquid-solid or solid-solid phase transformations, as Maxwell relations and phase diagrams. The students can apply statistical methods to connect physical quantities such as temperature, hydrostatic pressure and stress tensor to atomic and molecular features. They memorize approximate microscopic models and can apply them to describe heat capacity, electric conductivity, mechanical properties and magnetism. On the mesoscopic side, they can employ variational approaches to examine phase separation and domain growth.			
3	**Subject aims** • Introduction to mechanical properties of materials and their assessment methods • Microscopic origin of plastic deformation and fracture • Thermodynamical concepts to describe phase equilibria and phase transformations in liquid and solid states • Introduction to functional (electrical, magnetic, optical) properties of materials • Introduction to probability theory and statistical ensembles • Classical and quantum statistics (Boltzmann, Fermi and Bose-Einstein) • Heat capacity of crystalline solids (Debye theory) • Magnetism (para-magnetism and mean field theory of ferro-magnetism)			
4	**Teaching methods** lecture, group work			
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 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** 6/113			
10	**Responsibility for module** Prof. Dr. Alexander Hartmaier, 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.			

THEORETICAL AND APPLIED MATERIALS SCIENCE: QUANTUM MECHANICS IN MATERIALS SCIENCE

Module code	Student workload	Credits	Semester	Frequency	Duration
3a	120 hours	4 ECTS	2nd	summer term	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** 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

successful completion of "Introduction to Quantum Mechanics in Solid State Physics" or equivalent course.

6 Assessment methods

written examination (together with submodule 3b; 3 hours for entire module 3).

7 Prerequisites for the assignment of credit points

Passing the written examination and successful participation in exercise classes (achieving min. 50% of points from exercise sheets and presenting the solution for at least one exercise in class).

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

None

9 Impact of grade on total grade

4/113

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.

THEORETICAL AND APPLIED MATERIALS SCIENCE: MICROSTRUCTURE AND MECHANICAL PROPERTIES					
Module code 3b	**Student workload** 120 hours	**Credits** 4 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) 15 hrs (1 SWS)	**Independent study** 75 hours	**Class size** a) 30 students b) 10-15 students
2	**Learning outcomes** The students understand the definitions of mechanical equilibrium and are able to apply it to simple problems. Based on this understanding they are able to implement and to apply a simple Finite Element code for elastic problems. They learn and understand the basics of continuum plasticity and can motivate classical plasticity models from microstructural principles. Based on this understanding, the students are able to discuss the correlation between microstructure and mechanical properties of materials and they develop the skills to apply this knowledge to materials science problems.			
3	**Subject aims** • Mechanical equilibrium definitions • Basics of the Finite Element Method/Implementation of Finite Element code in Matlab • Continuum plasticity and transition to micromechanics • Microstructural mechanisms and microscopic descriptions of mechanical properties of materials • Length scales in materials (phases, grain boundaries, defect densities) • Hardening mechanisms (grain boundary, dislocation, solid solution and precipitation hardening) • Micromechanical modelling of material properties			
4	**Teaching methods** lecture, class			
5	**Prerequisites for participation** successful completion of “Basics in Materials Science” (3a, 3b, 3c) or equivalent courses.			
6	**Assessment methods** written examination (together with submodule 3a; 3 hours for entire module 3). 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** 4/113			
10	**Responsibility for module** Prof. Dr. Markus Anthony Stricker			
11	**Other information** Lecture notes are provided online. 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 4	**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) 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” (2a) 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** 6/113			
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.			

ADVANCED NUMERICAL METHODS: CONTINUUM METHODS IN MATERIALS SCIENCE					
Module code 5a	**Student workload** 120 hours	**Credits** 4 ECTS	**Semester** 3rd	**Frequency** winter term	**Duration** 1 semester

1	**Types of courses:** a) lecture b) numerical exercises	**Contact hours** a) 30 hrs (2 SWS) b) 15 hrs (1 SWS)	**Independent study** 75 hours	**Class size** a) 30 students b) 10 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) • Introduction to the Finite Element/Finite Volume Method in solid mechanics as method to solve BVP • CALPHAD thermodynamics and kinetics of multicomponent diffusion • Mean field models of microstructure evolution • Rate equations for precipitation including numerical integration • Introduction to free boundary problems • Thermodynamic concept of the Phase-field method • Linking of microstructure and mechanical properties			
4	**Teaching methods** lecture, numerical exercises			
5	**Prerequisites for participation** background in mechanical engineering, physics or related discipline			
6	**Assessment methods** written examination together with submodule 5b (3 hours for entire module 5). 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** 4/113			
10	**Responsibility for module** Prof. Dr. Ingo Steinbach			
11	**Other information** Lecture notes are provided online.			

ADVANCED NUMERICAL METHODS: ATOMISTIC SIMULATION METHODS

Module code	Student workload	Credits	Semester	Frequency	Duration
5b	120 hours	4 ECTS	3rd	winter term	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** 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 “Theoretical and Applied Materials Science”(Module 3) is recommended			
6	**Assessment methods** written examination together with submodule 5a (3 hours for entire Module 5). 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** 4/113			
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.			

INTERFACES AND SURFACES

Module code	Student workload	Credits	Semester	Frequency	Duration
6-MS1	180 hours	6 ECTS	2nd	summer 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** 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** 6/113
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					
Module code 6-MS2	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 2nd	**Frequency** summer term	**Duration** 1 semester

1	**Types of courses:** a) lectures b) hands-on practical studies	**Contact hours** a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** a) 20 students b) 20 students
2	**Learning outcomes** After participating in the module students will: know and understand common data-driven methods (supervised and unsupervised learning, deep learning) be able to estimate limitations and applicability of these methods in context of materials science and select the proper methods for particular applications. be able to write Python code to implement and apply these methods be able to organize and manipulate the data more efficiently			
3	**Subject aims** • Overview and taxonomy of data science • Supervised learning, regression and classification • Unsupervised learning, clustering, dimensionality reduction • Data storage and organization, ontologies, databases of relevance in materials science • Design and management of SQL and noSQL databases • Data visualization and reporting • Image and text mining • Python tools and libraries for data science • Multi-purpose notebooks for interactive data analytics			
4	**Teaching methods** lectures and hands-on computer classes			
5	**Prerequisites for participation** Basic knowledge in materials science, basic knowledge in Python. Completion of “Statistical methods in data analysis and design of experiments” recommended.			
6	**Assessment methods** successful completion of project work, written project report			
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** 6/113			
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); K. Rajan (Editor): Informatics for Materials Science and Engineering, Butterworth-Heinemann (2013); 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).			

PHASE-FIELD THEORY AND APPLICATION

Module code	Student workload	Credits	Semester	Frequency	Duration
6-MS3	180 hours	6 ECTS	2nd	summer 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) 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** 6/113			
10	**Responsibility for module** Prof. Dr. Ingo Steinbach, Prof. Dr. Fathollah Varnik, Dr. Oleg Shchyglo			
11	**Other information** Lecture notes will be provided online.			

INTRODUCTION TO PARALLEL- & SCIENTIFIC-COMPUTING

Module code	Student workload	Credits	Semester	Frequency	Duration
6-MS4	180 hours	6 ECTS	2nd	summer term	1 semester

1	**Types of courses:** lecture	**Contact hours** 60 hrs (4 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** 6/113
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.

CONTINUUM MECHANICS

Module code	Student workload	Credits	Semester	Frequency	Duration
6-MS5	180 hours	6 ECTS	2nd	summer 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** 120 hours	**Class size** a) 10 students b) 10 students

2 Learning outcomes

Extended knowledge in continuum-mechanical modeling and solution techniques as a prerequisite for computer-oriented structural analysis. After successfully completing the module, the students will

- possess extended knowledge of continuum mechanics
- be able to formulate problems of structural and material mechanics within the framework of continuum mechanics
- have mastered solution techniques for mechanical problems as a prerequisite for computer-oriented analysis
- be able to create mathematical models for engineering systems and processes
- be able to interpret modeling results and revise models accordingly.

3 Subject aims

Starting with an introduction to the advanced analytical techniques of linear elasticity theory, the course moves on to the continuum-mechanical concepts of the nonlinear elasticity and ends with the discussion of material instabilities and microstructures. Numerous examples and applications will be given.

- Advanced Linear Elasticity
- Beltrami equation, Navier equation
- Stress-functions
- Scalar- and vector potentials
- Galerkin-vector, Love-function
- Solution of Papkovich - Neuber
- Nonlinear Deformation
- Strain tensor, stress-tensors
- Polar decomposition
- Equilibrium, strain-rates
- Nonlinear Elastic Materials
- Covariance and isotropy
- Hyperelastic materials, constrained materials, hypoelastic materials
- Objective rates, material stability, microstructures

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

Master of Science Computational Engineering (Import lecture)

9 Impact of grade on total grade

6/113

10 Responsibility for module

Prof. Dr. rer. nat. Klaus Hackl

11 Other information

Literature: P.C. Chou, N.J. Pagano: Elasticity: Tensor, dyadic, and engineering approaches, Dover (1997); T.C. Doyle, J.L. Ericksen: Nonlinear elasticity. Advances in appl. mech. IV, Academic Press (1956); C. Truesdell, W. Noll: The nonlinear field theories of mechanics, Springer (2004); Handbuch der Physik (Flügge, Hrsg.), Bd. III/3, Springer-Verlag (1965); J.E. Marsden, T.J.R. Hughes: Mathematical foundation of elasticity, Prentice Hall (1983); R.W. Ogden: Nonlinear elastic deformation, Wiley & Sons (1984).

PHYSICS OF COMPLEX PHASE TRANSITIONS IN SOLIDS					
Module code 6-MS6	**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** 6/113			
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 6-MS7	**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** 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** 6/113
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).

MODERN COATING TECHNOLOGIES					
Module code 7-PC1	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 3rd	**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) 40 students b) 40 students

2	**Learning outcomes** Students have gained insight into the art of thin films science and technology and broadened their knowledge in disciplines such a materials processing. The focus is on processing of functional materials especially in use for microelectronics, optoelectronics, catalysis etc. Successful students understand the basic techniques and fundamental processes of thin film deposition and are able to select the most appropriate film deposition process to achieve a desired outcome for specific applications. In addition, state-of-the art technologies are discussed with representative materials examples, especially using physical and chemical vapour deposition techniques.
3	**Subject aims** • Physical and chemical routes to thin film fabrication: evaporation, sputtering, pulsed laser deposition (PLD), molecular beam epitaxy (MBE), chemical vapour deposition (CVD), atomic layer deposition (ALD), sol-gel process, plasma deposition process etc. • Fundamental process during film deposition: adsorption, surface diffusion, nucleation, growth and microstructure development, defects, epitaxy, mechanism (using relevant theory and models) • Material types with characteristic examples (emphasis on fundamentals and applications of each technique) • Thin film properties and characterization • Process control and industrial applications (case studies)
4	**Teaching methods** lecture, class, seminar, guest lectures
5	**Prerequisites for participation** background in physics, chemistry, or materials science
6	**Assessment methods** written examination (1,5 hours) and presentation of seminars
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** 6/113
10	**Responsibility for module** Prof. Dr. Anjana Devi
11	**Other information** Lecture notes will be provided online.

FUNDAMENTAL ASPECTS OF MATERIALS SCIENCE AND ENGINEERING (FAMSE)

Module code	Student workload	Credits	Semester	Frequency	Duration
7-PC2	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) 10 students b) 10 students
2	**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.			
3	**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)			
4	**Teaching methods** lecture, class			
5	**Prerequisites for participation** successful completion of “Elements of Microstructure” (2a) and “Statistical Mechanics and Fundamental Materials Physics” (2c) recommended			
6	**Assessment methods** oral examination (0.5 hours)			
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- und Microengineering			
9	**Impact of grade on total grade** 6/113			
10	**Responsibility for module** Prof. Dr.-Ing. Gunther Eggeler			
11	**Other information** A list with recommended literature and class notes will be available online.			

MEMS & NANOTECHNOLOGY					
Module code 7-PC3	**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** 90 hours	**Class size** a) 10 students b) 10 students
2	**Learning outcomes / Lernergebnisse/Kompetenzen** • Die Studierenden verstehen die Konzepte, Fertigungsverfahren und kennen die Werkstoffe und Besonderheiten von mikrofluidischen Mikrosystemen und BioMEMS. • Die Studierenden kennen und verstehen die Konzepte und Fertigungsverfahren von Nanomaterialien und Nanosystemen • Sie können Nanoobjekte unterscheiden und können Charakterisierungsmethoden für die unterschiedlichen Nanoobjekte bewerten • Sie können Prozessabläufe für die Entwicklung von Mikro- und Nanosystemen entwerfen. • Im Rahmen der Übungen praktizieren die Studierenden wissenschaftliches Lernen und Denken und übertragen die Erkenntnisse/Fertigkeiten auf konkrete und neue Problemstellungen.			
3	**Subject aims / Inhalte** • Das Modul MEMS & Nanotechnologie vermittelt vertiefte Kenntnisse über den Einsatz von Mikrosystemen in aktuellen Gebieten der Ingenieurtechnik und der biomedizinischen Technik sowie über die Konzepte, Methoden und Werkstoffe der Nanotechnologie. • Einführung in aktuelle Gebiete der wissenschaftlichen Forschung in unterschiedlichen Bereichen des Micro-Engineering (MEMS, BioMEMS) mit besonderem Blick auf die ingenieursgemäße Umsetzung der Ergebnisse in technische und biomedizintechnische Anwendungen • Überblick zu Konzepten und Technologien des Micro-Engineering • Schnittmengen zwischen Technik und Biologie (Biosensorik, Bionik, Biomimetik) • Relevante Grundlagen der Biologie und der biomedizinischen Technik • Konzepte der Nanotechnologie (u.a. “bottom up”, “top down”) • Methoden zur Herstellung und Charakterisierung nanoskaliger Systeme • Nanoskalige Werkstoffe (z.B. Carbon Nanotubes, Nanopartikel) • Nanostrukturierte Oberflächen (z.B. mittels GLAD hergestellte Nanosäulen) • Anwendungen aus dem Bereich Nanotechnologie			
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** Master of Science in Mechanical Engineering: Werkstoff-Engineering			
9	**Impact of grade on total grade** 6/113			
10	**Responsibility for module** Prof. Dr. Alfred LudwigLie			
11	**Other information** The lecture will be held in German language.			

POLYMERS AND SHAPE MEMORY ALLOYS

Module code	Student workload	Credits	Semester	Frequency	Duration
7-PC4	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) 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” (2a) 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** 6/113
10	**Responsibility for module** Dr. Klaus Neuking, Prof. Dr.-Ing. Jan Frenzel
11	**Other information** Lecture notes will be provided.

MULTISCALE MECHANICS OF MATERIALS

Module code	Student workload	Credits	Semester	Frequency	Duration
8-MS1	180 hours	6 ECTS	3rd	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** 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** 6/113
10	**Responsibility for module** PD Dr. habil. Rebecca Janisch
11	**Other information** Lecture notes will be provided.

<table>
<tr><th colspan="6">ADVANCED ATOMISTIC SIMULATION METHODS</th></tr>
<tr><td>Module code
8-MS2</td><td>Student workload
180 hours</td><td>Credits
6 ECTS</td><td>Semester
3rd</td><td>Frequency
winter term</td><td>Duration
1 semester</td></tr>
</table>

<table>
<tr><td>1</td><td>Types of courses:
a) lecture
b) classes focusing on hands-on computational tasks</td><td>Contact hours
a) 30 hrs (2 SWS)
b) 30 hrs (2 SWS)</td><td>Independent study
120 hours</td><td>Class size
20 students</td></tr>
<tr><td>2</td><td colspan="4">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.</td></tr>
<tr><td>3</td><td colspan="4">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</td></tr>
<tr><td>4</td><td colspan="4">Teaching methods
lecture, exercises</td></tr>
<tr><td>5</td><td colspan="4">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.</td></tr>
<tr><td>6</td><td colspan="4">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.</td></tr>
<tr><td>7</td><td colspan="4">Prerequisites for the assignment of credit points
passing the exam (bonus points will be taken into account)</td></tr>
<tr><td>8</td><td colspan="4">This module is used in the following degree programmes as well
none</td></tr>
<tr><td>9</td><td colspan="4">Impact of grade on total grade
6/113</td></tr>
<tr><td>10</td><td colspan="4">Responsibility for module
Prof. Dr. Anna Grünebohm and Dr. Matous Mrovec</td></tr>
<tr><td>11</td><td colspan="4">Other information</td></tr>
</table>

COMPUTATIONAL FRACTURE MECHANICS					
Module code 8-MS3	**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 failue 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 diffent types of fracture models, to study the relevant literature independently. On an engineering level, the students are able to 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-plstic fracture mechanics • R curve behavior of materials • Concepts of cohesive zones (CZ), extended finite elements (XFEM) and damage mechanics • Finite element based fracture simulations for static and dynamic cracks • Application to brittle fracture & ductile failure for different geometries and loading situations			
4	**Teaching methods** lecture, seminar, computer simulations (guided and independent)			
5	**Prerequisites for participation** basic knowledge about solid mechanics and plasticity (e.g. by module 3b or equivalent)			
6	**Assessment methods** written examination (2 hours, 90%), evaluation of independent computer models (10 %)			
7	**Prerequisites for the assignment of credit points** passing the written exam			
8	**This module is used in the following degree programmes as well** Computational Engineering, Master course: Maschinenbau			
9	**Impact of grade on total grade** 6/113			
10	**Responsibility for module** Prof. Dr. Alexander Hartmaier			
11	**Other information** Lecture notes will be provided.			

MECHANICAL MODELLING OF MATERIALS					
Module code 8-MS4	**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) 5 students b) 5 students
2	**Learning outcomes** On successful completion of the MMM module, students will be able to: • analyse and understand different classes of engineering materials and correctly formulate the constitutive models for each class of materials, • select appropriate material models for every specific class of engineering materials with the view of making engineering structures more economic, • implement modified material models in finite element software to enable advanced finite element simulations of new engineering problems.			
3	**Subject aims** • Basic concepts of continuum mechanics (introduction) • Mechanical characterization of materials (mainly solids) • Basic concepts of constitutive equations for engineering materials • Classical (1-dimensional) models of elastic and inelastic materials • Boundary value problems of linear elasticity • Basic problems of inelastic behavior of materials (viscoelasticity, plasticity and damage) • Basic concepts of strength and failure of engineering materials			
4	**Teaching methods** lecture, class			
5	**Prerequisites for participation** basic knowledge in mathematics and mechanics (statics, dynamics and strength of materials)			
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 Course: Computational Engineering (Import lecture)			
9	**Impact of grade on total grade** 6/113			
10	**Responsibility for module** Prof. Dr.-Ing. Daniel Balzani			
11	**Other information** Literature: R. Lakes: Viscoelastic materials. Cambridge University Press (2009); R.M. Christensen: Theory of viscoelasticity. Academic Press, New York (1971); El.H. Dill: Continuum mechanics: Elasticity, plasticity, viscoelasticity. CRC Press (2007); Y.C. Fung: A first course in continuum mechanics. Englewood Cliffs, N.J., Prentice-Hall, Inc. (1977).			

ADVANCED STATISTICAL METHODS IN MATERIALS SCIENCE

Module code	Student work-load	Credits	Semester	Frequency	Duration
8-MS5	180 hours	6 ECTS	3rd	winter term	1 semester

	Types of courses	Contact hours	Independent study	Class size
1	a) lecture b) practical hands-on with Python and Jupyter notebook	a) 30 hrs (2 SWS) b) 30 hrs (2 SWS)	120 hours	a) 15 students b) 15 students

2 Learning outcomes

After participating in the module students will:

- know a variety of uncertainty indication methods and their limitations and applicability.
- be able to use active learning and Bayesian optimization methods in general and in application to materials properties optimization in particular,
- be able to construct deep generative models for materials properties generation.
- be able to assess limitations and applicability of these methods and select proper methods for particular tasks.
- will be able to write Python code to implement and use above-mentioned methods.

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)
- Data organization and storage

4 Teaching methods

lecture, including hands-on lectures and classes with hands-on computer exercises

5 Prerequisites for participation

Participation in “Data-driven materials science” course is recommended

6 Assessment methods

successful completion of project work, written project report

7 Prerequisites for the assignment of credit points

evaluation of project work above minimal threshold

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

none

9 Impact of grade on total grade

6/113

10 Responsibility for module

Prof. Dr. Hartmaier, 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);

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)

SOLIDIFICATION PROCESSING					
Module code 9-PC1	**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) 30 students b) 30 students
2	**Learning outcomes** Students know about different casting technologies like sand casting, continuous casting, investment casting, pressure die casting and miscellaneous advanced casting processes and memorize cases of their application and specific characteristics. Additionally, the causes of casting defects and strategies to avoid defects are understood. Students can relate casting microstructures to process conditions and are familiar with the principles of alloy thermodynamics and solidification. From the practical exercises, students are memorize different simulation tools for casting and solidification processes.			
3	**Subject aims** • History of metal casting, field of application and economic importance • Shape-, pressure-, die-, continuous-, and precision casting • Directional solidification, rapid solidification, rheo- and thixo casting • Mold material, molding and recycling • Mold filling and heat transfer (radiation and conduction) • Simulation of mold filling, solidification and casting microstructure • During the exercises, practical casting and microstructure analysis is demonstrated in the laboratory and during excursions to different foundries specialized on different casting techniques. The use of commercial software products for casting and microstructure evolution simulation is demonstrated and trained on the computer.			
4	**Teaching methods** lecture, classes			
5	**Prerequisites for participation** Bachelor degree in mechanical engineering, physics or similar			
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** 6/113			
10	**Responsibility for module** Prof. Dr. Ingo Steinbach			
11	**Other information** Literature: W. Kurz, D. Fisher: Fundamentals of solidification, Trans Tech Publications (1998); D. Stephanescu: Science and engineering of casting solidification, Springer (2008).			

ADVANCED MATERIALS PROCESSING AND MICROFABRICATION					
Module code 9-PC2	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 3rd	**Frequency** winter term	**Duration** 1 semester

1	**Types of courses:** a) lecture (German) b) class (German)	**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

After successful completion of the module, the students are able to,

- apply the Calphad method independently to materials engineering problems and correlate the calculated results with experimental data.
- establish connections between the basics of thermodynamics of multi-material systems, thermodynamic calculations and materials engineering processes using the example of metallic elements and alloys.
- evaluate and select special manufacturing technology processes for applications in research and industrial manufacturing with regard to their advantages and disadvantages.
- design and plan new material systems and manufacturing processes through cooperation in small groups on a theoretical basis.
- understand the importance of interface-dominated materials
- select and assess processes for surface modification as well as micro and nano technology.

3 Subject aims

The course contents are divided into the lecture and the accompanying exercise. They are summarized below according to these teaching formats.

Lecture

- Introduction to the Calphad method (Calculation of Phase Diagrams).
- Theoretical principles and use of a Calphad program.
- Theoretical consideration of solidification processes in thermodynamic equilibrium and based on the Scheil-Gulliver model.
- Linking theoretical approaches with application examples from current materials research and industrial practice, including:
- Solidification Structure and Heat Treatment of Ni-based Superalloys
- Multiphase Steels (e.g. DP and TRIP steels)
- Hydrogen Environment Embrittlement
- High Interstitial Steels
- High Entropy Alloys
- Super-Solidus Liquid Phase Sintering
- Thixotropic Shaping
- Thermophysical Properties of Metallic Materials
- Powder Metallurgy of High Alloyed Steels
- Additive Manufacturing
- Multistep Heat Treatment Processes
- Multiphase Equilibria in Novel High-speed Steels
- Property Distribution Mapping
- Possibilities and limits of the use of thermodynamic equilibrium calculations in materials research.
- Basic concepts and processes of micro and nano technology
- Advanced and special method of materials processing
- Interface dominated high-performance materials

Exercise

In the course of the exercise, there is first a practical introduction to the use of Calphad software. Subsequently, simple exercises (e.g. Fe-Fe_3C phase diagram) are calculated by the students independently, supported by the lecturer. More complex application examples from the lecture are worked on by the students as far as possible independently in small groups and on the basis of prepared tasks. In the same way, an introduction to a software for calculating diffusion processes in

	metallic multi-component systems is given. Here, too, an introduction with simple exercises (e.g. Darken experiment) is given first, followed by more complex questions with a direct reference to the contents of the lecture. During the exercise, the small groups prepare a short documentation during the semester, which is then discussed in the plenary.
4	**Teaching methods** Lecture Exercises on the PC in small groups (2-3 students) Moderated Moodle course with interactive elements for self-study Language: **German**
5	**Prerequisites for participation** none
6	**Assessment methods** written examination (3 hours)
7	**Prerequisites for the assignment of credit points** Successful completion of the MAP (written examination) Completion of an exercise with short documentation (academic performance)
8	**This module is used in the following degree programmes as well** None
9	**Impact of grade on total grade** 6/113
10	**Responsibility for module** Prof. Dr.-Ing. Sebastian Weber (Responsibility & Teaching) Prof. Dr.-Ing. Alfred Ludwig (Teaching)
11	**Other information** The use of the Calphad method is taught using the "ThermoCalc" software, supplemented by the solution of diffusion problems in metallic multi-component systems using the "Dictra" simulation software.

SURFACE SCIENCE AND CORROSION

Module code	Student workload	Credits	Semester	Frequency	Duration
9-PC3	180 hours	6 ECTS	3rd	winter 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) 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** 6/113
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 9-PC4	**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) 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** 6/113			
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 9-PC5	**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** -			
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** 6/113			
10	**Responsibility for module** Prof. Dr. Tong Li			
11	**Other information** -			

GENERAL OPTIONAL SUBJECT					
Module code 10	**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 will be recognized. Some suggested courses are listed in the following as modules 10-1 to 10-6			
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** 6/113			
10	**Responsibility for module** see specific module description			
11	**Other information**			

APPLICATION AND IMPLEMENTATION OF ELECTRONIC STRUCTURE METHODS					
Module code 10-1	**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** 6/113			
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	Student work-load	Credits	Semester	Frequency	Duration
10-2	180 hours	6 ECTS	3rd	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) 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** 6/113
10	**Responsibility for module** Prof. Dr. Fathollah Varnik
11	**Other information** Lecture notes will be provided.

THEORY AND APPLICATION OF BOND ORDER POTENTIALS					
Module code 10-3	**Student work-load** 180 hours	**Credits** 6 ECTS	**Semester** 1st/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** After participating in the module, students are able to understand fundamental physical concepts of approximate electronic structure methods such as tight binding and bond order potentials (BOPs). They are able to carry out atomistic simulations for various materials using these methods and analyze and interpret the outcomes.			
3	**Subject aims** • Tight-binding approximation • Lanczos algorithm and Greens functions • Recursion method and continued fraction, terminators • Numerical BOP • Analytic BOP • Kernel-polynomial method • Onsite-levels and self-consistency • Magnetism, charge-transfer • Forces • Parameterization and validation • Applications			
d4	**Teaching methods** lecture, computer exercises, seminars			
5	**Prerequisites for participation** completion of module 2 or equivalent			
6	**Assessment methods** individual project and/or oral (0.5 hours) examination, depending on the size of the class			
7	**Prerequisites for the assignment of credit points** successful completion of the project/passing the exam			
8	**This module is used in the following degree programmes as well** none			
9	**Impact of grade on total grade** 6/113			
10	**Responsibility for module** Dr. Matous Mrovec, PD Dr. habil. Thomas Hammerschmidt			
11	**Other information** Lecture notes will be provided.			

COMPUTATIONAL PLASTICITY

Module code	Student workload	Credits	Semester	Frequency	Duration
10-4	180 hours	6 ECTS	2nd	summer term	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 the classifications of mechanical behavior and to which materials the different types of behavior can be associated. 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 can discuss the basic concepts of the numerical implementation of plasticity models and can identify the method which is most suited to solve a given mechanical problem. Students are able to implement and apply a numerical scheme for the solution of elasto-plastic problems within the finite element method and are able to review the use of homogenization methods to describe plasticity in polycrystals.
3	**Subject aims** • Basics of continuum mechanics and FEM • 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) • Plasticity of polycrystals (Sachs, Taylor and self-consistent model) • Numerical solution schemes of the crystal plasticity method • Structure, implementation and application of an Abaqus UMAT
4	**Teaching methods** lecture (2h/week), exercises (2h/week) / team project incl. Seminar talk/English
5	**Prerequisites for participation** none
6	**Assessment methods** Portfolio exam including report on project and seminar
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** 6/113
10	**Responsibility for module** Prof. Dr. Alexander Hartmaier
11	**Other information**

ADVANCED FINITE ELEMENT METHODS

Module code	Student workload	Credits	Semester	Frequency	Duration
10-5	180 hours	6 ECTS	2nd	summer 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) 30-40 students b) 30-40 students

2	**Learning outcomes** This course enables students to numerically solve nonlinear problems in engineering sciences by providing the methodological basis of the geometrically and physically nonlinear finite element method. The successful student can apply the basics of the Advanced Finite Element Methods in seminar papers and is able to solve nonlinear structural-mechanical problems by means of hand calculations. Furthermore the students are able to program and validate problems in geometrically and physically nonlinear structural analysis.
3	**Subject aims** • Non-linear continuum mechanics • The weak form, consistent linearization and finite element discretization of non-linear elastomechanics and elastodynamics • One-dimensional spatial truss elements • The principles of the formulation of geometrically nonlinear finite elements. Overview on nonlinear constitutive models including elasto-plastic and damage models • Algorithms to solve the resulting non-linear equilibrium equations by load- and arc-length controlled Newton-type iteration schemes • Application of the non-linear finite element method non-linear stability analysis of structures • Exercises to demonstrate the application of the non-linear finite element method for the solution of selected examples • Practical applications of the non-linear finite element method demonstrated by means of a commercial finite element programme.
4	**Teaching methods** lecture, class, homework
5	**Prerequisites for participation** basics in mathematics, mechanics and structural analysis; finite element methods in linear structural mechanics
6	**Assessment methods** written examination (2 hours). Bonus points can be gained by submitting solutions to the homework distributed during 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** Master of Science in Computational Engineering
9	**Impact of grade on total grade** 6/113
10	**Responsibility for module** Prof. Dr. Günther Meschke
11	**Other information** Lecture notes will be provided as printed manuscript. Recommended Literature: Manuscript and Lecture notes T. Belytschko and W.K. Liu: Nonlinear finite elements for continua and structures, Wiley (2000); O.C. Zienkiewicz, R.L. Taylor: The finite element method for solid and structural mechanics, Elsevier (2005).

FINITE ELEMENT METHODS IN LINEAR STRUCTURAL MECHANICS					
Module code 10-6	**Student workload** 180 hours	**Credits** 6 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) 30 hrs (2 SWS)	**Independent study** 120 hours	**Class size** a) 30-40 students b) 30-40 students
2	**Learning outcomes** This course enables students to numerically solve linear engineering problems by providing a sound methodological basis of the finite element method. Students can apply the method to numerical analysis of trusses, beams and plates, and also analyses of transport processes such as heat conduction. In seminar papers the students shall apply the basics of the Linear Finite Element Methods and solve structural-mechanical problems by means of hand calculations. Furthermore, the students are able to independently implement corresponding user-defined elements in FE programs and perform numerical analyses of beam and shell structures.			
3	**Subject aims** • Introduction to the finite element method in the framework of linear elastomechanics and elastodynamics • Step by step explanation of principles of spatial discretization using the finite element method. • One-dimensional isoparametric truss elements and development of two- (plane stress and plane strain) and three-dimensional isoparametric finite elements for linear structural mechanics • Application of the finite element method to the spatial discretization of problems associated with transport processes within structures (e.g. heat conduction, coupled problems) is demonstrated • Finite element models for beams and plates • Aspects of element locking and possible remedies and practical application of the finite element method for the solution of selected examples.			
4	**Teaching methods** lecture, class, homework			
5	**Prerequisites for participation** basics in mathematics, mechanics and structural analysis			
6	**Assessment methods** written examination (3 hours). Bonus points can be gained by submitting solutions to the homework distributed during 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** Master of Science in Computational Engineering			
9	**Impact of grade on total grade** 6/113			
10	**Responsibility for module** Prof. Dr. Günther Meschke			
11	**Other information** Lecture notes will be provided as online manuscript. Recommended Literature: Manuscript and Lecture Notes; J. Fish and T. Belytschko: A first course in finite elements, Wiley (2007); K.-J. Bathe: Finite element procedures, Prentice Hall (1996); T.J.R. Hughes: The finite element method. Linear static and dynamic finite element analysis, Prentice Hall (1987); O.C. Zienkiewicz, R.L. Taylor, The finite element method. Part I: Basis and fundamentals, Elsevier Science & Technology (2005).			

OPTIONAL SCIENTIFIC OR ENGINEERING SUBJECT					
Module code 11	**Student workload** 120 hours	**Credits** 4 ECTS	**Semester** 3rd	**Frequency** free choice of available modules	**Duration** 1 semester

1	**Types of courses:** lecture and class	**Contact hours** 40 hrs	**Independent study** 80 hours	**Class size**
2	**Learning outcomes** Students broaden their skill or method spectrum and set an individual focus to their curriculum matching their personal interests.			
3	**Subject aims** • Deepen knowledge about specific topics in Materials Science and Simulation according to own interests • Any module from engineering or science master´s courses will be recognized.			
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** 4/113			
10	**Responsibility for module** see specific module description			
11	**Other information**			

MATHEMATICS FOR MATERIALS MODELLING					
Module code 11-1	**Student workload** 120 hours	**Credits** 4 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) 15 hrs (1 SWS)	**Independent study** 75 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** 4/113			
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.			

ENGINEERING CERAMICS & COATING TECHNOLOGY

Module code	Student workload	Credits	Semester	Frequency	Duration
11-2	120 hours	4 ECTS	2nd	summer term	1 semester

	Types of courses:	Contact hours	Independent study	Class size
1	a) lecture b) class	a) 30 hrs (2 SWS) b) 15 hrs (1 SWS)	75 hours	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
5	**Prerequisites for participation** knowledge in materials properties is recommended.
6	**Assessment methods** oral examination (20 minutes) or written examination (90 min.)
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** 4/113
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.

MATERIALS INFORMATICS					
Module code 11-3	**Student workload** 120 hours	**Credits** 4 ECTS	**Semester** 3rd	**Frequency** winter term	**Duration** 1 semester

1	**Type(s) of course(s):** seminar	**Contact hours** 45 hrs (3 SWS)	**Independent study** 75 hours	**Class size** 10 students
2	**Learning outcomes** After successful participation in the module, students are able to read a scientific article and to put its content in the context of current literature. They can analyse the presented approach, contrast it with other, similar articles, and assess the novelty of its contribution to the field of 'Materials Informatics'. They can further present a critical summary of a scientific article in front of master-level students and co-lead a discussion about the topic. They have learned to exercise a critical approach towards current, scientific literature and to critically defend the statements in an article.			
3	**Subject aims** • understanding the ideas of the emerging field of Materials Informatics • gaining an overview of the current state of the art in this research field • being able to read, assess and evaluate scientific literature • presenting a complex scientific subject to an informed audience • judging and arguing for or against a research approach/idea			
4	**Teaching methods** lecture			
5	**Prerequisites for participation** basic understanding in mathematics, physics, mechanics, and materials science			
6	**Assessment methods** Students read one article per week and will write a short review about the article. Every week, one student will gather the reviews, present the topic, and lead the discussion. Discussions will evaluate the approach and identify open questions. Presentation (40%), oral exam 30 min (60%)			
7	**Prerequisites for the assignment of credit points** Submission of all but one summary and presentation of one article			
8	**This module is used in the following degree programmes as well** none			
9	**Impact on total grade** 4/113			
10	**Responsibility for module** Prof. Dr.-Ing. Markus Stricker			
11	**Other information** Literature: t.b.a.			

NON-TECHNICAL/NON-SCIENTIFIC OPTIONAL MODULE					
Module code 12	**Student workload** 120 hours	**Credits** 4/3 ECTS	**Semester** $1^{st}/3^{rd}$	**Frequency** 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 • Any module from a Master´s course will be recognized. Module 12a is an example of a course offered at ICAMS.			
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** Only one language course will be taken into account for this module.			

DOCUMENTING AND COMMUNICATING SCIENCE					
Module code 12a	**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** 5-20 students
2	**Learning outcomes** Successful participants are able to prepare different types of scientific documents. They know structural elements of different formats and tools for scientific typesetting, plotting and producing graphics. Students are able to carry out a literature research on a topic in materials research independently, as well as to summarise their findings in a written report, using adequate citing techniques and avoiding plagiarism. The students learn how to summarize their findings in a short oral presentation. They are aware of the rules of good scientific practice.			
3	**Subject aims** • Structures, style, and types of scientific documents • Principles and application of LaTeX • Literature research • Citations, quotations, copyright issues, plagiarism • Presenting and structuring scientific data • Graphics and images • Plots and tables • 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** 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** ---			
10	**Responsibility for module** Prof. Dr. Anna Grünebohm, Dr. Manuel Piacenza			
11	**Other information** Recommended Literature: J. Schimel: Writing Science – How to write papers that get cited and proposals that get funded, Oxford University Press (2012); M. Alley, The Craft of scientific presentations: Critical steps to succeed and critical errors to avoid, Springer (2013); W. Strunk and E.B. White: The elements of style, Pearson Education Inc. (2000); H. Glasman-Deal: Science research writing – for non-native speakers of English, Imperial College Press (2010); R.A. Day and B. Gastel: How to write and publish a scientific paper, Greenwood/ABC-CLIO, LLC (2011); L. Lamport: LaTex – A document preparation system, Addison-Wesley (1994); F. Mittelbach et al: The LaTex companion, Addison-Wesley (2004); E.R. Tufte: Visual display of quantitative information, Graphics Press (2001); S. Few: Show me the numbers, Analytics Press (2012).			

PROJECT WORK					
Module code 13	**Student workload** 180 hours	**Credits** 6 ECTS	**Semester** 3rd	**Frequency** continuous offers of topics	**Duration** 1 semester

1	**Types of courses:** practical work	**Contact hours** 80 hrs	**Independent study** 100 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** 6/113			
10	**Responsibility for module** all lecturers of the Master course			
11	**Other information**			

MASTER THESIS					
Module code 14	**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 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 13) and a total of at least 80 ECTS from all modules			
6	**Assessment methods** written thesis (40 to 150 pages)			
7	**Prerequisites for the assignment of credit points** positively evaluated thesis			
8	**This module is used in the following degree programmes as well** none			
9	**Impact of grade on total grade** 30/113			
10	**Responsibility for module** all lecturers of the Master course			
11	**Other information**			