MASTER COURSE
“MATERIALS SCIENCE AND SIMULATION”

MODULE DESCRIPTIONS

March 2018
# Module Descriptions

<table>
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<tr>
<td></td>
<td><strong>Basic modules</strong></td>
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<td>Elements of Microstructure</td>
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<td>2b</td>
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<td>Theoretical and Applied Materials Science</td>
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<td>Microstructure and Mech. Properties</td>
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<td>Profile module (Modelling &amp; Simulation)</td>
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<td>6</td>
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<td><strong>Scientific Theses</strong></td>
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<td>13</td>
<td>Project work (180 h)</td>
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<td>14</td>
<td>Master thesis (900 h)</td>
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<td>30</td>
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<tr>
<td></td>
<td><strong>Sum Weekly Hours</strong></td>
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</table>

**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 Partly individual module
   2a Compulsory module for all students
   2b Submodule to be chosen according to student’s background

for Bachelors of Science:
- Assessment and Description of Materials Properties (2b-N1)
- Materials Processing (2b-N2)
- If students wish their Master’s degree to be recognized by the faculty of Physics, e.g. to continue their studies by acquiring a doctoral degree in Physics, they can choose from those modules that are in accordance with the doctoral regulations of the faculty and under the condition that they fulfil the respective requirements as fixed at the beginning of their studies together with their adviser of studies.

for Bachelors of engineering:
- Introduction to Quantum Mechanics in Solid State Physics (2b-E1)
- Statistical Physics and Thermodynamics (2b-E2)

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)
- Application and implementation of electronic structure methods (6-MS2)
- The CALPHAD Method (6-MS3)
- Continuum Mechanics (6-MS4)

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 Modelling in Materials Science (8-MS1)
- Advanced Atomistic Simulation Methods (8-MS2)
- Computational Fracture Mechanics (8-MS3)
- Lattice Boltzmann Modelling: From Simple Flows to Interface Driven Phenomena (8-MS4)
- Mechanical Modelling of Materials (8-MS5)
- Theory and Application of Micromechanical Modelling (8-MS6)
- 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 Any module from a science or engineering Master’s programme will be recognized.

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 2 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

<table>
<thead>
<tr>
<th>Semester</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>Σ</th>
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<tr>
<td>Compulsory modules: 1, 2a, 3, 4, 5</td>
<td>9</td>
<td>14</td>
<td>8</td>
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<td>31</td>
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<td>Optional modules: 2b, 6, 7, 8, 9, 10, 11</td>
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<td>12</td>
<td>16</td>
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<td>46</td>
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<td>Key qualifications: module 12</td>
<td>3</td>
<td>4</td>
<td></td>
<td></td>
<td>7</td>
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<td>Project work: module 13</td>
<td></td>
<td>6</td>
<td></td>
<td>6</td>
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<td>Master's thesis: module 14</td>
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<td>Σ</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>120</td>
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</table>

Credits are allocated according the the following scheme:

- Compulsory 31 CP = 26%
- Optional 46 CP = 38%
- Key qualifications 7 CP = 6%
- Project report and Master's thesis 36 CP = 30%
# Module Scheme and Credits

<table>
<thead>
<tr>
<th>Semester I</th>
<th>Semester II</th>
<th>Semester III</th>
<th>Semester IV</th>
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<tbody>
<tr>
<td>Programming Concepts in Materials Science: 6 CP</td>
<td>Quantum Mechanics in Materials Science: 4 CP</td>
<td>Continuum Methods in Materials Science: 4 CP</td>
<td>Master Thesis and Seminar: 30 CP</td>
</tr>
<tr>
<td>Elements of Microstructure: 3 CP</td>
<td>Microstructure and Mechanical Properties: 4 CP</td>
<td>Atomistic Simulation Methods: 4 CP</td>
<td></td>
</tr>
<tr>
<td>Basic Lectures (Theoretical Physics or Materials Science): 12 CP</td>
<td>Advanced Characterization Methods: 6 CP</td>
<td>Free Specialization Module I: 6 CP</td>
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<tr>
<td>General Optional Lecture: 6 CP</td>
<td>Module Modelling &amp; Simulation: 6 CP</td>
<td>Free Specialization Module II: 6 CP</td>
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</tr>
<tr>
<td>Soft Skills I: 3 CP (e.g. Scientific Writing)</td>
<td>Module Processing &amp; Characterization: 8 CP</td>
<td>Optional Scientific Lecture: 4 CP</td>
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</tr>
<tr>
<td>Soft Skills II: 4 CP (e.g. Management Skills)</td>
<td>Soft Skills II: 4 CP</td>
<td>Research Project and Seminar: 6 CP</td>
<td></td>
</tr>
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</table>

Course scheme: the size of the fields represents the allocated credit point.
### Programming Concepts in Materials Science

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>1st</td>
<td>winter</td>
<td>1 semester</td>
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<table>
<thead>
<tr>
<th>Types of courses:</th>
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<tbody>
<tr>
<td>a) lecture</td>
</tr>
<tr>
<td>b) class</td>
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<table>
<thead>
<tr>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
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<tbody>
<tr>
<td>a) 30 hrs (2 SWS)</td>
<td>120 hours</td>
<td>a) 30 students</td>
</tr>
<tr>
<td>b) 30 hrs (2 SWS)</td>
<td></td>
<td>b) 10 students</td>
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</tbody>
</table>

**Learning outcomes**

On successful completion of this module the students will be able to analyse, write and test Python and C++ language programs of moderate complexity. Furthermore, they will be able to program and to solve basic numerical problems that may be useful or required for course work, assignments and projects. The students will also be able to make independent steps towards formulating a numerical problem from materials science problem as an abstract algorithm and to implement this algorithm in one of the taught structured programming languages.

#### Subject aims

- Introduction to operating systems (Linux and Unix)
- Introduction to modern programming languages (Python, C++)
- Introduction to relevant mathematical and graphical software
- Examples that will gain an overview of modern programming approaches and tools will comprise:
  - data interpolation and fitting
  - linear algebra
  - numerical integration
  - theory and numerical solution of ordinary and partial differential equations
  - fundamental solutions of boundary value problems

#### Teaching methods

- lectures, numerical exercises (homework)

#### Prerequisites for participation

none

#### Assessment methods

- final exam consists of numerical exercises (20%) and written examination (3 hours) (80%)

#### Prerequisites for the assignment of credit points

- passing the written examination (bonus points will be taken into account)

This module is used in the following degree programmes as well

none

#### Impact of grade on total grade

6/120

#### Responsibility for module

- Prof. Dr. Ralf Drautz, Prof. Dr. Godehard Sutmann

#### Other information

Lecture notes will be provided. The book “A primer on scientific programming with python” by Hans Petter Langtangen will be covered.
Module Descriptions

BASICS IN MATERIALS SCIENCE: ELEMENTS OF MICROSTRUCTURE

<table>
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<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
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<tbody>
<tr>
<td>2a</td>
<td>90 hours</td>
<td>3 ECTS</td>
<td>1st</td>
<td>winter</td>
<td>1 semester</td>
<td></td>
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</table>

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

2. Learning outcomes
   Students will develop a first qualitative and comprehensive view of all basic elements of materials science and engineering, which are important to understand the evolution of materials microstructure during processing and service. They learn 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
   - 3/120

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

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<tr>
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<th>2b-E1</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
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<tr>
<td></td>
<td></td>
<td>240 hours</td>
<td>8 ECTS</td>
<td>1st</td>
<td>winter term</td>
<td>1 semester</td>
</tr>
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</table>

| 1 | Types of courses: |
|   | a) lecture |
|   | b) class |
| 2 | Contact hours |
|   | a) 45 hrs (3 SWS) |
|   | b) 30 hrs (2 SWS) |
| 3 | Independent study |
|   | 165 hours |
| 4 | Class size |
|   | a) 20 students |
|   | b) 10 students |

## 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 solve 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.

## 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

## Teaching methods
lecture, class

## Prerequisites for participation
none

## Assessment methods
written examination (2 hours), bonus points can be gained by providing solutions to the problem sheets in class.

## Prerequisites for the assignment of credit points
passing the written examination (bonus points will be taken into account)

## This module is used in the following degree programmes as well
none

## Impact of grade on total grade
8/120

## Responsibility for module
Dr. Tilmann Hickel, Prof. Dr. Ralf Drautz, Prof. Dr. Jörg Neugebauer

## Other information
Lecture notes will be provided.
# BASICS IN MATERIALS SCIENCE:
## STATISTICAL PHYSICS AND THERMODYNAMICS

<table>
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<tr>
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<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
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<table>
<thead>
<tr>
<th>Types of courses:</th>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) lecture</td>
<td>a) 30 hrs (2 SWS)</td>
<td>75 hours</td>
<td>a) 20 students</td>
</tr>
<tr>
<td>b) class (exercise and seminars)</td>
<td>b) 15 hrs (1 SWS)</td>
<td></td>
<td>b) 10 students</td>
</tr>
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</table>

## Learning outcomes

In the thermodynamic part, the students are guided to formulate realistic material systems and processes in an energy framework of thermodynamics. The ability of defining simple systems with determining thermodynamic properties are exercised. Thereafter, they learn to apply extremal principles to thermodynamic problems. Concepts such as Maxwell relations and phase diagrams are exemplified. Finally, the importance of modelling approaches in a thermodynamic framework are briefly addressed. For the statistical physics part, the students will become familiar with fundamental concepts of probability and statistical ensembles and will learn to derive basic thermodynamic quantities such as entropy and free energy in terms of microscopic system variables. They will also develop the necessary skills to transfer and apply these concepts to materials modelling and solid state physics. Examples will be worked out for rubber elasticity, random walk and diffusion, specific heat of crystalline solids, compressibility of metallic systems as well as para and ferro-magnetism.

## Subject aims

- Introduction to key concepts of probability theory: probability distributions, expectation values, central limit theorem
- Physical concepts in classical mechanics required for the understanding of statistical mechanics
- Basic concepts in classical thermodynamics: state variables, thermodynamic potentials, entropy, extremal principles, Legendre transformations, Maxwell relations, phase equilibria, phase diagrams, phase coexistence and interfaces, reversibility and irreversibility, adiabatic processes
- Linking classical mechanics to statistical mechanics: microcanonical, canonical and grand canonical ensemble, equipartition theorem, Maxwell distribution
- Basic aspects of quantum statistics

## Teaching methods

lecture, class, group work

## Prerequisites for participation

background in mechanical engineering, materials science or related disciplines

## Assessment methods

written examination (2 hours)

## Prerequisites for the assignment of credit points

passing the written examination

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

iMOS (Molecular Science and Simulation)

## Impact of grade on total grade

4/120

## Responsibility for module

Prof. Dr. Ingo Steinbach, Prof. Dr. Fatollah Varnik, Dr.-Ing. Reza Darvishi Kamachali

## Other information

Literature:
# BASICS IN MATERIALS SCIENCE: ASSESSMENT AND DESCRIPTION OF MATERIAL PROPERTIES

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
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<tbody>
<tr>
<td>2b-N1</td>
<td>240 hours</td>
<td>8 ECTS</td>
<td>1st</td>
<td>winter term</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

## 1 Types of courses:
- a) lecture
- b) class

## 2 Contact hours
- a) 45 hrs (3 SWS)
- b) 30 hrs (2 SWS)

## 3 Independent study
- 165 hours

## 4 Class size
- a) 20 students
- b) 10 students

## 2 Learning outcomes
Students know the basic mechanical and functional properties of materials, the quantities by which these properties are described and how to assess these quantities. They can explain the metallurgical and physical origin of materials properties and are able to apply the related materials descriptions to engineering problems. The students understand the relation between microstructure and properties and know typical ranges of mechanical and functional (e.g. conductivity, coercitivity, remanence) properties of the main classes of materials (metals, ceramics, glasses, polymers).

## 3 Subject aims
- Introduction to concepts of mechanical properties of materials (stress-strain curves, stiffness, strength, ductility)
- Origin of plastic deformation and fracture
- Relation between microstructure and mechanical properties
- Strengthening concepts for engineering materials
- Assessment methods for mechanical properties (mechanical testing)
- Introduction to concepts of functional (electrical, magnetic, optical) properties of materials
- Physical origin of functional properties, key quantities and their relations
- Methods to measure the different functional properties

## 4 Teaching methods
- lecture, class, seminar paper

## 5 Prerequisites for participation
- background in physics, chemistry or related discipline

## 6 Assessment methods
- written examination together with submodule 2b-N2 (4 hours for entire sub-module 2b-N). Bonus points can be gained by submitting solutions to the problem sheets that are distributed in class.

## 7 Prerequisites for the assignment of credit points
- passing the 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
- 8/120

## 10 Responsibility for module
- PD Dr. habil. Rebecca Janisch, Prof. Dr.-Ing. Alfred Ludwig

## 11 Other information
- Lecture notes will be provided online.
- Recommended Literature:
  - G. Gottstein: Physical foundations of materials science, Springer Verlag (2004);
### BASICS IN MATERIALS SCIENCE: MATERIALS PROCESSING

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>2b-N2</td>
<td>120 hours</td>
<td>4 ECTS</td>
<td>1st</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

#### 1 Types of courses:
- a) lecture
- b) lab

#### 2 Contact hours
- a) 30 hrs (2 SWS)
- b) 15 hrs (1 SWS)

#### 3 Independent study
- 75 hours

#### 4 Class size
- a) 20 students
- b) 10-15 students

#### 2 Learning outcomes
Students possess knowledge of the basic principles and technologies of materials processing including production and refining of metals from ores, alloying, melting, casting, forming, joining, heat treatment, and surface modification. This knowledge enables them to understand how processing affects the microstructure and properties of technologically important metals. Thus they have developed the competence to select materials and processing routes that take into account technological and economic requirements and constraints.

#### 3 Subject aims
- Introduction to key engineering ferrous and non-ferrous metallic materials
- Primary processes: refining, melting, casting
- Knowledge of important engineering manufacturing processes
- Metal forming: forging, rolling, extrusion, swaging, bending, deep drawing
- Joining: welding, brazing, soldering
- Knowledge of important surface-treatment and heat-treatment processes
- Surface treatment: case hardening, nitriding, carburizing, coating
- Heat treatment: annealing, hardening, tempering, precipitation hardening

#### 4 Teaching methods
- lecture, lab exercises

#### 5 Prerequisites for participation
- background in physics, chemistry or related discipline

#### 6 Assessment methods
- written examination together with submodule 2b-N1 (4 hours for entire sub-module 2b-N)

#### 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
- 4/120

#### 10 Responsibility for module
- Dr. Fabian Pöhl

#### 11 Other information
- Lecture notes will be provided.
- Recommended books:
# THEORETICAL AND APPLIED MATERIALS SCIENCE: QUANTUM MECHANICS IN MATERIALS SCIENCE

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>3a</td>
<td>120 hours</td>
<td>4 ECTS</td>
<td>2nd</td>
<td>summer</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Types of courses:</th>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>a) lecture</td>
<td>a) 30 hrs (2 SWS)</td>
<td>75 hours</td>
<td>a) 30 students</td>
</tr>
<tr>
<td></td>
<td>b) class</td>
<td>b) 15 hrs (1 SWS)</td>
<td></td>
<td>b) 10-15 students</td>
</tr>
</tbody>
</table>

## Learning outcomes
Students have acquired an overview of the fundamentals and the application of quantum mechanics in materials science. They are able to read and 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 have some insight in the numerical implementation of electronic structure methods. The students can relate electronic structure properties to the crystal structure and other properties of materials.

## 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

## Teaching methods
lecture, class

## Prerequisites for participation
successful completion of “Introduction to Quantum Mechanics in Solid State Physics” or equivalent course

## Assessment methods
written examination (together with submodule 3b; 3 hours for entire module 3). Bonus points can be gained by providing solutions to the problem sheets in class.

## Prerequisites for the assignment of credit points
passing the written examination (bonus points will be taken into account)

## This module is used in the following degree programmes as well
none

## Impact of grade on total grade
4/120

## Responsibility for module
Prof. Dr. Ralf Drautz

## 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

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>3b</td>
<td>120 hours</td>
<td>4 ECTS</td>
<td>2nd</td>
<td>summer term</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

#### 1 Types of courses:
- a) lecture
- b) class

#### 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: Assessment and description of material properties" or equivalent course

#### 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
4/120

#### 10 Responsibility for module
Prof. Dr. Alexander Hartmaier

#### 11 Other information
Lecture notes are provided online.

Literature:
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
   a) 30 students
   b) 30 students

2 Learning outcomes
   Students develop a clear view on the structure of solids. They know 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 origins. 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
   6/120

10 Responsibility for module
   Prof. Dr.-Ing. Gunther Eggeler

11 Other information
   A list with recommended literature and class notes is available online.
## ADVANCED NUMERICAL METHODS:
### CONTINUUM METHODS IN MATERIALS SCIENCE

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>5a</td>
<td>120 hours</td>
<td>4 ECTS</td>
<td>3rd</td>
<td>winter term</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

### Types of courses:
- a) lecture
- b) numerical exercises

<table>
<thead>
<tr>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) 30 hrs (2 SWS)</td>
<td>75 hours</td>
<td>a) 30 students</td>
</tr>
<tr>
<td>b) 15 hrs (1 SWS)</td>
<td></td>
<td>b) 10 students</td>
</tr>
</tbody>
</table>

### Learning outcomes
Students understand the underlying principles of the finite element/finite volume method to solve problems in continuum mechanics including phase transformations. They are familiar with 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 have acquired the skills to model and solve materials science problems and they also understand the limitations of these methods.

### 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

### Teaching methods
lecture, numerical exercises

### Prerequisites for participation
background in mechanical engineering, physics or related discipline

### Assessment methods
written examination together with submodule 5b (3 hours for entire module 5)

### Prerequisites for the assignment of credit points
passing the written examination

### This module is used in the following degree programmes as well
none

### Impact of grade on total grade
4/120

### Responsibility for module
Prof. Dr. Ingo Steinbach

### Other information
Lecture notes are provided online.
# ADVANCED NUMERICAL METHODS: ATOMISTIC SIMULATION METHODS

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>5b</td>
<td>120 hours</td>
<td>4 ECTS</td>
<td>3rd</td>
<td>winter term</td>
<td>1 semester</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>1</th>
<th>Types of courses:</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) lecture</td>
<td>a) 30 hrs (2 SWS)</td>
</tr>
<tr>
<td>b) class</td>
<td>b) 15 hrs (1 SWS)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td>75 hours</td>
<td>a) 30 students</td>
</tr>
<tr>
<td></td>
<td>b) 10-15 students</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2</th>
<th>Learning outcomes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Students will be acquainted with models for the interatomic interaction and understand how these interactions can be represented by potentials. They learn how to use 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 understand 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.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>3</th>
<th>Subject aims</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Empirical and semi-empirical potentials for ionic, covalent and metallic materials</td>
<td></td>
</tr>
<tr>
<td>• Atomic dynamics</td>
<td></td>
</tr>
<tr>
<td>• Statistics of atomic ensembles</td>
<td></td>
</tr>
<tr>
<td>• Observables in atomistic simulations (MSD, RDF, specific heat and free energy)</td>
<td></td>
</tr>
<tr>
<td>• Monte Carlo (kinetic, Metropolis) and Transition-state theory</td>
<td></td>
</tr>
<tr>
<td>• Lattice-gas-Hamiltonian (Ising-model, cluster expansion)</td>
<td></td>
</tr>
<tr>
<td>• Magnetism (Heisenberg-model)</td>
<td></td>
</tr>
<tr>
<td>• Linking atomistic simulations to the electronic, microstructural and macroscopic models</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>Teaching methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>lecture, class, problem sheets</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>5</th>
<th>Prerequisites for participation</th>
</tr>
</thead>
<tbody>
<tr>
<td>successful completion of “Theoretical and Applied Materials Science” (Module 3) is recommended</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>6</th>
<th>Assessment methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>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.</td>
<td></td>
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</table>

<table>
<thead>
<tr>
<th>7</th>
<th>Prerequisites for the assignment of credit points</th>
</tr>
</thead>
<tbody>
<tr>
<td>passing the written examination (bonus points will be taken into account)</td>
<td></td>
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</table>

<table>
<thead>
<tr>
<th>8</th>
<th>This module is used in the following degree programmes as well</th>
</tr>
</thead>
<tbody>
<tr>
<td>none</td>
<td></td>
</tr>
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<table>
<thead>
<tr>
<th>9</th>
<th>Impact of grade on total grade</th>
</tr>
</thead>
<tbody>
<tr>
<td>4/120</td>
<td></td>
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</table>

<table>
<thead>
<tr>
<th>10</th>
<th>Responsibility for module</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prof. Dr. Ralf Drautz</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>11</th>
<th>Other information</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lecture notes will be provided. Relevant literature will be discussed in the first lecture.</td>
<td></td>
</tr>
</tbody>
</table>
**INTERFACES AND SURFACES**

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>6-MS1</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>2nd</td>
<td>summer</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

**Types of courses:**
- **a)** lecture
- **b)** class

<table>
<thead>
<tr>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) 30 hrs (2 SWS)</td>
<td>120 hours</td>
<td>a) 20 students</td>
</tr>
<tr>
<td>b) 30 hrs (2 SWS)</td>
<td></td>
<td>b) 10 students</td>
</tr>
</tbody>
</table>

**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 apply them to material science problems.

**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

**Teaching methods**
lecture, computer exercises

**Prerequisites for participation**
background in physics, chemistry or related discipline

**Assessment methods**
written or oral examination (1.5 hours). Bonus points can be gained by complementary tasks distributed in the lecture.

**Prerequisites for the assignment of credit points**
passing the examination (bonus points will be taken into account)

**This module is used in the following degree programmes as well**
one

**Impact of grade on total grade**
6/120

**Responsibility for module**
PD Dr. habil. Rebecca Janisch, Dr. Jutta Rogal, Dr. Thomas Hammerschmidt

**Other information**
Lecture notes will be provided.
Recommended Literature:
J. M. Howe: Interfaces in materials, Wiley Interscience (1997);
APPLICATION AND IMPLEMENTATION OF ELECTRONIC STRUCTURE
METHODS

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>6-MS2</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>2nd</td>
<td>summer term</td>
<td>1 semester</td>
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</tbody>
</table>

1. Types of courses:
   a) lecture + group seminar
   b) practical studies

<table>
<thead>
<tr>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) 30 hrs (2 SWS)</td>
<td>120 hours</td>
<td>a) 10 students</td>
</tr>
<tr>
<td>b) 30 hrs (2 SWS)</td>
<td></td>
<td>b) 10 students</td>
</tr>
</tbody>
</table>

2. Learning outcomes
   Students will learn how 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 have the basic knowledge required to use and implement the most common numerical solvers that are employed in quantum mechanical problems. In this way they will be able to contribute to the implementation of quantum mechanical codes. Students will also be enabled to choose the most appropriate electronic structure computational method and code 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
   - The Plane-Wave Pseudo-Potential Method (iterative diagonalization, self-consistency)
   - The 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
   6/120

10. Responsibility for module
    Prof. Dr. Ralf Drautz, Prof. Dr. Jörg Neugebauer

11. Other information
    Lecture notes will be provided.
# THE CALPHAD METHOD

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
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<td>6-MS3</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>2nd</td>
<td>summer</td>
<td>1 semester</td>
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</table>

<table>
<thead>
<tr>
<th>Types of courses:</th>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) lecture</td>
<td>a) 30 hrs (2 SWS)</td>
<td>120 hours</td>
<td>a) 15 students</td>
</tr>
<tr>
<td>b) class</td>
<td>b) 30 hrs (2 SWS)</td>
<td></td>
<td>b) 15 students</td>
</tr>
</tbody>
</table>

## Learning outcomes

Students understand the concept of single and multiphase equilibrium, learn how to model Gibbs energy and its derivatives using fundamental theories and the connection to experimental determined thermodynamic properties. They learn about the experimental techniques used to determine that properties. They are able to connect the thermodynamic of materials to several applications which use thermodynamics as input as, for example, phase field simulations. They learn to evaluate thermodynamic descriptions. They develop skills that enable them to optimise materials’ constitutions and to transfer this knowledge to strategies to solve problems and to design new materials. They learn to take decisions based on the available resources.

## Subject aims

- Thermodynamic Functions
- Modelling of ordered and disordered multicomponent phases
- Calculation of phase diagrams
- Construction of Gibbsian Databases after critical evaluation of experimental information as well as first-principles calculated data
- Use of stable and metastable thermodynamic quantities in microstructure simulations

## Teaching methods

lecture, class, individual project and group work, case studies, discussions, presentations of modelling results

## Prerequisites for participation

basic knowledge in thermodynamics and statistical physics

## Assessment methods

written report (10 to 30 pages) of individual project on thermodynamic modelling

## Prerequisites for the assignment of credit points

positively evaluated written report

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

none

## Impact of grade on total grade

6/120

## Responsibility for module

Dr. Suzana G. Fries

## Other information

Literature:
## CONTINUUM MECHANICS

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>6-MS4</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>2nd</td>
<td>summer term</td>
<td>1 semester</td>
</tr>
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<table>
<thead>
<tr>
<th>Types of courses</th>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) lecture</td>
<td>a) 30 hrs (2 SWS)</td>
<td>120 hours</td>
<td>a) 10 students</td>
</tr>
<tr>
<td>b) class</td>
<td>b) 30 hrs (2 SWS)</td>
<td></td>
<td>b) 10 students</td>
</tr>
</tbody>
</table>

### Learning outcomes

Students will gain extended knowledge of continuum mechanics and learn to formulate problems of structural and material mechanics within this framework. They furthermore learn different solution techniques for mechanical problems as a prerequisite for computer-oriented analysis.

### 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

### Teaching methods

lecture, class

### Prerequisites for participation

none

### Assessment methods

written examination (2 hours)

### Prerequisites for the assignment of credit points

passing the written examination

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

Master of Science Computational Engineering (Import lecture)

### Impact of grade on total grade

6/120

### Responsibility for module

Prof. Dr. rer. nat. K. Hackl, Prof. Dr. rer. nat. K.C. Le

### 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);
MODERN COATING TECHNOLOGIES

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
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<td>7-PC1</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</td>
<td>summer</td>
<td>1 semester</td>
</tr>
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</table>

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 as 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**
   - 6/120

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)

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
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<th>Semester</th>
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<table>
<thead>
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<th>1</th>
<th>Types of courses:</th>
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<tr>
<td>a) lecture</td>
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<td>b) class</td>
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<th>Contact hours</th>
<th>Independent study</th>
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<tr>
<td>a) 45 hrs (3 SWS)</td>
<td>120 hours</td>
<td>a) 10 students</td>
<td></td>
</tr>
<tr>
<td>b) 15 hrs (1 SWS)</td>
<td></td>
<td>b) 10 students</td>
<td></td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>3</th>
<th>Learning outcomes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Students will be able to apply elements from the materials science curriculum to actual engineering problems in advanced materials technology. They are aware of the strong link between elementary atomistic, crystallographic, thermodynamic/kinetic and microstructural processes and the behaviour of materials/components on the macro scale. They will be able to use the understanding of basic processes to develop new and improve classical materials, to assess the mechanical and functional properties of materials and to understand kinetic processes in solids and at surfaces. In addition to an increased familiarity with advanced basic concepts, the students will be able to apply materials science theory to four fascinating material classes: High entropy alloys, intermetallic phases, single crystal Ni-base superalloys and shape memory alloys.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>Subject aims</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Importance of atoms and electrons in materials engineering and the transition from atoms to alloys and from alloys to components</td>
<td></td>
</tr>
<tr>
<td>• Thermodynamic concepts in materials engineering and fundamentals of alloy design (with a special focus on ternary phase diagrams)</td>
<td></td>
</tr>
<tr>
<td>• Kinetic concepts in materials science and engineering (especially precipitation processes)</td>
<td></td>
</tr>
<tr>
<td>• Basic concepts of solid state phase transformations</td>
<td></td>
</tr>
<tr>
<td>• Understanding and application of knowledge to four materials classes: high entropy alloys, intermetallic phases, single crystal superalloys and shape memory alloys</td>
<td></td>
</tr>
<tr>
<td>• Acquisition of knowledge about high temperature strength (example: superalloys)</td>
<td></td>
</tr>
<tr>
<td>• Acquisition of knowledge about fracture mechanics and fatigue (example: shape memory alloys)</td>
<td></td>
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</table>

<table>
<thead>
<tr>
<th>5</th>
<th>Teaching methods</th>
</tr>
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<tbody>
<tr>
<td>lecture, class</td>
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<table>
<thead>
<tr>
<th>6</th>
<th>Prerequisites for participation</th>
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<tbody>
<tr>
<td>successful completion of “Elements of Microstructure” (2a) and “Statistical Physics and Thermodynamics” (2b-E2) recommended</td>
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<table>
<thead>
<tr>
<th>7</th>
<th>Assessment methods</th>
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</thead>
<tbody>
<tr>
<td>oral examination (30 min.)</td>
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<table>
<thead>
<tr>
<th>8</th>
<th>Prerequisites for the assignment of credit points</th>
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</thead>
<tbody>
<tr>
<td>passing the exam</td>
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</table>

<table>
<thead>
<tr>
<th>9</th>
<th>This module is used in the following degree programmes as well</th>
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</thead>
<tbody>
<tr>
<td>Master of Science in Mechanical Engineering: Werkstoff- und Microengineering</td>
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<table>
<thead>
<tr>
<th>10</th>
<th>Impact of grade on total grade</th>
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<td>6/120</td>
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<table>
<thead>
<tr>
<th>11</th>
<th>Responsibility for module</th>
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<tbody>
<tr>
<td>Prof. Dr.-Ing. Gunther Eggeler</td>
<td></td>
</tr>
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<table>
<thead>
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<th>12</th>
<th>Other information</th>
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<tbody>
<tr>
<td>A list with recommended literature and class notes will be available online.</td>
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### MEMS & NANOTECHNOLOGY

<table>
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<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
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<tbody>
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<td>7-PC3</td>
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<td>6 ECTS</td>
<td>2nd</td>
<td>summer</td>
<td>1 semester</td>
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<table>
<thead>
<tr>
<th>Types of courses:</th>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) lecture</td>
<td>a) 45 hrs (3 SWS)</td>
<td>120 hours</td>
<td>a) 10 students</td>
</tr>
<tr>
<td>b) class</td>
<td>b) 15 hrs (1 SWS)</td>
<td></td>
<td>b) 10 students</td>
</tr>
</tbody>
</table>

### Learning outcomes / Lernergebnisse/Kompetenzen
- Das Modul MEMS & Nanotechnologie vermittelt vertiefte Kenntnisse über den Einsatz von Mikrosystemen (Mikro-Elektro-Mechanische Systeme, MEMS) in aktuellen Gebieten der Ingenieurtechnik und der biomedizinischen Technik sowie über die Konzepte, Methoden und Werkstoffe der Nanotechnologie.
- Zentraler Aspekt der Vorlesung ist, den Studierenden vertiefte ingenieurwissenschaftliche Grundlagen in diesen Bereichen zu vermitteln.
- Anhand von zahlreichen Beispielen lernen die Studierenden den Stand moderner ingenieurwissenschaftlicher Forschung im Bereich MEMS & Nanotechnologie kennen. Desweiteren erwerben die Studierenden vertiefte, auch interdisziplinäre Methodenkompetenz und können diese nach der Vorlesung auch situativ angepasst anwenden.
- Im Rahmen der angebotenen Übungen praktizieren die Studierenden wissenschaftliches Lernen und Denken und lernen die Erkenntnisse/Fertigkeiten auf konkrete und neue Problemstellungen zu übertragen.
- Das Modul bereitet die Studierenden auf die Durchführung einer Masterarbeit vor.

### Subject aims / Inhalte
- Überblick zu Konzepten und Technologien des Micro-Engineering
- 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
- 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)
- Nanostrukturierte Oberflächen (z.B. mittels GLAD hergestellte Nanosäulen)
- Anwendungen aus dem Bereich Nanotechnologie

### Teaching methods
lecture, class

### Prerequisites for participation
none

### Assessment methods
written examination (2 hours)

### Prerequisites for the assignment of credit points
passing the written examination

### This module is used in the following degree programmes as well
- Master of Science in Mechanical Engineering: Werkstoff-Engineering

### Impact of grade on total grade
6/120

### Responsibility for module
Prof. Dr. Alfred Ludwig

### Other information
The lecture will be held in German language
### POLYMERS AND SHAPE MEMORY ALLOYS

<table>
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<th>Module code</th>
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<th>Student workload</th>
<th>180 hours</th>
<th>Credits</th>
<th>6 ECTS</th>
<th>Semester</th>
<th>2nd</th>
<th>Frequency</th>
<th>summer term</th>
<th>Duration</th>
<th>1 semester</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Types of courses:</td>
<td></td>
<td>Contact hours</td>
<td></td>
<td>Independent study</td>
<td>120 hours</td>
<td>Class size</td>
<td></td>
<td>a) 10 students</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>a) lecture</td>
<td>b) class</td>
<td>a) 45 hrs (3 SWS)</td>
<td>b) 15 hrs (1 SWS)</td>
<td></td>
<td></td>
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<tr>
<td>Learning outcomes</td>
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<tr>
<td>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.</td>
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</tbody>
</table>

| 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 | |

| Teaching methods | lecture, class |

| Prerequisites for participation | successful completion of “Elements of Microstructure” (2a) or equivalent recommended |

| Assessment methods | written examination (2 hours) |

| Prerequisites for the assignment of credit points | passing the written examination |

| This module is used in the following degree programmes as well | Master of Science in Mechanical Engineering: Werkstoff-Engineering |

| Impact of grade on total grade | 6/120 |

| Responsibility for module | Dr. Klaus Neuking (polymers), Dr.-Ing. Jan Frenzel (shape memory alloys) |

| Other information | Lecture notes will be provided. |
MULTISCALE MODELLING IN MATERIALS SCIENCE

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
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<tbody>
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<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</td>
<td>winter</td>
<td>1 semester</td>
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</table>

1. **Types of courses:**
   - a) lecture
   - b) class

2. **Contact hours**
   - a) 30 hrs (2 SWS)
   - b) 30 hrs (2 SWS)

3. **Independent study**
   - 120 hours

4. **Class size**
   - a) 20 students
   - b) 10 students

2. **Learning outcomes**
   The students gain knowledge about the different length and time scales on which the phenomena and mechanisms of material behaviour occur. They furthermore understand the different levels of how to describe these phenomena and the existing approaches to bridge and integrate these scales including their range of validity. The students build up the skills to independently develop scale-bridging models that integrate all necessary scales and employ these models to describe and predict materials behaviour under given conditions.

3. **Subject aims**
   - Characterization of relevant length and times scales in materials science
   - Concepts of concurrent and hierarchical multi-scale approaches
   - Classical homogenization techniques (Taylor/Sachs and Voigt/Reuss)
   - Micromechanical modeling (crystal plasticity, polycrystalline and multiphase materials)
   - Dislocation-based plasticity models
   - Total energy methods in atomistics
   - Atomistic calculation of fundamental physical and material properties
   - Calculation of free energy
   - Basics of the Monte Carlo method
   - Examples and applications of different multiscale methods in the class

4. **Teaching methods**
   - lecture, computer exercises, seminars

5. **Prerequisites for participation**
   - completion of module 2 or equivalent

6. **Assessment methods**
   - oral (30 minutes) or written (2 hours) examination, depending on size of the class.

7. **Prerequisites for the assignment of credit points**
   - passing the exam

8. **This module is used in the following degree programmes as well**
   - none

9. **Impact of grade on total grade**
   - 6/120

10. **Responsibility for module**
    - Prof. Dr. Alexander Hartmaier, Dr. Thomas Hammerschmidt

11. **Other information**
    - Lecture notes will be provided
ADVANCED ATOMISTIC SIMULATION METHODS

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
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<tbody>
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<td>6 ECTS</td>
<td>3rd</td>
<td>winter</td>
<td>1 semester</td>
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</table>

1 Types of courses:
   a) lecture
   b) class

2 Contact hours
   a) 30 hrs (2 SWS)
   b) 30 hrs (2 SWS)

3 Independent study
   120 hours

4 Class size
   a) 20 students
   b) 10 students

2 Learning outcomes
   Atomistic simulations in materials science are challenging since they often involve large system sizes and long-time scales to capture the physical properties of interest. This requires the application of simulation techniques that go beyond the standard methods. Students will have an understanding of the basic concepts of advanced atomistic simulation techniques. They will have an overview of a variety of methods that have been developed to overcome the shortcomings of standard approaches. This includes e.g. methods for extending the accessible time scale compared to those reached with regular molecular dynamics.

3 Subject aims
   - Derivation of molecular dynamics algorithms in various ensembles
   - Hybrid approaches, quantum mechanics/molecular mechanics (QM/MM)
   - Biased sampling, configurational biased Monte Carlo, Wang-Landau, parallel tempering
   - Accelerating the dynamics: hyperdynamics, bond boost method, parallel replica molecular dynamics, temperature accelerated molecular dynamics
   - Coarse graining the dynamics: separation of time scales, markovian state models
   - Transition State Theory, Transition State search: dimer method, nudged elastic band method, string method, drag method, transition path sampling
   - State-to-state dynamics: kinetic Monte Carlo, lattice approximation, adaptive kinetic Monte Carlo
   - Free energy calculations

4 Teaching methods
   lecture, discussions, computer exercises

5 Prerequisites for participation
   background in physics, chemistry or related discipline

6 Assessment methods
   Oral (30 minutes) or written (2 hours) examination. Bonus points can be gained by submitting solutions to the problem sheets that are distributed in class.

7 Prerequisites for the assignment of credit points
   passing the exam (bonus points will be taken into account)

8 This module is used in the following degree programmes as well
   none

9 Impact of grade on total grade
   6/120

10 Responsibility for module
    Prof. Dr. Ralf Drautz, Dr. Jutta Rogal

11 Other information
## COMPUTATIONAL FRACTURE MECHANICS

<table>
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<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
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<td>6 ECTS</td>
<td>3rd</td>
<td>winter term</td>
<td>1 semester</td>
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</table>

1. **Types of courses:**
   - a) lecture
   - b) class

   **Contact hours:**
   - a) 30 hrs (2 SWS)
   - b) 30 hrs (2 SWS)

   **Independent study:**
   - 120 hours

   **Class size:**
   - a) 20 students
   - b) 10 students

2. **Learning outcomes**
   The students attain the ability to independently simulate fracture including plasticity for a wide range of materials and geometries. Based on the acquired understanding of the different types of brittle fracture and ductile failure of materials, they are enabled to choose appropriate fracture models and to implement them in a finite element environment. They gain sufficient knowledge about the theoretical background of the different types of fracture models, to study the relevant literature independently. On an engineering level, the students 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-plastic 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**
   6/120

10. **Responsibility for module**
    Prof. Dr. Alexander Hartmaier

11. **Other information**
    Lecture notes will be provided
# LATTICE BOLTZMANN MODELLING:
FROM SIMPLE FLOWS TO INTERFACE DRIVEN PHENOMENA

<table>
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<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
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<td>6 ECTS</td>
<td>3rd</td>
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<td>1 semester</td>
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<table>
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<th>Types of courses</th>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
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<tbody>
<tr>
<td>a) lecture</td>
<td>a) 30 hrs (2 SWS)</td>
<td>120 hours</td>
<td>a) 10 students</td>
</tr>
<tr>
<td>b) class</td>
<td>b) 30 hrs (2 SWS)</td>
<td></td>
<td>b) 10 students</td>
</tr>
</tbody>
</table>

## Learning outcomes
On successful completion of this module, students will be familiar with fundamental equations of hydrodynamics such as the continuity and the Navier-Stokes equations. They will be able to obtain analytic solutions of these equations for a number of simple cases such as the hydrostatic pressure in an ideal gas, planar Couette flow, Poiseuille flow and momentum diffusion equation. Moreover, they will learn the mathematical foundations of the Boltzmann equation and derive from it the lattice Boltzmann method (LBM). Using the above mentioned analytical results, they will benchmark the LBM and will thus gain confidence in its reliability. Moreover, they will also gain insight into modelling multiphase flows via the LBM, which will be applied to study capillarity and wetting phenomena. Also in this case, the multiphase-LBM will be tested via simple, analytically solvable examples.

## Subject aims
- Introduction to fluid dynamics on continuum level (Euler and Navier-Stokes equations)
- Relation between the Boltzmann equation and the lattice Boltzmann method (LBM)
- Application of the Chapman-Enskog multiscale expansion analysis to obtain macroscopic equations from the LBM
- The difference between real and ideal fluids and how this issue may be tackled within the LBM
- Simulation of two phase system (e.g. droplet + vapor) within the LBM
- Study of complex objects such as red blood cells within the lattice Boltzmann method

## Teaching methods
lecture, group work, case studies, discussions

## Prerequisites for participation
successful completion of "Programming concepts in Materials Science" (module 1) or equivalent

## Assessment methods
oral examination (30 minutes)

## Prerequisites for the assignment of credit points
passing the exam (for active participation in the lecture, bonus points will be considered)

## This module is used in the following degree programmes as well
none

## Impact of grade on total grade
6/120

## Responsibility for module
Prof. Dr. Fathollah Varnik

## Other information
Lecture notes will be provided.
## MECHANICAL MODELLING OF MATERIALS

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student work-load</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>8-MS5</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1</th>
<th>Types of courses</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) lecture</td>
<td></td>
</tr>
<tr>
<td>b) class</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2</th>
<th>Learning outcomes</th>
</tr>
</thead>
<tbody>
<tr>
<td>on successful completion of the MMM module, students will be able to:</td>
<td></td>
</tr>
<tr>
<td>1. analyse different classes of engineering materials and correctly formulate the constitutive models for each class of materials,</td>
<td></td>
</tr>
<tr>
<td>2. rationally design machines and structures (using the commercial programs) and reduce uncertainty in the design process,</td>
<td></td>
</tr>
<tr>
<td>3. select appropriate material models for every specific class of engineering materials with the view of making engineering structures more economic.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>3</th>
<th>Subject aims</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Basic concepts of continuum mechanics (introduction)</td>
<td></td>
</tr>
<tr>
<td>• Mechanical characterization of materials (mainly solids) – test methods and data analysis</td>
<td></td>
</tr>
<tr>
<td>• Basic concepts of constitutive equations for engineering materials</td>
<td></td>
</tr>
<tr>
<td>• Classical (1-dimensional) models of elastic and inelastic materials</td>
<td></td>
</tr>
<tr>
<td>• Boundary value problems of linear elasticity</td>
<td></td>
</tr>
<tr>
<td>• Basic problems of inelastic behavior of materials (viscoelasticity, plasticity and damage,)</td>
<td></td>
</tr>
<tr>
<td>• Basic concepts of strength of failure of engineering materials</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>Teaching methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>lecture, class</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>5</th>
<th>Prerequisites for participation</th>
</tr>
</thead>
<tbody>
<tr>
<td>basic knowledge in mathematics and mechanics (statics, dynamics and strength of materials)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>6</th>
<th>Assessment methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>written examination (2 hours)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>7</th>
<th>Prerequisites for the assignment of credit points</th>
</tr>
</thead>
<tbody>
<tr>
<td>passing the written examination</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>8</th>
<th>This module is used in the following degree programmes as well</th>
</tr>
</thead>
<tbody>
<tr>
<td>Master Course: Computational Engineering (Import lecture)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>9</th>
<th>Impact of grade on total grade</th>
</tr>
</thead>
<tbody>
<tr>
<td>6/120</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>10</th>
<th>Responsibility for module</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prof. Daniel Balzani</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>11</th>
<th>Other information</th>
</tr>
</thead>
<tbody>
<tr>
<td>Literature:</td>
<td></td>
</tr>
<tr>
<td>R. Lakes: Viscoelastic materials. Cambridge University Press (2009);</td>
<td></td>
</tr>
<tr>
<td>E.H. Dill: Continuum mechanics: Elasticity, plasticity, viscoelasticity. CRC Press (2007);</td>
<td></td>
</tr>
</tbody>
</table>
THEORY AND APPLICATION OF MICROMECHANICAL MODELLING

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>8-MS6</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

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 possess fundamental understanding of the principles of micromechanical modelling. They understand the concepts of crystal plasticity, representative volume elements (RVE), and homogenization techniques and for which types of problems these techniques can be applied. They are able to apply micromechanical modelling methods to predict mechanical properties at both micro- and macroscopic scales for simple problems based on the numerical exercise classes and assignments. They will also possess a basic understanding of the modelling of fatigue and damage problems and the principle differences in the required homogenization techniques, which are current challenges of the frontier of research.

3. Subject aims
   - Crystal plasticity
   - Representative volume elements (RVE)
   - Voronoi tessellation
   - Homogenization techniques for mechanical properties
   - Deformation of single and polycrystals
   - Prediction of mechanical properties for macroscopic scale from microscopic simulation
   - Micromechanical damage modeling

4. Teaching methods
   - Lecture, computer exercises, and seminar

5. Prerequisites for participation
   - Basics in material science and continuum mechanics

6. Assessment methods
   - Oral (30 minutes) or written (2 hours) examination, depending on size of the class

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
   - 6/120

10. Responsibility for module
    - Prof. Dr. Alexander Hartmaier, Dr. Napat Vajragupta

11. Other information
    - Lecture notes will be provided.
## Module Descriptions

### SOLIDIFICATION PROCESSING

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9-PC1</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

**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

### Learning outcomes

Students know about different casting technologies like sand casting, continuous casting, investment casting, pressure die casting and miscellaneous advanced casting processes. This includes knowledge 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 familiar with different simulation tools for casting and solidification processes.

### Subject aims

- History of metal casting, field of application and economic importance
- Shape-, pressure-, die-, continuous-, 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.

### Teaching methods

- Lecture, classes

### Prerequisites for participation

Bachelor degree in mechanical engineering, physics or similar

### Assessment methods

Written examination (120 minutes)

### Prerequisites for the assignment of credit points

Passing the written examination

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

- Master of Science in Mechanical Engineering: Werkstoff-Engineering

### Impact of grade on total grade

6/120

### Responsibility for module

Prof. Dr. Ingo Steinbach

### Other information

Literature:
# ADVANCED MATERIALS PROCESSING AND MICROFABRICATION

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9-PC2</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>2nd</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

1. **Types of courses:**
   - a) lecture
   - b) class

2. **Contact hours**
   - a) 45 hrs (3 SWS)
   - b) 15 hrs (1 SWS)

3. **Independent study**
   - 120 hours

4. **Class size**
   - a) 10 students
   - b) 10 students

### Learning outcomes

Students will be able to understand the fundamentals and basic aspects of the materials science fields of advanced steel technology, high-entropy alloys and microsystems technology and microfabrication. These key technologies of modern materials and microsystems technology are presented within this module and discussed with the help of actual industrial applications and recent developments of materials engineering. The topics presented cover basic and special processes of the cast production line (solidification, directional solidification and special thermomechanical treatments such as the separate zone-refining treatment) and the powder metallurgical processing route. Related topics like integrated micro-structural processes during manufacturing and application will be additionally discussed, focusing especially on industrial applications and processes. Besides the aspects of materials science, which focus on bulk materials processing and properties, a focus is laid on the topics of microsystems technologies (processing and integrity of small scale systems). Presented topics are the processing and application of thin layers and the materials used. These engineering subjects will be presented by the professors of the Institute of Materials and discussed with current issues and research priorities. Groups of topics are: Processing fundamentals, high-entropy alloys (Prof. George), microsystems technology and integrity of small scale systems (Prof. Ludwig), powder metallurgy, integrated material-technical processes and advanced steel technology (Prof. Theisen).

### Subject aims

- Acquisition of knowledge about advanced steel technologies, including powder metallurgy and integrated material-technical processes
- Acquisition of knowledge about solidification fundamentals, including directional solidification and single-crystal growth
- Special concepts of thermomechanical treatments (example: selective zone refining)
- Basic concepts of the processing of special material like high-entropy alloys
- Fundamentals of microsystems technology and integrity of small scale systems

### Teaching methods

- lecture, class

### Prerequisites for participation

- none

### Assessment methods

- written examination (180 min.)

### Prerequisites for the assignment of credit points

- passing the written examination

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

- Master of Science in Mechanical Engineering: Werkstoff- und Microengineering

### Impact of grade on total grade

- 6/120

### Responsibility for module

- Prof. Dr.-Ing. Werner Theisen

### Other information

- A list with recommended literature and class notes will be available online.
# SURFACE SCIENCE AND CORROSION

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9-PC3</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

## Types of courses:
- a) lecture
- b) class

<table>
<thead>
<tr>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) 45 hrs (3 SWS)</td>
<td>120 hours</td>
<td>a) 25 students</td>
</tr>
<tr>
<td>b) 15 hrs (1 SWS)</td>
<td></td>
<td>b) 25 students</td>
</tr>
</tbody>
</table>

## 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 also obtain knowledge about the basics of applied surface technologies providing corrosion protection, including an outlook of novel technological developments. Furthermore, the students will be acquainted with engineering aspects of materials selection, analysing corrosion damage and measures for counteracting corrosion.

## Subject aims

- Short introduction into surface science and electrochemistry
- Fundamental aspects of corrosion science: thermodynamics and kinetics (Pourbaix diagrams, Butler-Volmer equation etc.)
- Understanding passivity of materials
- Understanding of typical corrosion problems, such as atmospheric corrosion, bimetal corrosion, localised corrosion, corrosion under biofilms, basics of high temperature corrosion
- Learning how to make 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
- Learning to assess which counteracting methods best to use for different cases

## Teaching methods

lecture, class, including a short lab course

## Prerequisites for participation

successful completion of “Statistical Physics and Thermodynamics” (2b-E2) and “Elements of Microstructure” (2a) recommended

## Assessment methods

written examination (2 hours)

## Prerequisites for the assignment of credit points

passing the written examination

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

Master of Science in Mechanical Engineering: Werkstoff-Engineering

## Impact of grade on total grade

6/120

## Responsibility for module

Dr. habil. Michael Rohwerder

## Other information

Lecture notes will be provided
# MATERIALS FOR AEROSPACE APPLICATIONS

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9-PC4</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

## 1 Types of courses:
- a) lecture
- b) class

## 2 Learning outcomes
Students have 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 will know about the degradation and damage mechanisms and learn how characterization and testing methods are used for qualifying materials and joints for aerospace applications. They know and can handle 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 mechanisms 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 (30 minutes) 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
- 6/120

## 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

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9-PC5</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</td>
<td>winter term</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1</th>
<th>Types of courses:</th>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>a) lecture</td>
<td>a) 30 hrs (2 SWS)</td>
<td>120 hours</td>
<td>a) 15 students</td>
</tr>
<tr>
<td></td>
<td>b) exercises</td>
<td>b) 30 hrs (2 SWS)</td>
<td></td>
<td>b) 15 students</td>
</tr>
</tbody>
</table>

## Learning outcomes
This course provides an introduction to a range of three-dimensional nanoscale and atomic scale materials characterization technique, e.g. 3D X-ray microscopy, electron tomography, and atom probe tomography etc. The working principles of each technique will be covered in detail. The students will learn how to use the three-dimensional materials characterization technique to solve scientific questions related with material science. Applications in a vast range of applications, such as engineering alloys, catalyst materials, semiconductors will be introduced. The students will acquire a good understanding of three-dimensional nanoscale and atomic scale materials characterization methods, which are currently extremely important in both industry and academia. Additionally the students will achieve some basic hands-on experience on sample preparation and sample analysis on one of these technique (depends on the availability of instrument).

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.

## 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

## Teaching methods
lecture, exercises

## Prerequisites for participation
-

## Assessment methods
written exam (50%), report/seminar talk (50%)

## Prerequisites for the assignment of credit points
passing the exam

## This module is used in the following degree programmes as well
Masters Mechanical Engineering: Werkstoff-Engineering

## Impact of grade on total grade
6/120

## Responsibility for module
Jun.-Prof. Dr. Tong Li

## Other information
-
### GENERAL OPTIONAL SUBJECT

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>1st</td>
<td>free choice of available modules</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

#### Learning outcomes

By freely choosing lectures students can widen their skill or method spectrum according to their personal interests.

#### 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 10-7

#### Teaching methods

see specific module description

#### Prerequisites for participation

none

#### Assessment methods

written or oral examination as given in specific module description

#### Prerequisites for the assignment of credit points

passing the examination

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

see specific module description

#### Impact of grade on total grade

6/120

#### Responsibility for module

see specific module description

#### Other information
ADVANCED FINITE ELEMENT METHODS

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-1</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>2nd</td>
<td>summer</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

1. **Types of courses:**
   - a) lecture
   - b) class

2. **Contact hours:**
   - a) 30 hrs (2 SWS)
   - b) 30 hrs (2 SWS)

3. **Independent study:**
   - 120 hours

4. **Class size:**
   - 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. In seminar papers the students shall apply the basics of the Advanced Finite Element Methods and solve nonlinear structural-mechanical problems by means of hand calculations. Furthermore the students are required 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**
   - 6/120

10. **Responsibility for module**
    - Prof. Dr. Günther Meschke and assistants

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);
## THEORETICAL AND COMPUTATIONAL PLASTICITY

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-2</td>
<td>90 hours</td>
<td>3 ECTS</td>
<td>1st</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

### Student workload
- Contact hours: 30 hrs (2 SWS)
- Independent study: 60 hours
- Class size: 5 students

### Learning outcomes
Students will learn the fundamentals of computational modelling of inelastic materials with emphasis on rate independent plasticity. They will be provided with a sound basis for approximation methods and the finite element method and a good understanding of different methodologies for discretisation of time evolution problems, and rate independent elasto-plasticity in particular.

### Subject aims
- Physical motivation, rate independent plasticity, rate dependence, creep, rheological models
- 1-D Mathematical Model: yield criterion, flow rule, loading/unloading conditions, isotropic and kinematic hardening models
- Computational aspects of 1-D elasto-plasticity: integration algorithms for 1-D elasto-plasticity, operator split, return mapping, incremental elasto-plastic BVP, consistent tangent modulus
- Classical model of elasto-plasticity: physical motivation; Classical mathematical model of rate-independent elasto-plasticity: yield criterion, flow rule, loading/unloading conditions
- Computational aspects of elasto-plasticity: integration algorithms for elasto-plasticity, operator split, the trial elastic state, return mapping, incremental elasto-plastic BVP, consistent tangent modulus
- Integration algorithms for generalized elasto-plasticity: stress integration algorithm
- Computational aspects of large strain elasto-plasticity: multiplicative elasto-plastic split, yield criterion, flow rule, isotropic hardening operator split, return mapping, exponential map, incremental elasto-plastic BVP

### Teaching methods
- Lecture, class

### Prerequisites for participation
- Basic knowledge of continuum mechanics

### Assessment methods
- 60% by examination (open book exam), 40% by course work (three small projects that will require both hand calculation and computer simulation. Computer simulation will require a certain amount of programming).

### Prerequisites for the assignment of credit points
- Passing the exam

### This module is used in the following degree programmes as well
- Master of Science Computational Engineering

### Impact of grade on total grade
3/120

### Responsibility for module
- Prof. Dr. rer. nat. Klaus Hackl

### Other information
- Literature:
  - Lecture notes;
  - J. Lubliner: Plasticity theory, Macmillan (1990);
  - J.C. Simo and T.J. Hughes: Computational inelasticity, Springer (1998);
### Module Descriptions

#### FINITE ELEMENT METHODS IN LINEAR STRUCTURAL MECHANICS

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-3</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>1st</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

**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

**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 and pollutant transport. In seminar papers the students shall apply the basics of the Advanced Finite Element Methods and solve structural-mechanical problems by means of hand calculations. Furthermore the students are required to program and validate problems in structural analysis and transport processes.

**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 p-truss elements and development of two-(plane stress and plane strain) and three-dimensional isoparametric p-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, moisture transport, coupled problems) is demonstrated
- Finite element models for beams and plates
- Aspects of element locking and possible remedies practical application of the finite element method for the solution of selected examples. Introduction of finite element programs

**Teaching methods**

lecture, class, homework

**Prerequisites for participation**

basics in mathematics, mechanics and structural analysis

**Assessment methods**

written examination (3 hours). Bonus points can be gained by submitting solutions to the homework distributed during class.

**Prerequisites for the assignment of credit points**

passing the written examination

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

Master of Science in Computational Engineering

**Impact of grade on total grade**

6/120

**Responsibility for module**

Prof. Dr. Günther Meschke and assistants

**Other information**

Lecture notes will be provided as printed 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);
## ADAPTIVE FINITE ELEMENT METHODS

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-4</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>1st</td>
<td>once per year, usually winter term</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

### 1 Types of courses:
- a) lecture
- b) class

### 2 Learning outcomes
Students will be familiar with advanced finite element methods for the numerical solution of partial differential equations and with advanced solution techniques for the resulting discrete problems. Concerning the first topic adaptive mesh-refinement methods based on a posteriori error estimators and the required data structures will be in the focus. Concerning the second topic taking advantage of the adaptive structure of the discretizations and the use of multigrid-techniques will be central.

### 3 Subject aims
- Need for efficient solvers, error estimation, and adaptivity
- Basic a posteriori error estimates, their structure and their application to examples
- A catalogue of error estimators, their common structure and their comparison
- Mesh adaptation, in particular refinement, coarsening and smoothing
- Required data structures and possible implementations
- Review of stationary iterative solvers, in particular conjugate gradient algorithms
- Multigrid methods, their structure, their properties, and their realization

### 4 Teaching methods
lecture, class

### 5 Prerequisites for participation
basic knowledge about partial differential equations and their variational formulation, finite element methods, numerical methods for the solution of large linear and non-linear systems of equations.

### 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 Computational Engineering

### 9 Impact of grade on total grade
6/120

### 10 Responsibility for module
Prof. Dr. Rüdiger Verfürth

### 11 Other information
Lecture Notes (http://www.rub.de/num1/skripten/AdaptiveFEM.pdf);
M. Ainsworth, J.T. Oden: A posteriori error estimation in finite element analysis, Wiley (2000);
D. Braess: Finite elements: Theory, fast solvers and applications in solid mechanics. Cambridge University Press (2001);
Demonstration software and user guide (www.rub.de/num1/demo/index.html)
# ENERGY METHODS IN MATERIALS MODELING

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-5</td>
<td>120 hours</td>
<td>4</td>
<td>1st</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

1. **Types of courses**
   - lecture and class

2. **Contact hours**
   - 45 hrs (3 SWS)

3. **Independent study**
   - 75 hours

4. **Class size**
   - 20 students

## Learning outcomes
On successful completion of this module, students will be able to:
- Apply energy methods to simulate the behavior of solids including microstructural aspects.
- Understand and make use of the underlying mathematical concepts.
- Assess the quality of of an energy based material model with regard to its performance in energy minimization algorithms.
- Develop suitable numerical estimates for material models that suffer from convexity problems.

## Subject aims
- Energy minimization for phase transforming materials: boundedness, coercivity, notions of convexity
- Estimates of the energetically optimal microstructure: quasiconvexification, convexification, polyconvexification, rank-1-convexification
- Examples: trip-steels; shape memory alloys: introduction and material model, convexification, translation method, lamination

## Teaching methods
- lecture, class

## Prerequisites for participation
- basics in mathematics and continuum mechanics

## Assessment methods
- written examination (2 hours, weighted 75%), participation in class (weighted 25%)

## Prerequisites for the assignment of credit points
- passing the exam (bonus points will be taken into account).

This module is used in the following degree programmes as well:
- Master of Science Computational Engineering

## Impact of grade on total grade
- 4/120

## Responsibility for module
- Priv.-Doz. Dr.-Ing. Rainer Fechte-Heinen

## Other information
- Lecture notes will be provided.
- Literature:
  - K. Bhattacharya: Microstructure of martensite – Why it forms and how it gives rise to the shape-memory effect. Oxford University Press (2003);
  - M. Silhavý: The mechanics and thermodynamics of continuous media. Springer (1997);
  - G. Gottstein: Physical foundations of materials science, Springer Verlag (2004);
ENGINEERING CERAMICS & COATING TECHNOLOGY

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-6</td>
<td>120 hours</td>
<td>4 ECTS</td>
<td>2nd</td>
<td>summer term</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

1. **Types of courses:**
   - a) lecture
   - b) class

2. **Contact hours**
   - a) 30 hrs (2 SWS)
   - b) 15 hrs (1 SWS)

3. **Independent study**
   - 75 hours

4. **Class size**
   - a) 10 students
   - b) 10 students

2. **Learning outcomes**
   The students obtain a profound knowledge about engineering ceramics and their technical applications. This will include details on the processing of engineering ceramics and an overview on the typical property spectrum of ceramics allowing the selection of ceramics for specific needs.
   A broad knowledge in different coating technologies gives the students the ability to select suitable coating methods especially for wear, corrosion and high temperature applications as thermal barrier coatings. Special emphasis will be laid on different thermal spray technologies.

3. **Subject aims**
   - Powder synthesis, shaping, sintering and characterization methods for ceramic materials
   - Physical, chemical and thermodynamic basics
   - Applications of engineering ceramics
   - Basic knowledge on different coatings technologies (PVD, CVD, thermal spray processes and others)
   - Coating technologies to improve the useful properties of materials

4. **Teaching methods**
   - lecture, class

5. **Prerequisites for participation**
   Knowledge equivalent to contents from “Assessment and Description of Material Properties” (2b-N1) or similar is recommended

6. **Assessment methods**
   - oral examination (20 minutes) or written examination

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**
   - 4/120

10. **Responsibility for module**
    - Prof. Dr. Robert Vaßen

11. **Other information**
    - Literature:
      - L. Michalowsky: Neue keramische Werkstoffe, Wiley (1994);
      - W. Schatt: Sintervorgänge, Grundlagen, VDI Verlag (1992);
    - Slides will be available online.
### PHASE-FIELD THEORY AND APPLICATION

<table>
<thead>
<tr>
<th><strong>Module code</strong></th>
<th><strong>Student workload</strong></th>
<th><strong>Credits</strong></th>
<th><strong>Semester</strong></th>
<th><strong>Frequency</strong></th>
<th><strong>Duration</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>10-7</td>
<td>120 hours</td>
<td>4 ECTS</td>
<td>2nd</td>
<td>summer term</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

1. **Types of courses:**
   - a) lecture
   - b) exercises

2. **Contact hours:**
   - a) 15 hrs (1 SWS)
   - b) 30 hrs (2 SWS)

3. **Independent study:** 75 hours

<table>
<thead>
<tr>
<th><strong>Class size</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>a) 30 students</td>
</tr>
<tr>
<td>b) 10-15 students</td>
</tr>
</tbody>
</table>

#### 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

- Dendritic solidification, scale invariant solution and microscopic solvability
- Traveling wave solution of a phase front, sharp and thin interface limit
- Anisotropy and the $\xi$-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 (1,5 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

4/120

#### 10 Responsibility for module

Prof. Dr. Ingo Steinbach, Prof. Dr. Fathollah Varnik, Dr. Oleg Shchyglo

#### 11 Other information

Lecture notes will be provided online.
<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>120 hours</td>
<td>4 ECTS</td>
<td>3rd</td>
<td>free choice of available modules</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

1. Types of courses: lecture and class

2. Contact hours: 40 hrs

3. Independent study: 80 hours

4. Class size

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<table>
<thead>
<tr>
<th>Learning outcomes</th>
</tr>
</thead>
<tbody>
<tr>
<td>By freely choosing lectures students can widen their skill or method spectrum and set an individual focus to their curriculum matching their personal interests.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Subject aims</th>
</tr>
</thead>
<tbody>
<tr>
<td>- Develop knowledge and skills in fields beyond engineering and science</td>
</tr>
<tr>
<td>- Deepen knowledge about specific topics in Materials Science and Simulation according to own interests</td>
</tr>
</tbody>
</table>

Any module from engineering or science master’s courses will be recognized.

<table>
<thead>
<tr>
<th>Teaching methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>see specific module description</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Prerequisites for participation</th>
</tr>
</thead>
<tbody>
<tr>
<td>none</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Assessment methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>written or oral examination as given in specific module description</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Prerequisites for the assignment of credit points</th>
</tr>
</thead>
<tbody>
<tr>
<td>passing the examination</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>This module is used in the following degree programmes as well</th>
</tr>
</thead>
<tbody>
<tr>
<td>see specific module description</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Impact of grade on total grade</th>
</tr>
</thead>
<tbody>
<tr>
<td>4/120</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Responsibility for module</th>
</tr>
</thead>
<tbody>
<tr>
<td>see specific module description</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Other information</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
<tr>
<td><strong>NON-TECHNICAL/NON-SCIENTIFIC OPTIONAL MODULE</strong></td>
</tr>
<tr>
<td>-----------------------------------------------</td>
</tr>
<tr>
<td><strong>Module code</strong></td>
</tr>
<tr>
<td>12</td>
</tr>
</tbody>
</table>

1. **Types of courses:**
   - Lecture and class

2. **Contact hours**
   - 45 hrs

3. **Independent study**
   - 75 hours

4. **Class size**

<table>
<thead>
<tr>
<th><strong>Learning outcomes</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>By freely choosing lectures students can widen their skill or method spectrum according to their personal interests.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Subject aims</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>• Develop knowledge and skills in fields beyond engineering and science</td>
</tr>
<tr>
<td>• Gain and develop knowledge in non-technical subjects, related to materials engineering, like business administration according to own interests</td>
</tr>
<tr>
<td>• Develop and practice communication skills</td>
</tr>
<tr>
<td>• Any module from a Master’s course will be recognized. Module 12a is an example of a course offered at ICAMS.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Teaching methods</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>see specific module descriptions</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Prerequisites for participation</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>none</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Assessment methods</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>written or oral examination as given in specific module description</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Prerequisites for the assignment of credit points</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>passing the examination</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>This module is used in the following degree programmes as well</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>none</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th><strong>Impact of grade on total grade</strong></th>
</tr>
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<tbody>
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<td>---</td>
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</table>

<table>
<thead>
<tr>
<th><strong>Responsibility for module</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>see specific module description</td>
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</table>

<table>
<thead>
<tr>
<th><strong>Other information</strong></th>
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<tbody>
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<td></td>
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</tbody>
</table>
## DOCUMENTING AND COMMUNICATING SCIENCE

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>12a</td>
<td>120 hours</td>
<td>4 ECTS</td>
<td>1st</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

### 1 Types of courses:
- a) lecture
- b) class

### 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 summarise 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. Ralf Drautz, PD Dr. habil. Rebecca Janisch, 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);
- S. Few: Show me the numbers, Analytics Press (2012).
## PROJECT WORK

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</td>
<td>continuous offers of topics</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1</th>
<th>Types of courses: practical work</th>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>80 hrs</td>
<td>100 hours</td>
<td>1-3 students</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2</th>
<th><strong>Learning outcomes</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>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.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>3</th>
<th><strong>Subject aims</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>• Treatment of a scientific subject in a given time</td>
</tr>
<tr>
<td></td>
<td>• Scientific solution for a given practical problem</td>
</tr>
<tr>
<td></td>
<td>• Application of learned techniques from previous modules</td>
</tr>
<tr>
<td></td>
<td>• Teamwork</td>
</tr>
<tr>
<td></td>
<td>• Written presentation of the results</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th><strong>Teaching methods</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>continuous contact periods to advice the student, presentation of progress during group seminars and discussions</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>5</th>
<th><strong>Prerequisites for participation</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>successful completion of all compulsory modules of first and second semester</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>6</th>
<th><strong>Assessment methods</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>written report (20 to 50 pages)</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>7</th>
<th><strong>Prerequisites for the assignment of credit points</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>positively evaluated written report</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>8</th>
<th><strong>This module is used in the following degree programmes as well</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>none</td>
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</table>

<table>
<thead>
<tr>
<th>9</th>
<th><strong>Impact of grade on total grade</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>6/120</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>10</th>
<th><strong>Responsibility for module</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>all lecturers of the Master course</td>
</tr>
</tbody>
</table>

| 11 | **Other information** |
## MASTER THESIS

<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>900 hours</td>
<td>30 ECTS</td>
<td>4th</td>
<td>continuous offers of topics</td>
<td>1 semester</td>
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</table>

<table>
<thead>
<tr>
<th>1</th>
<th>Types of courses:</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Contact hours</td>
</tr>
<tr>
<td>3</td>
<td>Independent study</td>
</tr>
<tr>
<td>4</td>
<td>Class size</td>
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</table>

<table>
<thead>
<tr>
<th>1</th>
<th>practical work</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>100 hrs</td>
</tr>
<tr>
<td>3</td>
<td>800 hours</td>
</tr>
<tr>
<td>4</td>
<td>1 student</td>
</tr>
</tbody>
</table>

### 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.

### 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

### Teaching methods
Continuous contact to advice the student, presentation of progress during group seminars and discussions.

### Prerequisites for participation
Successful completion of project work (module 13) and a total of at least 80 ECTS from all modules.

### Assessment methods
Written thesis (40 to 150 pages)

### Prerequisites for the assignment of credit points
Positively evaluated thesis

### This module is used in the following degree programmes as well
None

### Impact of grade on total grade
30/120

### Responsibility for module
All lecturers of the Master course

### Other information