MASTERS COURSE
“MATERIALS SCIENCE AND SIMULATION”

MODULE DESCRIPTIONS
## COURSE SCHEDULE

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<td>Basic modules</td>
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<td>3</td>
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<td>Microstructure and Mech. Properties</td>
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<td>Atomistic Simulation Methods</td>
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<td>4 6</td>
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<td>Profile module (free choice)</td>
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<td>Optional modules</td>
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<td>Optional scientific or engineering subject</td>
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<td>12</td>
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<tr>
<td>12b</td>
<td>Key qualification</td>
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<td>x</td>
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<td></td>
<td>Scientific Theses</td>
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<tr>
<td>13</td>
<td>Project work (180 h)</td>
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<td>6</td>
<td>x</td>
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<tr>
<td>14</td>
<td>Master thesis (900 h)</td>
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<td>30</td>
<td>x</td>
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| Sum Weekly Hours | 84 | 21 | 22 | 21 | 20 |
| Sum Workload     | 36 | 900| 900| 900| 900|
| Sum Credit Points | 120| 30 | 30 | 30 | 30 |

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

Basic Modules
1. Compulsory module in numerical methods
2. Compulsory modules in materials science

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

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

7. Profile module 7 (PC) has to be chosen from:
   - Modern Coating Technologies (7-PC1)
   - Fundamental Aspects of Materials Science and Engineering (7-PC2)
   - MEMS and Nanotechnology (7-PC3)
   - Polymers and Shape Memory Alloys (7-PC4)

8 - 9. Profile modules 8 and 9 can be chosen freely from:
   - Multiscale Mechanics of Materials (8-MS1)
   - Advanced Atomistic Simulation Methods (8-MS2)
   - Computational Fracture Mechanics (8-MS3)
   - Mechanical Modelling of Materials (8-MS4)
   - 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.
Selection of courses offered:
   - Application and Implementation of Electronic Structure Methods (10-1)
   - Lattice Boltzmann Modeling: From Simple Flows to Interface Driven Phenomena (10-2)
   - Theory and Application of Bond Order Potentials (10-3)
   - Computational Plasticity (10-4)
   - Advanced Finite Elemente Methods (10-5)
   - Finite Element Methods in Linear Structural Mechanics (10-6)
• Machine Learning Methods in Data Analysis and Processing (11-1)
• Engineering Ceramics and Coating Technology (11-2)
• Materials Informatics (11-3)
• Practical Applications of Material Informatics with R (11-4)
• Mathematics for Materials Modelling (11-5)

Non-technical/Non-scientific optional Module

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

The project work and the Master thesis represent practical self-guided research and make up 30% of all credit points.
EXAMINATIONS, CREDITS AND GRADES

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

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

CREDIT ALLOCATION

<table>
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<tr>
<th>Semester</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>Σ</th>
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<td>Compulsory modules: 1, 2, 3, 4, 5</td>
<td>21</td>
<td>14</td>
<td>8</td>
<td>43</td>
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<tr>
<td>Optional modules: 6, 7, 8, 9, 10, 11</td>
<td>6</td>
<td>12</td>
<td>16</td>
<td>34</td>
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<td>Key qualifications: module 12</td>
<td>3</td>
<td>4</td>
<td>7</td>
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<td>Project work: module 13</td>
<td>6</td>
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<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>120</td>
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Credits are allocated according the the following scheme:

- Compulsory 43 CP = 36%
- Optional 34 CP = 28%
- Key qualifications 7 CP = 6%
- Project report and Master’s thesis 36 CP = 30%
Course scheme: the size of the fields represents the allocated credit points
ALL MODULES

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

2 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.

3 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

4 Teaching methods
lectures, numerical exercises (homework)

5 Prerequisites for participation
none

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

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

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

9 Impact of grade on total grade
6/113

10 Responsibility for module
PD Dr. habil. Thomas Hammerschmidt, Prof. Dr. Godehard Sutmann

11 Other information
Lecture notes will be provided. The book "A primer on scientific programming with python" by Hans Petter Langentangen will be covered.
## BASICS IN MATERIALS SCIENCE: ELEMENTS OF MICROSTRUCTURE

<table>
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<th>Student workload</th>
<th>Credits</th>
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<td>1 semester</td>
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<th>Types of courses:</th>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
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<tr>
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<td>lecture</td>
<td>30 hrs (2 SWS)</td>
<td>60 hours</td>
<td>30 students</td>
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</table>

### 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

3/113

### 10 Responsibility for module

Prof. Dr.-Ing. Gunther Eggeler

### 11 Other information

A list with recommended literature and class notes will be available online.
# BASICS IN MATERIALS SCIENCE:  
INTRODUCTION TO QUANTUM MECHANICS IN SOLID-STATE PHYSICS

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<tr>
<th>Module code</th>
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<th>Student workload 180 hours</th>
<th>Credits 6 ECTS</th>
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<td>Types of courses:</td>
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<td>Class size a) 20 students b) 10 students</td>
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<tr>
<td>a) lecture</td>
<td>a) 30 hrs (2 SWS)</td>
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<tr>
<td>b) class</td>
<td>b) 30 hrs (2 SWS)</td>
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</table>

## 2 Learning outcomes
Students will acquire a basic understanding of quantum mechanics and the necessary conceptual and mathematical background. This will enable the students to transfer knowledge gained in this course to applications in chemistry, materials science and solid-state physics. They will be able to independently 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.

## 3 Subject aims
- Fundamental quantum mechanics (history and Heisenberg relation)
- Schrödinger equation and interpretation of wave functions
- Stationary solutions (quantum wells, tunneling)
- The hydrogen atom and the periodic system of elements
- Electrons in a periodic potential and band formation
- Harmonic oscillator and lattice vibrations
- Crystallography in solid-state physics
- Fundamentals of magnetism

## 4 Teaching methods
lecture, class

## 5 Prerequisites for participation
none

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

## 7 Prerequisites for the assignment of credit points
passing the 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
6/113

## 10 Responsibility for module
Dr. Tilmann Hickel, Prof. Dr. Ralf Drautz, Prof. Dr. Anna Grünebohm

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

<table>
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<tr>
<th>Module code</th>
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<th>Frequency</th>
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<td>1 semester</td>
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<th>Class size</th>
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<td>a) 45 hrs (3 SWS)</td>
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<td>a) 20 students</td>
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<tr>
<td>b) class</td>
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<td>b) 15 hrs (1 SWS)</td>
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<td>b) 20 students</td>
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<tr>
<th>2</th>
<th>Learning outcomes</th>
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<tr>
<td>Students possess knowledge of the basic principles and technologies of materials processing including casting, sintering, forming, heat treatment and surface modification. They also understand basic thermodynamic concepts for phase stability and liquid-solid or solid-solid phase transformations, as Maxwell relations and phase diagrams, and can apply them to solve simple materials science problems. Concerning mechanical behaviour of materials, the students understand the definition of mechanical equilibrium and are able to apply it to simple problems. They have an overview on the different mechanical properties and their assessment methods, including the microstructural strengthening mechanisms of materials. The students know the basic physical properties of functional materials and how they are related to the microstructure. They are able to discuss the correlation between processing, microstructure and properties of materials and have the basic skills to apply their knowledge to solve materials science problems.</td>
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The students are familiar with fundamental concepts of statistical mechanics and know how to connect macroscopic material properties to atomic and molecular features by using probability theory and statistical methods. They are able to derive the Boltzmann distribution of energies by using the equal probability principle of equilibrium states. Using statistical mechanics, they are able to relate properties such as temperature, pressure and specific heat to atomistic variables for a number of cases such as ideal gases and crystalline solids (Debye theory). They understand how magnetic properties such as para-and ferromagnetism are connected to spin degrees of freedom and can derive from a simple statistical starting point the magnetization curve for a paramagnet and the Curie-law for a ferromagnetic material. They are also familiar with basic principles of quantum statistics and know and the difference between fermions and bosons. The students can use the variational approach to study the evolution of a system towards equilibrium (Ginzburg-Landau theory). |

<table>
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<tr>
<th>3</th>
<th>Subject aims</th>
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<tbody>
<tr>
<td>Overview on important engineering manufacturing processes: Casting, powder processing, metal forming, surface treatment, heat treatment</td>
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<tr>
<td>Thermodynamical concepts to describe phase equilibria and phase transformations in liquid and solid states</td>
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<tr>
<td>Introduction to mechanical properties of materials and their assessment methods</td>
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<tr>
<td>Microscopic origin of plastic deformation and fracture</td>
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<tr>
<td>Fundamental relations between microstructure and mechanical properties, incl. strengthening mechanisms for engineering materials</td>
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<tr>
<td>Introduction to functional (electrical, magnetic, optical) properties of materials</td>
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<tr>
<td>Physical origin of functional properties, key quantities and their relations</td>
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<tr>
<td>Introduction to key concepts of probability theory: probability distributions, expectation values, central limit theorem</td>
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<td>Basics of ensemble theory; microcanonical, canonical and grand canonical ensemble</td>
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<tr>
<td>Boltzmann distribution and equipartition theorem</td>
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<tr>
<td>Statistical approach to temperature and pressure: Virial theorem and equation of state of ideal gases</td>
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<tr>
<td>Specific heat of crystalline solids (Debye theory)</td>
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<tr>
<td>Introduction to variational formalism (Euler-Lagrange)</td>
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<tr>
<td>Ginzburg-Landau theory of magnetism</td>
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<tr>
<th>4</th>
<th>Teaching methods</th>
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<tbody>
<tr>
<td>lecture, group work</td>
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<thead>
<tr>
<th>5</th>
<th>Prerequisites for participation</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Assessment methods</td>
</tr>
<tr>
<td>---</td>
<td>-------------------</td>
</tr>
<tr>
<td>6</td>
<td>written examination (2 hours), bonus points can be gained by providing solutions to the problem sheets in class.</td>
</tr>
<tr>
<td></td>
<td><strong>Prerequisites for the assignment of credit points</strong></td>
</tr>
<tr>
<td>7</td>
<td>passing the exam</td>
</tr>
<tr>
<td></td>
<td><strong>This module is used in the following degree programmes as well</strong></td>
</tr>
<tr>
<td>8</td>
<td>None (IMOS informieren!)</td>
</tr>
<tr>
<td></td>
<td><strong>Impact of grade on total grade</strong></td>
</tr>
<tr>
<td>9</td>
<td>6/113</td>
</tr>
<tr>
<td></td>
<td><strong>Responsibility for module</strong></td>
</tr>
<tr>
<td>10</td>
<td>Prof. Dr. Alexander Hartmaier, Prof. Dr. Fathollah Varnik</td>
</tr>
<tr>
<td></td>
<td><strong>Other information</strong></td>
</tr>
</tbody>
</table>
### Module Descriptions

**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>

#### 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) 30 students
- b) 10-15 students

#### 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).

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

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

#### Impact of grade on total grade
- 4/113

#### 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</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></td>
</tr>
<tr>
<td>b) class</td>
<td></td>
</tr>
<tr>
<td>Contact hours</td>
<td></td>
</tr>
<tr>
<td>a) 30 hrs (2 SWS)</td>
<td></td>
</tr>
<tr>
<td>b) 15 hrs (1 SWS)</td>
<td></td>
</tr>
<tr>
<td>Independent study</td>
<td></td>
</tr>
<tr>
<td>75 hours</td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>3</th>
<th>Subject aims</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Mechanical equilibrium definitions</td>
<td></td>
</tr>
<tr>
<td>• Basics of the Finite Element Method/Implementation of Finite Element code in Matlab</td>
<td></td>
</tr>
<tr>
<td>• Continuum plasticity and transition to micromechanics</td>
<td></td>
</tr>
<tr>
<td>• Microstructural mechanisms and microscopic descriptions of mechanical properties of materials</td>
<td></td>
</tr>
<tr>
<td>• Length scales in materials (phases, grain boundaries, defect densities)</td>
<td></td>
</tr>
<tr>
<td>• Hardening mechanisms (grain boundary, dislocation, solid solution and precipitation hardening)</td>
<td></td>
</tr>
<tr>
<td>• Micromechanical modelling of material properties</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>successful completion of “Basics in Materials Science” (3a, 3b, 3c) or equivalent courses</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 3a; 3 hours for entire module 3). Bonus points can be gained by providing solutions to the problem sheets in class.</td>
<td></td>
</tr>
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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>
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</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>none</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>4/113</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>10</th>
<th>Responsibility for module</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prof. Dr. Markus Anthony Stricker</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>11</th>
<th>Other information</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lecture notes are provided online.</td>
<td></td>
</tr>
<tr>
<td>Literature:</td>
<td></td>
</tr>
</tbody>
</table>
# ADVANCED CHARACTERIZATION 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>4</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

## Contact hours
- a) 45 hrs (3 SWS)
- b) 15 hrs (1 SWS)

## Independent study
- 120 hours

## Class size
- a) 30 students
- b) 30 students

### 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.

### 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 [HAADF], 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)

### Teaching methods
lecture, class, lab

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

### 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- and Microengineering

### Impact of grade on total grade
6/113

### Responsibility for module
Prof. Dr.-Ing. Jan Frenzel, Prof. Dr. Tong Li

### 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>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>5a</td>
<td>4 ECTS</td>
<td>3rd</td>
<td>winter term</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Student workload</th>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td>120 hours</td>
<td>a) 30 hrs (2 SWS)</td>
<td>75 hours</td>
<td>a) 30 students</td>
</tr>
<tr>
<td></td>
<td>b) 15 hrs (1 SWS)</td>
<td></td>
<td>b) 10 students</td>
</tr>
</tbody>
</table>

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

#### 2. 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.

#### 3. Subject aims
- Introduction into Partial Differential Equation and Boundary Value Problems (BVP)
- Introduction to the Finite Element/Finite Volume Method in solid mechanics as method to solve BVP
- CALPHAD thermodynamics and kinetics of multicomponent diffusion
- Mean field models of microstructure evolution
- Rate equations for precipitation including numerical integration
- Introduction to free boundary problems
- Thermodynamic concept of the Phase-field method
- Linking of microstructure and mechanical properties

#### 4. Teaching methods
lecture, numerical exercises

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

#### 6. Assessment methods
written examination together with submodule 5b (3 hours for entire module 5). Bonus points can be gained by providing solutions to the problem sheets in class.

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

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

#### 9. Impact of grade on total grade
4/113

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

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

<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>
</tbody>
</table>

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

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

### Independent study
- 75 hours

### Class size
- a) 30 students
- b) 10-15 students

### Learning outcomes
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.

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

### Teaching methods
- Lecture, class, problem sheets

### Prerequisites for participation
Successful completion of “Theoretical and Applied Materials Science” (Module 3) is recommended.

### Assessment methods
- Written examination together with submodule 5a (3 hours for entire Module 5). Bonus points can be gained by providing solutions to the problem sheets in class.

### 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
- 4/113

### Responsibility for module
- Prof. Dr. Ralf Drautz

### Other information
- Lecture notes will be provided. Relevant literature will be discussed in the first lecture.
### 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>

#### 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 (2 hours) or oral examination (30 minutes) depending on size of the class. 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
none

#### Impact of grade on total grade
6/113

#### Responsibility for module
PD Dr. habil. Thomas Hammerschmidt, PD Dr. habil. Rebecca Janisch

#### Other information
Lecture notes will be provided.
Recommended Literature:
- J. M. Howe: Interfaces in materials, Wiley Interscience (1997);
## Module Descriptions

### DATA-DRIVEN 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>6-MS2</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>1</th>
<th>Types of courses:</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) lectures</td>
<td></td>
</tr>
<tr>
<td>b) hands-on practical studies</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2</th>
<th>Contact hours</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) 30 hrs (2 SWS)</td>
<td></td>
</tr>
<tr>
<td>b) 30 hrs (2 SWS)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>3</th>
<th>Independent study</th>
</tr>
</thead>
<tbody>
<tr>
<td>120 hours</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>Class size</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) 20 students</td>
<td></td>
</tr>
<tr>
<td>b) 20 students</td>
<td></td>
</tr>
</tbody>
</table>

### Learning outcomes

The students have an overview of data science in the context of materials science. This will include the most important concepts of data science, their mathematical foundation as well as their practical application in the field of materials science. The course will enable the students to organize and analyse data more efficiently.

### Subject aims

- Overview and taxonomy of data science
- Supervised learning, regression and classification
- Unsupervised learning, clustering, dimensionality reduction
- Data storage and organization, ontologies, databases of relevance in materials science
- Design and management of SQL and noSQL databases
- Data visualization and reporting
- Image and text mining
- Python tools and libraries for data science
- Multi-purpose notebooks for interactive data analytics

### Teaching methods

- lectures and hands-on computer classes

### Prerequisites for participation

- Basic knowledge in materials science, basic knowledge in Python.
- Completion of “Statistical methods in data analysis and design of experiments” recommended.

### Assessment methods

- successful completion of project work, written project report

### Prerequisites for the assignment of credit points

- none

### Impact on total grade

- 6/113

### Responsibility for module

- Prof. Dr. Drautz, Dr. Yury Lysogorskiy

### Other information

- Literature:
  - T. Hastie, R. Tibshirani, J. Friedman: The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Springer (2009);
  - K. Rajan (Editor): Informatics for Materials Science and Engineering, Butterworth-Heinemann (2013);
<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-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>
<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) 30 students</td>
</tr>
<tr>
<td>b) exercises</td>
<td>b) 30 hrs (2 SWS)</td>
<td></td>
<td>b) 10-15 students</td>
</tr>
</tbody>
</table>

**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.

**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

**Teaching methods**

lecture, exercises

**Prerequisites for participation**

Students must have good knowledge in statistical and condensed matter physics. Programming skills in C++ are of advantage.

**Assessment methods**

written exam (2 hours)

**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**

6/113

**Responsibility for module**

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

**Other information**

Lecture notes will be provided online.
### INTRODUCTION TO PARALLEL- & SCIENTIFIC-COMPUTING

<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>
</tbody>
</table>

1. **Types of courses:**
   - lecture

2. **Contact hours**
   - 60 hrs (4 SWS)

3. **Independent study**
   - 120 hours

4. **Class size**
   - 20 students

#### Learning outcomes
The students gain an introductory knowledge about parallel computing, parallel algorithms and applications of scientific computing. Introduction to the main parallel communication libraries will be provided (MPI for distributed memory parallel architectures and OpenMP for shared memory devices). Hands-on with specific problem oriented examples will support the experience in applying parallel computing methods. For different applications (e.g. particle methods, Monte Carlo, linear algebra) parallel algorithms are introduced, compared and assessed. Numerical algorithms for linear algebra, Fourier transforms or solvers for differential equations are introduced and discussed together with their potential for parallelisation. The students will gain practical experience with numerical libraries in accompanying projects that will be presented by the students in short talks.

#### Subject aims
- Parallel communication libraries MPI and OpenMP
- Parallel algorithms for particle methods, linear algebra, fast Fourier transforms
- Performance evaluation
- Numerical optimisation
- Application of numerical libraries
- Atomistic simulations with ASE

#### Teaching methods
- lecture, project work

#### Prerequisites for participation
- basic knowledge in higher programming languages

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

#### Prerequisites for the assignment of credit points
- passing exam and presentation of project work

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

#### Impact of grade on total grade
- 6/113

#### Responsibility for module
- Prof. Dr. Godehard Sutmann

#### Other information
- Slides of lectures will be provided.
## 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-MS5</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

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

### Independent study
- 120 hours

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

### 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
6/113

### Responsibility for module
Prof. Dr. rer. nat. Klaus Hackl, Prof. Dr. rer. nat. Khanh Chau 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);
<table>
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<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>6-MS6</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>2nd</td>
<td>summer</td>
<td>1 semester</td>
</tr>
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<table>
<thead>
<tr>
<th>Frequency</th>
<th>Duration</th>
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</thead>
<tbody>
<tr>
<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) 30 hrs (2 SWS)</td>
<td>120 hours</td>
<td>20 students</td>
</tr>
<tr>
<td>b) seminar</td>
<td>b) 30 hrs (2 SWS)</td>
<td></td>
<td></td>
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</table>

<table>
<thead>
<tr>
<th>Learning outcomes</th>
</tr>
</thead>
</table>
Students possess a conceptional understanding of complex phase transitions in solid state materials (e.g. superconducting and ferroic phases). They are familiar with state of the art analytical and numerical scale-bridging modelling methods in this field. Students can judge, compare and utilize these concepts and methods. They can identify the underlying physical properties.

<table>
<thead>
<tr>
<th>Subject aims</th>
</tr>
</thead>
</table>
- Introduction to complex phase transitions in solid state materials (e.g. magnetic, ferroelectric and superconducting phases)
- Classification of phase transitions and critical phenomena
- Models and simulation methods (e.g. spin models, Landau theory)

<table>
<thead>
<tr>
<th>Teaching methods</th>
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</thead>
</table>
lecture, seminar/project

<table>
<thead>
<tr>
<th>Prerequisites for participation</th>
</tr>
</thead>
</table>
basic knowledge on quantum mechanics / solid state physics and thermodynamics / statistical physics

<table>
<thead>
<tr>
<th>Assessment methods</th>
</tr>
</thead>
</table>
presentation of project work and short oral examination related to project

<table>
<thead>
<tr>
<th>Prerequisites for the assignment of credit points</th>
</tr>
</thead>
</table>
taking part in the seminar, successful oral presentation of the project

<table>
<thead>
<tr>
<th>This module is used in the following degree programmes as well</th>
</tr>
</thead>
</table>
Physics

<table>
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<tr>
<th>Impact of grade on total grade</th>
</tr>
</thead>
</table>
6/113

<table>
<thead>
<tr>
<th>Responsibility for module</th>
</tr>
</thead>
</table>
Prof. Dr. Anna Grünebohm, Prof. Dr. Ilya Eremin

<table>
<thead>
<tr>
<th>Other information</th>
</tr>
</thead>
</table>
Lecture notes will be provided.
THE CALPHAD METHOD IN THERMODYNAMICS AND DIFFUSION

<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-MS7</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**
   - 15 students

**Learning outcomes**
Students understand the concept of phase equilibrium, learn how to model Gibbs energy and its derivatives using fundamental theories and the connection to experimental determined thermodynamic properties. They learn to handle thermodynamic and diffusion databases. After a successful participation of the course students know the mathematical models of diffusion and numerical methods as well as diffusion processes. They will be able to understand physical relationships in the diffusion process and the connection to the thermodynamic properties. They learn to select a suitable model according to a requirement profile and are able to carry out simple material-specific simulations of diffusion processes in materials.

**Subject aims**
- Thermodynamic functions and calculation of phase diagrams.
- Constructions of the CALPHAD-type computational thermodynamic databases after critical evaluation of experimental information as well first- principles calculated data.
- Microstructure simulations using thermodynamic quantities
- Mathematical basics of the diffusion equation, diffusivity, mobility coefficients
- Diffusion as a coupling of mobility and thermodynamics
- Multicomponent Diffusion
- Introduction to DICTRA
- Mobility databases

**Teaching methods**
lecture, exercises, individual project, case studies, discussions, presentation of modeling results

**Prerequisites for participation**
basic knowledge in thermodynamics and statistical physics, basic knowledge of structure and properties of materials, ordinary differential equations.

**Assessment methods**
written report (10 to 15 pages) of individual project

**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**
6/113

**Responsibility for module**
Prof. Dr. Ingo Steinbach, Dr. Julia Kundin

**Other information**
Literature:
## 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>
</tr>
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<tbody>
<tr>
<td>7-PC1</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</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) 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
- 6/113

### 10. Responsibility for module
- Prof. Dr. Anjana Devi

### 11. Other information
- Lecture notes will be provided online.
### FUNDAMENTAL ASPECTS OF MATERIALS SCIENCE AND ENGINEERING (FAMSE)

<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>7-PC2</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) 45 hrs (3 SWS)
- b) 15 hrs (1 SWS)

#### 3 Independent study
120 hours

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

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

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

#### 4 Teaching methods
lecture, class

#### 5 Prerequisites for participation
successful completion of “Elements of Microstructure” (2a) and “Statistical Mechanics and Fundamental Materials Physics” (2c) recommended

#### 6 Assessment methods
oral examination (30 min.)

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

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

#### 9 Impact of grade on total grade
6/113

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

#### 11 Other information
A list with recommended literature and class notes will be available online.
### MEMS & NANOTECHNOLOGY

<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-PC3</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) 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 / 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 in Bereichen 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
- 6/113

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

### Other information
- The lecture will be held in German language.
<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>
<tr>
<td>7-PC4</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>2nd</td>
<td>summer</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) 15 hrs (1 SWS)

3. **Independent study**
   - 120 hours

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

**Learning outcomes**
Students will be familiar with the morphology/microstructure of polymers and shape memory alloys and know how to process these materials. They will understand the basic mechanical and functional properties of these two materials classes with a special focus on engineering applications and be familiar with scale bridging concepts, i.e. they can discuss macroscopic properties in view of atomistic interactions and morphological/microstructural features. Most importantly, they will understand the relation between morphology/microstructure and mechanical and functional properties.

**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**
6/113

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

**Other information**
Lecture notes will be provided.
### Module Descriptions

#### MULTISCALE MECHANICS OF MATERIALS

<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>8-MS1</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</td>
<td>winter term</td>
<td>1 semester</td>
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</table>

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

<table>
<thead>
<tr>
<th>2</th>
<th>Learning outcomes</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Students possess a fundamental understanding of the multiscale nature of the mechanical behaviour of materials and of the different approaches to take this into account in mechanical modelling of microstructures. They can identify the relevant length- and timescales of the microscopic processes that lead to meso-/macroscopic structure-property relationships. The students understand the principles of effective theory construction, coarse graining and homogenisation methods, and they can apply them to identify, analyse and model multiscale problems, such as plastic deformation, hardening behaviour, and fracture of microstructures. They are familiar with state of the art numerical and theoretical scale-bridging modelling methods. They can apply numerical tools on different length scales, and understand the underlying principles (atomistic modelling, discrete dislocation dynamics, crystal and continuum plasticity). Finally, students build up the skill to independently develop scale-bridging models that integrate all necessary scales and employ these models to describe and predict mechanical properties of materials under given conditions.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>3</th>
<th>Subject aims</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>- Introduction to problems in materials mechanics that involve multiple length and time scales</td>
</tr>
<tr>
<td></td>
<td>- Overview over principles and concepts of concurrent and hierarchical multiscale modeling of materials</td>
</tr>
<tr>
<td></td>
<td>- Principles of effective theory construction and its application in numerical modeling (extracting and passing information in hierarchical models); coarse graining and homogenisation</td>
</tr>
<tr>
<td></td>
<td>- Numerical models and technical aspects of hierarchical multiscale simulations (atomistic modeling, discrete dislocation dynamics, continuum and crystal plasticity)</td>
</tr>
<tr>
<td></td>
<td>- Overview over the state of the art in bridging length-scales in modeling of elasticity, plasticity, and fracture</td>
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<table>
<thead>
<tr>
<th>4</th>
<th>Teaching methods</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>lecture, computer exercises, and seminar</td>
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</table>

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<thead>
<tr>
<th>5</th>
<th>Prerequisites for participation</th>
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<tbody>
<tr>
<td></td>
<td>successful completion of “Basics in Materials Science” (module 2) or equivalent</td>
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<table>
<thead>
<tr>
<th>6</th>
<th>Assessment methods</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>oral (30 minutes) or written (2 hours) examination, depending on size of the class</td>
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<thead>
<tr>
<th>7</th>
<th>Prerequisites for the assignment of credit points</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>taking part in the exercises, passing the examination.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>8</th>
<th>This module is used in the following degree programmes as well</th>
</tr>
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<tbody>
<tr>
<td></td>
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<table>
<thead>
<tr>
<th>9</th>
<th>Impact of grade on total grade</th>
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<tbody>
<tr>
<td></td>
<td>6/113</td>
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<table>
<thead>
<tr>
<th>10</th>
<th>Responsibility for module</th>
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<tbody>
<tr>
<td></td>
<td>PD Dr. habil. Rebecca Janisch</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>11</th>
<th>Other information</th>
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<tbody>
<tr>
<td></td>
<td>Lecture notes will be provided.</td>
</tr>
<tr>
<td>Module code</td>
<td>Student workload</td>
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<td>-------------</td>
<td>------------------</td>
</tr>
<tr>
<td>8-MS2</td>
<td>180 hours</td>
</tr>
</tbody>
</table>

1. **Types of courses:**
   - a) lecture
   - b) classes focusing on hands-on computational tasks

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

3. **Independent study**
   - 120 hours

4. **Class size**
   - 20 students

2. **Learning outcomes**
The students gain fundamental knowledge of techniques and methods used in advanced atomistic simulations that address large system sizes, long-time scales, and long-range interactions. They can classify simulation methods including molecular statics, molecular dynamics and Monte Carlo simulations, and apply appropriate models of interatomic interactions (DFT, tight binding, empirical potentials). The students can evaluate the validity of the simulation outcomes and their relation to measurable material properties for several case studies. The students are able to plan, execute and monitor atomistic simulations.

3. **Subject aims**
   - Generation, analysis and optimization of atomic structures
   - Molecular statics and relaxation algorithms
   - Molecular dynamics in various ensembles, thermostats
   - Monte Carlo methods, spin lattice models, transition state theory
   - Accelerated techniques and hybrid approaches
   - Rigorous coarse-graining of atomic interaction models
   - Workflows for atomistic simulations
   - Case studies: e.g. elasticity and phonons, diffusion, ferroelectricity, melting

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

5. **Prerequisites for participation**
   - background in physics, chemistry or related discipline, knowledge of linux/unix environment and Python/C/ Fortran programming languages
   - participation in “advanced numerical methods: atomistic simulation methods” or similar course.

6. **Assessment methods**
   - oral (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**
   - 6/113

10. **Responsibility for module**
    - Prof. Dr. Anna Grünebohm and Dr. Matous Mrovec

11. **Other information**
    - ...
**Computational Fracture 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>8-MS3</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</td>
<td>winter 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) 30 hrs (2 SWS)

3. **Independent study:**
   120 hours

4. **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**
   6/113

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

11. **Other information**
    Lecture notes will be provided.
<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) 5 students</td>
</tr>
<tr>
<td>b) class</td>
<td>b) 30 hrs (2 SWS)</td>
<td></td>
<td>b) 5 students</td>
</tr>
</tbody>
</table>

### Learning outcomes
On successful completion of the MMM module, students will be able to:
1. Analyse different classes of engineering materials and correctly formulate the constitutive models for each class of materials.
2. Rationally design machines and structures (using the commercial programs) and reduce uncertainty in the design process.
3. Select appropriate material models for every specific class of engineering materials with the view of making engineering structures more economic.

### Subject aims
- Basic concepts of continuum mechanics (introduction)
- Mechanical characterization of materials (mainly solids) – test methods and data analysis
- Basic concepts of constitutive equations for engineering materials
- Classical (1-dimensional) models of elastic and inelastic materials
- Boundary value problems of linear elasticity
- Basic problems of inelastic behavior of materials (viscoelasticity, plasticity and damage)
- Basic concepts of strength of failure of engineering materials

### Teaching methods
Lecture, class

### Prerequisites for participation
Basic knowledge in mathematics and mechanics (statics, dynamics and strength of materials)

### 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 Course: Computational Engineering (Import lecture)

### Impact of grade on total grade
6/113

### Responsibility for module
Prof. Dr.-Ing. Daniel Balzani

### Other information
Literature:
- R. Lakes: Viscoelastic materials. Cambridge University Press (2009);
- El.H. Dill: Continuum mechanics: Elasticity, plasticity, viscoelasticity. CRC Press (2007);
# 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>
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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) 30 students</td>
</tr>
<tr>
<td>b) class</td>
<td>b) 30 hrs (2 SWS)</td>
<td></td>
<td>b) 30 students</td>
</tr>
</tbody>
</table>

## 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

6/113

## Responsibility for module

Prof. Dr. Ingo Steinbach

## Other information

Literature:
# ADVANCED MATERIALS PROCESSING AND MICROFABRICATION

<table>
<thead>
<tr>
<th>Module code</th>
<th>9-PC2</th>
<th>Student workload</th>
<th>180 hours</th>
<th>Credits</th>
<th>6 ECTS</th>
<th>Semester</th>
<th>3rd</th>
<th>Frequency</th>
<th>winter term</th>
<th>Duration</th>
<th>1 semester</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>Types of courses:</td>
<td></td>
<td></td>
<td>Contact hours</td>
<td></td>
<td>Independent study</td>
<td>120 hours</td>
<td></td>
<td>Class size</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>a) lecture</td>
<td></td>
<td></td>
<td>a) 45 hrs (3 SWS)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>a) 10 students</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>b) class</td>
<td></td>
<td></td>
<td>b) 15 hrs (1 SWS)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>b) 10 students</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

## 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

6/113

## 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>
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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) 45 hrs (3 SWS)
   - b) 15 hrs (1 SWS)

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

4. **Class size:**
   - a) 25 students
   - b) 25 students

2. **Learning outcomes**
   Students will gain a fundamental understanding of corrosion science, from basic electrochemistry of homogeneous metal corrosion to general aspects of localized corrosion, as well as of complex components and structures. They will 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.

3. **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

4. **Teaching methods**
   - lecture, class, including a short lab course

5. **Prerequisites for participation**
   - successful completion of “Statistical Mechanics and Fundamental Materials Physics” (2c) and “Elements of Microstructure” (2a) recommended.

6. **Assessment methods**
   - written examination (2 hours)

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

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

9. **Impact of grade on total grade**
   - 6/113

10. **Responsibility for module**
    - Prof. Dr. rer. nat. Martin Stratmann, Dr. rer. nat. Michael Rohwerder

11. **Other information**
    - Lecture notes will be provided.
## MATERIALS FOR AEROSPACE APPLICATIONS

<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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<td>6 ECTS</td>
<td>3rd</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

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

### Contact hours:
- a) 45 hrs (3 SWS)
- b) 15 hrs (1 SWS)

### Independent study:
- 120 hours

### Class size:
- a) 25 students
- b) 25 students

### 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.

### Subject aims
- Loading conditions for components of air- and space crafts (structures and engines)
- Development of materials and material systems for specific service conditions in aerospace applications (e.g. for aero-engines, rocket engines, thermal protection shields for re-entry vehicles, light weight structures for airframes, wings, and satellites)
- Degradation and damage mechanisms of aerospace materials and material systems under service conditions
- Characterization and testing methods for materials and joints for aerospace applications
- Concepts and methods for lifetime assessment. Introduction to concepts of mechanical properties of materials (stress-strain curves, stiffness, strength, ductility)

### Teaching methods
lecture, class

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

### Assessment methods
written (2 hours) or oral (30 minutes) examination, depending on number of students

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

### 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

### Impact of grade on total grade
6/113

### Responsibility for module
Prof. Dr.-Ing. Marion Bartsch

### Other information
Lecture notes will be provided online.
## INTRODUCTION TO THREE-DIMENSIONAL MATERIALS CHARACTERIZATION TECHNIQUES

<table>
<thead>
<tr>
<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>3rd</th>
<th>Frequency</th>
<th>winter term</th>
<th>Duration</th>
<th>1 semester</th>
</tr>
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</table>

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

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

3. **Independent study**
   - 120 hours

4. **Class size**
   - a) 15 students
   - b) 15 students

### Learning outcomes
This course provides an introduction to a range of three-dimensional nanoscale and atomic scale materials characterization techniques, 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
- submission of a report (100 %)

### 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
- 6/113

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

### Other information
- 

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Materials Science and Simulation
## GENERAL OPTIONAL SUBJECT

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<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
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<tr>
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<td>180 hours</td>
<td>6 ECTS</td>
<td>1st</td>
<td>free choice of available modules</td>
<td>1 semester</td>
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<table>
<thead>
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<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
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<tr>
<td>2</td>
<td>Learning outcomes</td>
<td>60 hrs</td>
<td>120 hours</td>
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<td>3</td>
<td>Subject aims</td>
<td></td>
<td></td>
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</tr>
<tr>
<td></td>
<td>• Develop knowledge and skills in fields beyond engineering and science</td>
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<tr>
<td></td>
<td>• Deepen knowledge about specific topics in Materials Science and Simulation according to own interests</td>
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<tr>
<td></td>
<td>Any module from a Master’s course will be recognized. Some suggested courses are listed in the following as modules 10-1 to 10-6</td>
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<table>
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<th>4</th>
<th>Teaching methods</th>
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<table>
<thead>
<tr>
<th>5</th>
<th>Prerequisites for participation</th>
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<table>
<thead>
<tr>
<th>6</th>
<th>Assessment methods</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>written or oral examination as given in specific module description</td>
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<table>
<thead>
<tr>
<th>7</th>
<th>Prerequisites for the assignment of credit points</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>passing the examination</td>
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<table>
<thead>
<tr>
<th>8</th>
<th>This module is used in the following degree programmes as well</th>
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<tbody>
<tr>
<td></td>
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<table>
<thead>
<tr>
<th>9</th>
<th>Impact of grade on total grade</th>
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<td></td>
<td>6/113</td>
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<table>
<thead>
<tr>
<th>11</th>
<th>Other information</th>
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## APPLICATION AND IMPLEMENTATION OF ELECTRONIC STRUCTURE METHODS

<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>
</tr>
</tbody>
</table>

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

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

3. **Independent study**
   - 120 hours

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

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#### 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.

#### 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)

#### Teaching methods

lecture, practical studies and group seminars

#### Prerequisites for participation

successful completion of “Introduction to Quantum Mechanics in Solid State Physics” is recommended.

#### Assessment methods

written examination (1.5 hours)

#### Prerequisites for the assignment of credit points

positively evaluated written report and passing of exam

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

none

#### Impact of grade on total grade

6/113

#### Responsibility for module

Prof. Dr. Ralf Drautz, Prof. Dr. Jörg Neugebauer

#### Other information

Lecture notes will be provided.
<table>
<thead>
<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
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<tr>
<td>10-2</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>3rd</td>
<td>winter</td>
<td>1 semester</td>
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<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>

### Learning outcomes

On successful completion of this module, students will be familiar with equations of hydrodynamics and their solutions for simple cases such as hydrostatic pressure in an ideal gas (barometric formula), planar Couette flow and the Poiseuille flow. The lecture also provides an introduction to the lattice Boltzmann method (LBM) and a simple code for simulating flow via LBM. Using the above mentioned simple cases, the students will be able to examine the validity of the LBM code and also address a number of interesting problems such as Laplace law for pressure difference in drops and their environments and wetting of liquids on solid surfaces.

### Subject aims

- Introduction to fluid dynamics on continuum level (Euler and Navier-Stokes equations)
- Basics of the lattice Boltzmann method (LBM)
- Simulation of multiphase fluids: drops, bubbles
- Wetting

### Teaching methods

lecture, group work, case studies, discussions

### Prerequisites for participation

familiarity with computer programming (C, Fortran, 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

6/113

### Responsibility for module

Prof. Dr. Fathollah Varnik

### Other information

Lecture notes will be provided.
<table>
<thead>
<tr>
<th>Module code</th>
<th>Student work-load</th>
<th>Credits</th>
<th>Semester</th>
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<th>Duration</th>
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<tbody>
<tr>
<td>10-3</td>
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<td>6 ECTS</td>
<td>1st/3rd</td>
<td>winter</td>
<td>1 semester</td>
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**Types of courses**
- a) lecture
- b) class

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

**Independent study** 120 hours

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

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**Learning outcomes**
The students will gain knowledge about the theory and applications of bond order potentials (BOPs) in atomistic simulations. The course will cover theoretical foundations of BOPs as well as their development, validation and applications. The lectures will be accompanied by practical exercises and individual projects to obtain hands-on experience with the BOP models for various materials and their properties.

**Subject aims**
- Tight-binding approximation
- Lanczos algorithm and Greens functions
- Recursion method and continued fraction, terminators
- Numerical BOP
- Analytic BOP
- Kernel-polynomial method
- Onsite-levels and self-consistency
- Magnetism, charge-transfer
- Forces
- Parameterization and validation
- Applications

**Teaching methods**
lecture, computer exercises, seminars

**Prerequisites for participation**
completion of module 2 or equivalent

**Assessment methods**
individual project and/or oral (30 minutes) examination, depending on the size of the class

**Prerequisites for the assignment of credit points**
successful completion of the project/passing the exam

This module is used in the following degree programmes as well

none

**Impact of grade on total grade**
6/113

**Responsibility for module**
Dr. Matous Mrovec, Dr. Thomas Hammerschmidt

**Other information**
Lecture notes will be provided.
## 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>10-4</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
- Lecture and class
- Contact hours: 60 hrs (4 SWS)
- Independent study: 120 hours
- Class size: no restrictions

### Learning outcomes
After successfully completing the module, the students can remember the definitions of the classifications of mechanical behavior and to which materials the different types of behavior can be associated. They understand the phenomenology and mechanisms of elastic and plastic behavior of crystalline materials and know the different types of plasticity models in solid mechanics. Furthermore, they understand the basic concepts and the mathematical formulation of continuum plasticity and crystal plasticity. They also understand the basic concepts of the numerical implementation of plasticity models and can assess which method is most suited to solve a given mechanical problem. Students are able to implement and apply a numerical scheme for the solution of elasto-plastic problems within the finite element method and have basic knowledge about the use of homogenization methods to describe plasticity in polycrystals.

### Subject aims
- Basics of continuum mechanics and FEM
- Phenomenology and atomistic origin of elastic and plastic deformation
- Concepts of continuum plasticity (yield criterion, flow rule, isotropic and kinematic hardening)
- Rate dependent and rate-independent formulations of continuum plasticity
- Numerical solution schemes for elasto-plasticity (operator split, return mapping, consistent tangent modulus)
- Computational aspects of small and large strain formulations
- Concepts of crystal plasticity (dislocation slip, flow rule, hardening models, consistent tangent modulus)
- Plasticity of polycrystals (Sachs, Taylor and self-consistent model)
- Numerical solution schemes of the crystal plasticity method
- Structure, implementation and application of an Abaqus UMAT

### Teaching methods
- Lecture (2h/week), exercises (2h/week) / team project incl. Seminar talk/English

### Prerequisites for participation
- None

### Assessment methods
- Portfolio exam including report on project and seminar

### Prerequisites for the assignment of credit points
- Passed final module examination

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

### Impact of grade on total grade
- 6/113

### Responsibility for module
- Prof. Dr. Alexander Hartmaier, assistants

### 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>10-5</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>2nd</td>
<td>summer</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

#### Contact hours
- a) lecture: 30 hrs (2 SWS)
- b) class: 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 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.

#### 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.

#### Teaching methods
lecture, class, homework

#### Prerequisites for participation
basics in mathematics, mechanics and structural analysis; finite element methods in linear structural mechanics

#### Assessment methods
written examination (2 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
6/113

#### 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
- T. Belytschko and W.K. Liu: Nonlinear finite elements for continua and structures, Wiley (2000);
**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>10-6</td>
<td>180 hours</td>
<td>6 ECTS</td>
<td>1st</td>
<td>winter</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 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.

3. **Subject aims**
   - Introduction to the finite element method in the framework of linear elastomechanics and elastodynamics
   - Step by step explanation of principles of spatial discretization using the finite element method.
   - One-dimensional isoparametric 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

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

5. **Prerequisites for participation**
   basics in mathematics, mechanics and structural analysis

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

7. **Prerequisites for the assignment of credit points**
   passing the written examination

8. **This module is used in the following degree programmes as well**
   Master of Science in Computational Engineering

9. **Impact of grade on total grade**
   6/113

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

11. **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);
## Module Descriptions

### Optional Scientific or Engineering 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>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>

<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>lecture and class</td>
<td>40 hrs</td>
<td>80 hours</td>
<td></td>
</tr>
</tbody>
</table>

### Learning outcomes

By freely choosing lectures students can widen their skill or method spectrum and set an individual focus to their curriculum matching 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 engineering or science master’s courses will be recognized.

### 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

4/113

### Responsibility for module

see specific module description

### Other information
### MACHINE LEARNING METHODS IN DATA ANALYSIS AND 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>11-1</td>
<td>120 hours</td>
<td>4 ECTS</td>
<td>2nd</td>
<td>summer</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

#### 1 Types of courses:
- Lecture incl. practical hands-on with Python using Jupyter notebook

#### 2 Learning outcomes
This course provides a basic understanding, knowledge and practical skills of data-science as well as the application of the main data-driven methods for analysing and processing material science data. The students understand the importance of a statistical description of data sets and can apply the concepts of moments of a distribution (average, median, variance, skewness) on arbitrary data sets. They can perform the significance test to identify influence parameters that show a strong impact on the data sets. Furthermore, they are able to formulate and test different hypotheses and to provide a significance level for the acceptance or rejection of a hypothesis. The students will be able to write their own Python code to conduct such tests and apply it to formulating mathematical (statistical learning) models to describe data sets. The students are given an overview of statistical methods for data analysis and processing, including main steps such as data preparation, outlier detection, identification of main influence parameters, formulation and solution of regression and classification problems. The lecture materials and practical hands-on in Python are provided for each topic.

#### 3 Subject aims
- Introduction into statistical description of data sets
- Differences between statistical analysis, machine learning and data mining: definitions, main ideas and principles
- Reliability of data and sources of error
- Data preparation and outlier detection
- Formulation of hypotheses and significance tests
- Fitting and smoothing of data
- Statistical validation of results and their presentation
- Quantitative description of data with empirical models
- Identification of true effects and interactions
- Classification and clustering
- Hands-on exercises on data analysis and processing

#### 4 Teaching methods
Lecture, practical class with hands-on computer exercises

#### 5 Prerequisites for participation
None

#### 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
4/113

#### 10 Responsibility for module
Dr. Irina Roslyakova

#### 11 Other information
Lecture notes (pdf slides) and practical hands-on (Jupyter notebook) will be provided.
### 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>11-2</td>
<td>120 hours</td>
<td>4 ECTS</td>
<td>2nd</td>
<td>summer</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

#### Learning outcomes

The students obtain a profound knowledge about engineering ceramics and their technical applications. This will include details on the manufacture of engineering ceramics covering examples of the major processing steps. Also manufacturing routes for fibre reinforced ceramic matrix composites will be presented. Furthermore, an overview on the typical thermo-mechanical as well as functional properties of ceramics will be given. This should allow the student the selection of ceramics for specific needs.

In addition, a basic knowledge on coating technologies for thick layers of especially ceramic materials will be given. This will include thermal spray and sintering technologies. The students will be able to select suitable coating methods for wear, corrosion, functional and high temperature applications.

#### Subject aims

- Powder synthesis & conditioning, shaping, sintering of ceramic materials
- Characterisation of ceramics with different methods
- Properties & applications of engineering ceramics
- Basic knowledge on different thick film deposition technologies (thermal spray processes and sintering techniques)
- Demonstration how coatings can improve the functionality of components

#### Teaching methods

- lecture, class

#### Prerequisites for participation

Knowledge in materials properties is recommended.

#### Assessment methods

- oral examination (20 minutes) or written examination

#### Prerequisites for the assignment of credit points

- passing the exam

#### Impact of grade on total grade

- 4/113

#### Responsibility for module

- Prof. Dr. Robert Vaßen

#### Other information

- Literature:
  - Plasma Spray Coating, Robert B. Heiman, Wiley, 2008
  - Slides will be available online.
<table>
<thead>
<tr>
<th></th>
<th>MATERIALS INFORMATICS</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><strong>Module code</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Student workload</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Credits</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Semester</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Frequency</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Duration</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Type(s) of course(s):</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Contact hours</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Independent study</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Class size</strong></td>
</tr>
<tr>
<td>2</td>
<td><strong>Learning outcomes</strong></td>
</tr>
<tr>
<td></td>
<td>The course covers selected mathematical topics encountered in materials modelling and in related</td>
</tr>
<tr>
<td></td>
<td>This seminar aims to be a discussion forum around the emerging field of ‘Material Informatics’ for</td>
</tr>
<tr>
<td></td>
<td>Master and PhD students. The seminar is a series of presentations followed by discussion, started</td>
</tr>
<tr>
<td></td>
<td>by the teacher and followed by the students. Presentations will tackle current articles in the scientific</td>
</tr>
<tr>
<td></td>
<td>literature which try to define ‘Materials Informatics’.</td>
</tr>
<tr>
<td>3</td>
<td><strong>Subject aims</strong></td>
</tr>
<tr>
<td></td>
<td>• outline the ideas of the emerging field of Materials Informatics and describe the current</td>
</tr>
<tr>
<td></td>
<td>• independently read, assess and evaluate scientific literature.</td>
</tr>
<tr>
<td></td>
<td>• present a complex scientific subject to an informed audience.</td>
</tr>
<tr>
<td></td>
<td>• can judge and argue for or against a research approach/idea.</td>
</tr>
<tr>
<td>4</td>
<td><strong>Teaching methods</strong></td>
</tr>
<tr>
<td>5</td>
<td><strong>Prerequisites for participation</strong></td>
</tr>
<tr>
<td>6</td>
<td><strong>Assessment methods</strong></td>
</tr>
<tr>
<td></td>
<td>Students read one article per week and will write a short review about the article. Every week, one</td>
</tr>
<tr>
<td></td>
<td>student will gather the reviews, present the topic, and lead the discussion. Discussions will evaluate</td>
</tr>
<tr>
<td></td>
<td>the approach and identify open questions.</td>
</tr>
<tr>
<td></td>
<td>Presentation (40%), oral exam 30 min (60%)</td>
</tr>
<tr>
<td>7</td>
<td><strong>Prerequisites for the assignment of credit points</strong></td>
</tr>
<tr>
<td>8</td>
<td><strong>This module is used in the following degree programmes as well</strong></td>
</tr>
<tr>
<td>9</td>
<td><strong>Impact on total grade</strong></td>
</tr>
<tr>
<td>10</td>
<td><strong>Responsibility for module</strong></td>
</tr>
<tr>
<td>11</td>
<td><strong>Other information</strong></td>
</tr>
</tbody>
</table>
### PRACTICAL APPLICATIONS OF MATERIAL INFORMATICS WITH R

<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>11-4</td>
<td>120 hours</td>
<td>4 ECTS</td>
<td>3rd</td>
<td>winter</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

1. **Types of courses:**
   - a) lectures
   - b) hands-on practical studies

2. **Contact hours**
   - a) 20 hrs (2 SWS)
   - b) 20 hrs (2 SWS)

3. **Independent study**
   - 80 hours
4. **Class size**
   - a) 20 students
   - b) 20 students

#### Learning outcomes

The students have an overview of material informatics, its main components, methods and tools. Lecture and hands-on cover a basic introduction into computational algorithms, database design, machine learning and statistical analysis methods as well as their mathematical foundations. The main goals of this course will focus on the analysis of data-driven modeling strategies of several application problems to identify the most appropriate solution in each considered case. The course materials cover the analysis of optimal data structure, required steps in data preparation process, selection and application of statistical and machine learning methods, analysis of implementation environment as well as efficient strategies for reporting and visualization of results. All exercises will be performed in R and the main differences to Python will be discussed.

#### Subject aims

- Introduction to Material informatics, its difference from other related disciplines
- Introduction to R, main data types and structures, main differences from Python
- Generic and user-defined functions
- Writing efficient code in R: comparison of possible solutions
- Efficient data management strategies: SQL vs. NoSQL database, existing materials databases
- Data preparation and outlier detection
- Statistical and machine learning: common points and main differences
- Supervised and unsupervised statistical/machine learning
- Data visualization and reporting
- Computer-based materials design

#### Teaching methods

lectures and hands-on computer classes

#### Prerequisites for participation

- basic knowledge in materials science, basic knowledge in Python
- completion of “Statistical methods in data analysis and design of experiments” and “Data-driven Materials Science” is recommended
- it is also recommended to participate in the course “Material Informatics” with Prof. M. Stricker

#### Assessment methods

oral (20 minutes) or written exam (1.5 hours/CIP-pool), depending on size of the class

#### Prerequisites for the assignment of credit points

none

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

none

#### Impact on total grade

4/113

#### Responsibility for module

Dr. Irina Roslyakova

#### Other information

Literature:
- F. Chollet, J.J.Allaire, Deep Learning with R, Manning Publications (2018);
### MATHEMATICS FOR MATERIALS 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>11-5</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>Types of courses:</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) lectures</td>
</tr>
<tr>
<td>b) exercises</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Contact hours</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) 30 hrs (2 SWS)</td>
</tr>
<tr>
<td>b) 15 hrs (1 SWS)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Independent study</th>
</tr>
</thead>
<tbody>
<tr>
<td>75 hours</td>
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</tbody>
</table>

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

#### 2 Learning outcomes

The course covers selected mathematical topics encountered in materials modelling and in related courses on quantum mechanics, statistical mechanics, thermodynamics and transport phenomena. The course will enable students to solve specific problems in integral and differential calculus and linear algebra that appear in physics and materials science and to understand common mathematical concepts in these fields.

#### 3 Subject aims

- Complex analysis (functions of complex variable, Cauchy’s and residue theorem)
- Analytic functions and their use in evaluation of definite integrals
- Vectors and matrices
- Linear transformations and tensors
- Fourier series
- Dirac’s delta function
- Integral transforms (Fourier, Laplace, convolution theorem)
- Sturm-Liouville theory of linear differential operators
- Partial differential equations

#### 4 Teaching methods

- lectures and exercises

#### 5 Prerequisites for participation

undergraduate level of mathematics for materials science and engineering

#### 6 Assessment methods

t.b.a.

#### 7 Prerequisites for the assignment of credit points

none

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

none

#### 9 Impact on total grade

4/113

#### 10 Responsibility for module

Dr. Matous Mrovec

#### 11 Other information

- Literature:
  - Erwin Kreyszig: Advanced Engineering Mathematics
  - George Arfken: Mathematical Methods for Physicists
  - Mary L. Boas: Mathematical Methods in Physical Sciences
## NON-TECHNICAL/NON-SCIENTIFIC OPTIONAL MODULE

<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>12</td>
<td>120 hours</td>
<td>4/3 ECTS</td>
<td>1st/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
- 45 hrs

### 3 Independent study
- 75 hours

### 4 Class size

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

### 6 Subject aims
- Develop knowledge and skills in fields beyond engineering and science
- Gain and develop knowledge in non-technical subjects, related to materials engineering, like business administration according to own interests
- Develop and practice communication skills
- Any module from a Master’s course will be recognized. Module 12a is an example of a course offered at ICAMS.

### 7 Teaching methods
see specific module descriptions

### 8 Prerequisites for participation
none

### 9 Assessment methods
written or oral examination as given in specific module description

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

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

### 12 Impact of grade on total grade
---

### 13 Responsibility for module
see specific module description

### 14 Other information
### 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>

#### Learning outcomes
Successful participants are able to prepare different types of scientific documents. They know structural elements of different formats and tools for scientific typesetting, plotting and producing graphics. Students are able to carry out a literature research on a topic in materials research independently, as well as to summarise their findings in a written report, using adequate citing techniques and avoiding plagiarism. The students learn how to summarize their findings in a short oral presentation. They are aware of the rules of good scientific practice.

#### 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

#### Teaching methods
lecture and hands-on tutorials in CIP-pool, literature-review as independent study

#### Prerequisites for participation
none

#### Assessment methods
written report, short oral presentation

#### 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.

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

#### Impact of grade on total grade
---

#### Responsibility for module
Prof. Dr. Anna Grünebohm, Dr. Manuel Piacenza

#### 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>
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</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>
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<table>
<thead>
<tr>
<th></th>
<th>Types of courses: practical work</th>
<th>Contact hours 80 hrs</th>
<th>Independent study 100 hours</th>
<th>Class size 1-3 students</th>
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<table>
<thead>
<tr>
<th></th>
<th>Learning outcomes</th>
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<tbody>
<tr>
<td>2</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>
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</table>

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

<table>
<thead>
<tr>
<th></th>
<th>Teaching methods</th>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>4</td>
<td>continuous contact periods to advice the student, presentation of progress during group seminars and discussions</td>
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<table>
<thead>
<tr>
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<tbody>
<tr>
<td>5</td>
<td>successful completion of all compulsory modules of first and second semester</td>
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<table>
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<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>6</td>
<td>written report (20 to 50 pages)</td>
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<tbody>
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<td>7</td>
<td>positively evaluated written report</td>
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<tr>
<th></th>
<th>This module is used in the following degree programmes as well</th>
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<tbody>
<tr>
<td>8</td>
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<table>
<thead>
<tr>
<th></th>
<th>Impact of grade on total grade</th>
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<tr>
<td>9</td>
<td>6/113</td>
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<tbody>
<tr>
<td>10</td>
<td>all lecturers of the Master course</td>
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<table>
<thead>
<tr>
<th></th>
<th>Other information</th>
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## MASTER THESIS

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<tr>
<th>Module code</th>
<th>Student workload</th>
<th>Student work</th>
<th>Credits</th>
<th>Semester</th>
<th>Frequency</th>
<th>Duration</th>
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<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>
<thead>
<tr>
<th>Types of courses: practical work</th>
<th>Contact hours</th>
<th>Independent study</th>
<th>Class size</th>
</tr>
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<tbody>
<tr>
<td>100 hrs</td>
<td>800 hours</td>
<td>1 student</td>
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<table>
<thead>
<tr>
<th>Learning outcomes</th>
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</thead>
<tbody>
<tr>
<td>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.</td>
</tr>
</tbody>
</table>

<table>
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<tbody>
<tr>
<td>- Independent scientific project</td>
</tr>
<tr>
<td>- Application of learned techniques from previous modules</td>
</tr>
<tr>
<td>- Independent identification and solution of scientific problems</td>
</tr>
<tr>
<td>- Literature survey</td>
</tr>
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<td>- Written and oral presentation of the results</td>
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<tr>
<td>successful completion of project work (module 13) and a total of at least 80 ECTS from all modules</td>
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<tr>
<th>Assessment methods</th>
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<tbody>
<tr>
<td>written thesis (40 to 150 pages)</td>
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<tr>
<td>positively evaluated thesis</td>
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