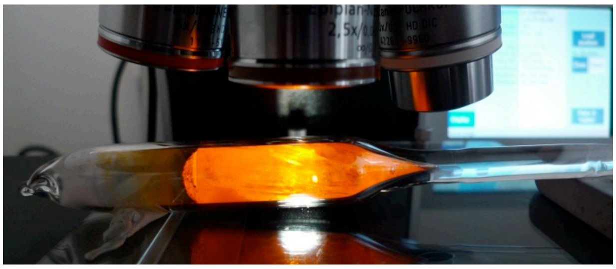
Crystallography, Institute of Earth and Environmental Sciences,
Albert-Ludwigs-University Freiburg

# Module guide M.Sc. Sustainable Materials – Crystalline Materials

(Examination Regulations 2017)



Freiburg, November 27, 2018

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# 1. Module guide M.Sc. Sustainable Materials – specialized Crystalline Materials

The M.Sc. Sustainable Materials - Crystalline Materials is an internationally accepted degree. The Master of Science (M.Sc.) is an internationally accredited certificate that can be completed within four semesters. The guide informs students about the vision, the structure, and the course of the master program and provides necessary details of the individual courses and modules. Based on Crystallography, the highly interdisciplinary courses cover the current state of the art materials research. Together with the other profiles of the M.Sc. Sustainable Materials it reflects the main areas of materials research in Freiburg. This module guide is for students taking the Crystalline Materials profile. It is intended to provide a description of the course aims and objectives, the course structure, content assessment and management. It also describes the regulations and processes associated with the course.

Crystalline Materials are the fundamental building blocks of modern materials science and technology. The solid state of a large variety of materials is a crystalline state. The topics of this master course are the understanding of the structure and the formation of the crystalline state, as well as the related technology. The study of crystalline materials is covered by many disciplines and the occupational area is broad. Chemistry, physics, mathematics, and engineering science are part of this master course. The student will learn the basics of crystal growth, material characterization, crystallography, and semiconductor technology. The teaching and training of these skills will provide an excellent position for the job market in the future. The list of possible applications is large. Here is just a selection of careers of recent alumni:

- Semiconductor industry for electronic and photonic devices
- Photovoltaic industry,
- Protein analysis in Pharmaceutical industry,
- Sensor and detector development for Medical and Industrial applications.
- Fuel Cells and Water Electrolysis,
- Ceramics-, Glass- and Cement industry.

## 1.1 Why choose the crystalline materials profile?

The crystalline materials profile is associated with the Chair of Crystallography at the Institute of Earth and Environmental Natural Sciences, which in turn belongs to the Faculty of Environment and Natural Resources. There are also strong connections to the Institutes of Inorganic and Analytical Chemistry in the Chemistry Faculty, the Faculty for Microsystems Engineering as well as to the Freiburg Materials Research Center (FMF) of the University, the

Fraunhofer Institutes for Solar Energy Systems (ISE), Applied Solid State Physics (IAF), Physical Measurement Techniques (IPM), and High-Speed Dynamics (EMI), as well as with the Swiss Federal Laboratories for Materials Testing and Research (EMPA) in Dübendorf, Switzerland. The Crystallography in Freiburg is housed in a recently renovated building and provides excellent conditions for study.

## 1.2 Freiburg´s core areas of expertise in research and education

The M.Sc. Sustainable Materials - Crystalline Materials program covers the areas of crystal growth for scientific and industrial applications, crystal growth experiments in space, semiconductor physics and technology, sensor and detector development, and a broad range of material characterization techniques. The scientific activities are carried out in close collaborations with national and international academic and industrial partners.

High technology laboratory equipment is available for practical training in the courses and for preparing the master thesis. At the Crystallography building and the Freiburg Materials research Center FMF the following facilities are part of the M.Sc. Crystalline Materials:

- Crystal growth facilities for melt, solution, and vapor growth
- Powder and single crystal X-ray diffractometers
- Polarized light and infrared microscopy
- Electron Microscopes with X-ray Energy Dispersive Analysis (EDS) and Electron Backscattered Diffractometry (EBSD)
- Molecular Beam Epitaxy facilities for growth of semiconductor films
- Cleanroom Facility with Lithography, Reactive Ion Etcher and Flip-Chip Bonder
- Hall-, van-der Pauw and related electrical characterization systems

## 1.3 The application

The application procedure for the graduate program is available online: http://www.cup.uni-freiburg.de/chemie/studium/msc_Crystalline%20Materials/studieninteressierte

Application deadline is July 15 each year, but for international students it is better to apply until May 15. The curriculum starts in the winter semester only.

The M.Sc. program Sustainable Materials - Crystalline Materials is accessible to all students, who have acquired a B.Sc. in Chemistry, Physics, Materials Science, Microsystems Engineering, and Geosciences from a German university, or from other universities and colleges world-wide (in accordance with certain quality control criteria). The applicant must have English-language skills that meet or exceed level B2 of the Common European Framework of Reference for Languages.

Questions concerning the general application and admission procedure should be addressed to the Application and Admission Coordinator Dr. Sabine Richter:

- **Application and Admission Coordinator**
  Dr. Sabine Richter: +49 (0)761/203-6063; sabine.richter@cup.uni-freiburg.de;
  Albertstr. 21, 79104 Freiburg im Breisgau, Germany

Specific questions concerning the major Crystalline Materials should be addressed to Prof. Dr. Andreas Danilewsky:

- **Head of the Crystalline Materials Program and Student Advisory Support**
  Prof. Dr. Andreas Danilewsky: +49 (0)761/203-6450; a.danilewsky@krist.uni-freiburg.de; Hermann-Herder-Strasse 5; 2nd floor, room 02 015, 79104 Freiburg im Breisgau, Germany

For organizational queries concerning the course of study, the program coordinator of the Crystalline Materials is the contact person:

- **Crystalline Materials Program Coordinator:**
  Ms. Wibke Kowalski, +49 (0)761/203-6398; wibke.kowalski@minpet.uni-freiburg.de
  Albertstr. 23-B, 1st floor, room 01 020, 79104 Freiburg im Breisgau, Germany

Questions about registration for examinations and Transcripts of Records should be addressed to the Examination Office:

- **Examination Office**
  http://www.cup.uni-freiburg.de/chemie/studium/pruefungsamt;
  Ms. Erika Dunai-Kovacs, +49 (0)761/203-6461; erika.dunai@cup.uni-freiburg.de
  Albert-Ludwigs-Universität, Prüfungsamt der Fakultät für Chemie und Pharmazie, Hebelstr. 27, D-79104 Freiburg

## 1.4 What constitutes our masters program?

The configuration and courses of the master program are providing a broad education in materials science and crystallography and is listed below. Official language of the program is English.

# 2. M.Sc. Sustainable Materials – Specialized Crystalline Materials

## 2.1 Compulsory Modules

**Annotations: B = Block Course, L = Lecture, P = Practical Course, F = Field Course**

| Module Name | Module Responsibility | Course Name | Type | ECTS Points | Sem. |
|---|---|---|---|---|---|
| **Crystal Growth** | **Danilewsky** | Crystal Growth Technology | L | **3** | 1 |
| | | Crystal Growth Methods I | P | **3** | 1 |
| | | Growth Kinetics | L | **1** | 2 |
| | | Crystal Growth Methods II | P | **2** | 2 |
| | | Crystal Preparation | P | **2** | 2 |
| | | Epitaxy | L | **1** | 2 |
| **Advanced Crystallography** | **Danilewsky** | Crystallographic Methodology | L+P | **3** | 1 |
| | | Space Groups and Crystal Struc-tures | L+P | **3** | 1 |
| **Physical and Chemical Ana-lytical Procedures** | **Danilewsky** | Physical and Chemical Analytical Procedures | L+P | **6** | 1/3 |
| **Sustainability** | **Hillebrecht** | See announcements | L+P | **6** | 1-3 |
| **Advanced Analytical Me-thods** | **Fiederle** | High-Resolution Spectroscopy | L+P | **3** | 2 |
| | | X-Ray Diffraction by Crystals | L+P | **3** | 2 |
| **Defects** | **Danilewsky** | Crystal Defects | L+P | **3** | 2 |
| | | Electrical and Optical Characte-rization Methods | L+P | **3** | 2 |

| | | | | | |
|---|---|---|---|---|---|
| **Applied Materials I** | **Fiederle** | Crystal Physics | L+P | **3** | 2 |
| | | Semiconductors | L+P | **3** | 2 |
| **Applied Materials II** | **Fiederle** | Semiconductor Technology | L+P | **3** | 3 |
| | | Electrical Characterization of Crystals and Devices | P | **3** | 3 |
| **X-Ray Methods** | **Danilewsky** | Structure Analysis by X-Ray Diffraction | L+P | **3** | 3 |
| | | Defect Analysis by Diffraction | L+P | **3** | 3 |
| **Technical and Applied Mineralogy** | **Sorgenfrei** | Modern Ceramics, Cements, and Glasses | L+P | **4** | 3 |
| | | Thermal Analysis | P | **2** | 3 |
| **Field Trips and Seminars** | **Danilewsky** | Seminar: Recent publications | L | **3** | 3 |
| | | Advanced Seminar on In-House Research | L | **1** | 3 |
| | | Field Trips to Industrial Facilities | F | **2** | 1-3 |

## 2.2 Methods and Concepts - Elective Module

| Module Name | Module Responsibility | Type | ECTS Points | Sem. |
|---|---|---|---|---|
| **Methods and Concepts** | **Danilewsky** | L, P, L + P | **18** | 1-3 |

See section 4, p.34, for a detailed course list.

# 3. Modules

## 3.1 Crystal Growth

**Lecturer(s)**

a) Prof. Dr. A. Danilewsky
b) Prof. Dr. A. Danilewsky; Prof. Dr. M. Fiederle; Dr. T. Sorgenfrei
c) Prof. Dr. A. Danilewsky
d) Prof. Dr. A. Danilewsky; Prof. Dr. A. Fiederle
e) Prof. Dr. A. Danilewsky; Prof. Dr. A. Fiederle
f) Prof. Dr. A. Fiederle

| Responsibility | Workload | Credits | Term | Cycle | Duration |
|---|---|---|---|---|---|
| Danilewsky | 360 h | 12 ECTS | WS & SS | annual | 2 terms |

| Course / Course Name | Presence | Private study | Participants |
|---|---|---|---|
| a) Crystal Growth Technology | 2 wh / 30 h | a) 60 h | a) 15 |
| b) Crystal Growth Methods I | 2 wh / 30 h | b) 60 h | b) 12 |
| c) Growth Kinetics | 1 wh / 15 h | c) 15 h | c) 15 |
| d) Crystal Growth Methods II | 1 wh / 15 h | d) 45 h | d) 8 |
| e) Crystal Preparation | 1 wh / 15 h | e) 45 h | e) 8 |
| f) Epitaxy | 1 wh / 15 h | f) 15 h | f) 15 |

### Learning goals and qualifications

Single crystals and single crystalline layers are at the heart of modern technology, and their synthesis is an important part of this curriculum. The first two courses deal exclusively with crystal growth, of which Crystal Growth Technology is the module covering the basics and the most common growth techniques. Other modules (e.g. Defects, the analytical modules) refer to the knowledge gained in this module. The following four courses deal with advanced studies on crystal growth by expanding the knowledgebase to important specialized topics such as epitaxy and kinetics. The knowledge is used in parts of the Applied Materials modules.

The students will be competent in choosing appropriate techniques for a given crystal growth. The practical experience of doing crystal growth enables them to actively apply a larger spectrum of methods and to avoid costly mistakes.

The individual qualifications and skills of the module are specified below:

1. On the successful completion of this module part students define the basics of crystal growth. They identify the different methods of crystal growth regarding the phase transition and configurations. They quantitatively predict the related physical as well as the chemical processes and identify the problems of industrial crystal growth techniques. They analyse the application of external fields and the use of simulation tools.
2. Students apply methods of crystal growth using the float-zone technique, aqueous solution growth, the gel or chemically induced growth, growth from the vapour phase, Bridgman growth and the Travelling Heater Method. They examine the different types of crystal growth methods and produce crystalline materials.
3. They identify growth mechanisms by the incorporation of atoms into a crystal lattice and the role of supersaturating and segregation phenomena. They recognize the procedures of crystal preparation and surface treatment. They differentiate between bulk crystal and growth of epitaxial films. The students apply these techniques and experiment with material preparation and the growth facilities.

## Syllabus

a) A short overview of crystal growth basics and methods is given. The overview is followed by a discussion of current aspects of bulk crystal growth for scientific and commercial production. These aspects are the use of external fields under high pressure and gravity fields like microgravity. The principles of thermodynamic equilibrium in growth systems are introduced and examples are applied. The problems of large industrial crystals and the solution with the use of simulation tools are shown.

b) This laboratory course introduces the students to the experiments of crystal growth with several setups. The industrial used method of float-zone growth is one important part of this course. The other growth methods are solution growth, gel or chemically induced growth, and growth from the vapour phase.

c) The macroscopically stable faces of a crystal are a function of the lattice structure. The incorporation of species into lattice positions depends on the real surface structure of the interface as well as on the growth mode. Anisotropies result in a non-uniform composition on a micro scale. The microscopic growth mechanisms, which produce such inhomogeneities and morphological instability, are the topic of this course. The microsegregation of impurities will be explained in terms of molecular kinetic models. Key words are: Lateral step flow, formation of macrosteps, interface supersaturation, faceting. Quantitative concentration measurements of dopants < $10^{18}$ atoms/$cm^3$ and a spatial resolution of about 1 µm with photoluminescence.

d) Laboratory crystal growth experiments in Bridgman growth ( e.g. $PbI_2$, SnS) and high temperature solution growth (e.g. Traveling Heater Method, Ge from Sn, Ge-Si from Ge) will be performed and the resulting crystals will be compared. The steps are: cleaning and preparation of starting materials and quartz glass ampoules, high purity filling of ampoules, planning of experiments (timeline, temperature, pulling speed etc.), crystal growth 1-2 weeks; long term stability of controllers, documentation.

e) Laboratory experiments on orientation (optical and Laue X-ray technique), cutting, grinding, and polishing, as well as selective etching of crystals; an introduction into Nomarski differential interference contrast microscopy will be given. From dopant striations in the crystals the growth history and quality of the crystals will be discussed.

f) Growth of epitaxial layers and deposition of thin films are playing an important role in development and applications of devices and tools. This course will give an overview of different epitaxial growth methods and deposition technologies from solution and vapor phase. Chemical Vapor Deposition (CVD), Physical Vapor Transport (PVT), Metal Organic CVD (MOCVD), and Molecular Beam Epitaxy (MBE) will be presented.

## Teaching form

a) Lecture with demonstrations using technologically important materials (e.g. Si, YAG) and audiovisual elements showing laboratory and industrial-scale processes.

b) Practice – Lab course: the students receive an introduction into each growth experiment, followed by a discussion of the experiment and possible problems. They then perform the different growth experiments under supervision, document the experiment and the results and present a written report for each experiment.

c) Multimedia presentation with 3D animations and discussion of light microscopy of real crystals

d) Lab course: practical preparation and execution of growth experiments in small groups

e) Lab course: practical preparation of grown crystals and characterization, discussion of results

f) Lecture: practical preparation and execution of characterization methods

## Examination form

Achievement of learning goals (unmarked): a) report (1h); b) discussion on the experiment; c) homework; d) report; e) report; f) exercises basics before conducting the experiment

Examination: Average of marked reports from b) and d) (50%) and one written examination (50%)

## Prerequisites for attending

a) None

b) None

c) a

d) a

e) a

f) None

## Usage of the module

M.Sc. Crystalline Materials

a) B.Sc. Physics and B.Sc. Chemistry

c) B.Sc. Physics and B.Sc. Chemistry

## Recommended reading

a) Dhanaraj, G., Byrappa, K., Prasad, V., Dudley, M. (Eds.) (2010): Handbook of Crystal Growth. Springer, Berlin, 1818.

Duffar, T. (Ed.) (2010): Crystal Growth processes based on capillarity. Wiley, Chichester, 566.

Hurle, D.T.J. (Ed.) (1993-1994): Handbook of Crystal Growth, vols 1a-2b. Elsevier, Amsterdam, 1352.

Rudolph, P. (Ed.) (2015): Handbook of Crystal Growth, 2nd Ed. vols 1a-2b. Elsevier, Amsterdam

b) Dhanaraj, G., Byrappa, K., Prasad, V., Dudley, M. (Eds.) (2010): Handbook of Crystal Growth(selected chapters). Springer, Berlin, 1818.

Hurle, D.T.J. (ed.) (1993-1994): Handbook of Crystal Growth(selected chapters). Elsevier, Amsterdam, 1352.

c) Sunagawa, I. (Ed.) (1987): Morphology of Crystals Part A, B and C, Terra Sci. Publ.

Tiller, W. A. (1991): The Science of Crystallization. Microscopic Interfacial Phenomena. Cambridge University Press, 424.

d) Dhanaraj, G., Byrappa, K., Prasad, V., Dudley, M. (Eds.) (2010): Handbook of Crystal Growth (selected chapters). Springer, Berlin, 1818.

Haussühl, S. (2007): Physical properties of crystals (chapter 1). Wiley-VCH, Weinheim,

439.

Hurle, D.T.J. (Ed.) (1993-1994): Handbook of Crystal Growth (selected chapters). Elsevier, Amsterdam, 1352.

Rudolph, P. (Ed.) (2015): Handbook of Crystal Growth, 2nd Ed. vols 1a-2b. Elsevier, Amsterdam

e) Sangwal, S. (1987): Etching of Crystals. North-Holland, Amsterdam, 520.

f) Herman, M.A. & Sitter, H. (1989): Molecular Beam Epitaxy, Springer-Verlag.

Sze, S.M. (2002): Semiconductor Devices Physics and Technology, Wiley,568.

## Lecture notes

https://ilias.uni-freiburg.de/login.php

## 3.2 Advanced Crystallography

**Lecturer(s)**

a) NN

b) NN

| **Responsibility** | **Workload** | **Credits** | **Term** | **Cycle** | **Duration** |
|---|---|---|---|---|---|
| Danilewsky | 180 h | 6 ECTS | WS | annual | 1 term |

| **Course / Course Name** | **Presence** | **Private study** | **Participants** |
|---|---|---|---|
| a) Crystallographic Methodology | a) 2 wh / 30 h | a) 60 h | a) 15 |
| b) Space Groups and Crystal Structures | b) 2 wh / 30 h | b) 60 h | b) 15 |

### Learning goals and qualifications

The two courses are grouped in that module because both impart important crystallographic knowledge about the symmetry of atomic arrangements in crystals and their analytical methods. The Advanced Crystallography courses provide the knowledge basis for most other modules, including the analytical X-ray methods, the crystal growth modules, and the semiconductor module.

The individual qualifications and skills of the module are specified below:

a) The students become competent in applying the basic principles of crystal lattices and symmetry to crystallographic analytical problems, especially X-ray crystallography.

b) The students calculate and operate with the concept of symmetry and group theory as applied to crystal structures. They differentiate space group symbols and classify the information given in the "International Tables" on a space group page. They recognize the construction principles of basic inorganic binary and ternary crystal structures.

### Syllabus

a) The course starts with a short introduction of the concepts of symmetry and crystallographic notation, followed by applied aspects of group theory, black and white groups, and colour groups and their applications. The concept and examples of quasi-crystals will be discussed.

b) The symmetry of any atomic arrangement in a crystal can be described by one of the 230 different crystallographic space groups. A first part of the course deals with principles of space group symmetry, notation and visualization. The most important basic crystallographic atomic arrangements (inorganic materials) are treated in a second part, starting from closest sphere packing structures.

## Teaching form

a) The students are introduced into the concept of symmetry through a mixture of lecturing and actively determining the symmetries of provided crystals models in small groups.

b) Lecture introducing the different symmetry operations in crystallography and the assignment of crystal structures to space groups by using 3D demonstrations of various technologically important and mineralogical popular crystal structures.

## Examination form

Achievement of learning goals (unmarked): a) completed homework assignments; b) solution of exercises

Examination: one written exam

## Prerequisites for attending

a) None

b) None

## Usage of the module

M.Sc. Sustainable Materials

## Recommended reading

a) Vainshtein, B.K. (1994): Fundamentals of Crystals, $2^{nd}$ Ed. Springer, Berlin, 482.

Haussühl, S. (2007): Physical properties of crystals (chapter 1). Wiley-VCH, Weinheim, 439.

b) Hahn, T. (ed.) (2005): International Tables for Crystallography, Vol. A. Springer.

Borchardt-Ott, W., Sowa H. (2013): Crystallography. Springer, Berlin, 307.

Hyde, B.G. & Anderson, S. (1989): Inorganic Crystal Structures. Wiley, New York, 430.

## Lecture notes

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| 3.3 Physical and Chemical Analytical Procedures | | | | | |
|---|---|---|---|---|---|
| **Lecturer(s)**<br>Prof. Dr. A. Danilewsky; Dr. H. Müller-Sigmund | | | | | |
| **Responsibility**<br>Danilewsky | **Workload**<br>180 h | **Credits**<br>6 ECTS | **Term**<br>WS | **Cycle**<br>annual | **Duration**<br>1 term |
| **Course /Course Name**<br>Physical and Chemical Analytical Procedures | | **Presence**<br>4 wh / 60 h | **Private study**<br>120 h | | **Participants**<br>12 |

## Learning goals and qualifications

This interdisciplinary module combines the physical, chemical, mineralogical and crystallographic methods for the full characterization of any material samples. The student gains key competences concerning quantitative material analysis by the use of state-of the-art equipment. The individual qualifications and skills of the module are specified below:

In the course of this practical module students acquaint themselves with a wide variety of physical and chemical analytical techniques available at the institute. Firstly, they identify which technique is the appropriate tool for a given problem. Secondly, they memorize the theoretical background of the technique, identify possible sources of error, and prepare the geological material for the subsequent analysis. Thirdly, they measure the samples, thereby collecting own practical experience. Fourthly, they undertake a critical data interpretation and evaluation.

## Syllabus

This course is designed to introduce the theory, applications, and operation of modern instrumental methods for chemical and physical analyses in environmental, Earth and materials science. Students are introduced to the spectrum of instrumental techniques, which are standard in research as well as in industry, and gain an understanding of the analytical approach to problem solving and data evaluation. To the extent feasible, students get hands-on experience with the machinery in the course of lab exercises, concentrating on concrete small analytical projects.

## Teaching form

Lecture + Practice, multimedia introduction into the basics of the methods, hands-on experience with different machinery in small groups (3-4 students), oral presentation of data and critical data discussion within groups

## Examination form

Achievement of learning goals (unmarked): Participation at the exercises

Examination: one marked written report

## Prerequisites for attending

Basic understanding of geological materials

B.Sc. level “Geochemical Methods” or equivalent knowledge

## Usage of the module

Compulsory course in M.Sc. Geology – Specialization Geochemistry and

M.Sc. Sustainable Materials- specialized Crystalline Materials, elective course in M.Sc Geology

## Recommended reading

Dinnebier, R. E. & Billinge, S.J.L. (2008): Powder Diffraction: Theory and Practice. RSC Publishing, RSC e-book collection.

Gill, R. (ed.) (1997): Modern Analytical Geochemistry: An Introduction to Quantitative Chemical Analysis for Earth, Environmental and Material Scientists: Addison Wesley Longman, UK, 344.

Reed, S. J. B. (2005): Electron microprobe analysis and scanning electron microscopy in geology. Cambridge University Press, 206.

Reimer, L (2010): Scanning Electron Microscopy. Springer Series in Optical Sciences Vol. 45, 511, Springer, Berlin.

## Lecture notes

https://ilias.uni-freiburg.de/login.php

## 3.4 Sustainability

| **Lecturer(s)** | | | | | |
|---|---|---|---|---|---|
| Prof. Dr. S. Hiermair, Prof. Dr. R. W. Lang, Dr. White, NN | | | | | |
| **Responsibility** | **Workload** | **Credits** | **Term** | **Cycle** | **Duration** |
| Hillebrecht | 180 h | 6 ECTS | WS & SS | annual | 2 terms |

| **Course /Course Name** | **Presence** | **Private study** | **Participants** |
|---|---|---|---|
| a) Material Life Cycles (Prof. Dr. Hiermaier, Dr. Ganzenmüller (Fraunhofer Inst.) (2 ECTS)<br>b) Sustainability (Prof. Lang, Uni Linz) (2 ECTS)<br>c) Sustainability (Dr. White) | a) 2 wh / 30 h<br>b) 1 wh / 15 h<br>c) 1 wh / 15 h | a) 30h<br>b) 15h<br>c) 15h | 60 |

### Learning goals and qualifications

Ability to assess sustainable development concepts in an engineering framework.

### Syllabus

The aim of the lecture is to introduce a framework within which a student can form critical, independent assessments of “Sustainable Developments”. With a focus on the role of materials it recognizes the complexity inherent in discussions of sustainability and shows how to deal with it in a systematic way. For that purpose the students are provided with procedures and tools, which allow them to analyze the financial, natural, human and social factors contributing to sustainable development. Within that context, the lecture addresses questions such as “How do we achieve sustainable development? How do we measure progress in achieving it? What does it mean in engineering practice? How do materials fit in?” The students will find that there is no completely “right“ answer to questions of sustainable development- instead, there is a thoughtful, well-researched response that recognizes the conflicting priorities of the environmental, the economic, the legal and the social aspects of a technological change.

### Teaching form

Lectures

## Examination form

Written exam (unmarked)

## Prerequisites for attending

a) None

b) None

c) None

## Usage of the module

M.Sc. Sustainable Materials

## Recommended reading

Variable

## Lecture notes

https://ilias.uni-freiburg.de/login.php

| 3.5 Defects | | | | | |
|---|---|---|---|---|---|
| **Lecturer(s)**<br>a) Prof. Dr. A. Danilewsky<br>b) Prof. Dr. M. Fiederle | | | | | |
| **Responsibility**<br>Danilewsky | **Workload**<br>180 h | **Credits**<br>6 ECTS | **Term**<br>SS | **Cycle**<br>annual | **Duration**<br>1 term |
| **Course /Course Name**<br>a) Crystal Defects<br>b) Electrical and Optical Characterization Methods | | **Presence**<br>a) 2 wh / 30 h<br>b) 2 wh / 30 h | **Private study**<br>a) 60 h<br>b) 60 h | | **Participants**<br>a) 15<br>b) 15 |

## Learning goals and qualifications

This module connects the modules of ideal crystal structures and crystal growth with the physical properties of real crystals. It contains two courses, which deal about real crystal structures containing lattice defects and different investigation methods to identify both crystals as well as defects.

As a consequence of the characterization of the crystal defects the students develop strategies to optimize the crystal growth and the material parameters.

The individual qualifications and skills of the module are specified below:

a) After learning the basics of crystalline material the students recognize the role of defects and the real structure of crystalline materials. They discover the formation of defects and identify the different types of structures. They apply tools of defect analysis for qualitative and quantitative results.

b) Students classify the principles of electrical and optical characterization methods. They apply the general techniques of material analysis and select the methods depending of the nature of the crystalline materials. They evaluate the results of physical methods and predict the quality and perfection of semiconductors.

## Syllabus

a) Crystals never have an ideal structure, and crystal defects influence physical properties and applications considerably. The course will introduce types (0-D to 3D), causes, and effects of crystal defects, such as point defects, color centers, dislocations, stacking faults, twinning. Analytical methods to investigate defects are discussed.

b) This course gives an overview of the optical and electrical characterization methods for crystalline materials. The measurement of resistivity of semiconductors and insulators is shown by the use of the Van-der-Pauw method and Four-Point-Probing. The precise analysis of mobility and charge carrier concentration is presented for the classical Hall and Van-Der-Pauw geometries. The advantages of optical characterization are demonstrated by the discussion of the methods Photoluminescence, Absorption and Transmission spectroscopy.

## Teaching form

a) Multimedia presentation supported by 3D models and animations, discussion and solution of problems.

b) Multimedia presentation supported by experimental data, discussion and solution of problems.

## Examination form

Achievement of learning goals (unmarked): a) participation at the lecture and discussions; b) participation at the lecture and discussions.

Examination: written exam

## Prerequisites for attending

a) None

b) None

## Usage of the module

M.Sc. Sustainable Materials

## Recommended reading

a) Hirth J. P., Lothe J. (1982): Theory of Dislocations, 2nd ed., Wiley New York.

Tiller, W. A. (1991): The Science of Crystallization. Microscopic Interfacial Phenomena. Cambridge University Press, 424 p.

b) Schroder, D.K. (2006): Semiconductor Material and Device Characterization 3rd Edition, Wiley, 800 p.

## Lecture notes

https://ilias.uni-freiburg.de/login.php

## 3.6 Advanced Analytical Methods

### Lecturer(s)

a) Prof. Dr. A. Danilewsky; Prof. Dr. M. Fiederle; Dr. T. Sorgenfrei; Dr. L. Kirste

b) Dr. T. Sorgenfrei; Dr. A. Remhof

| Responsibility | Workload | Credits | Term | Cycle | Duration |
|---|---|---|---|---|---|
| Fiederle | 180 h | 6 ECTS | SS | annual | 1 term |

| Course /Course Name | Presence | Private study | Participants |
|---|---|---|---|
| a) High-Resolution Spectroscopy | a) 2 wh / 30 h | a) 60 h | a) 15 |
| b) X-Ray Diffraction by Crystals | b) 2 wh / 30 h | b) 60 h | b) 15 |

### Learning goals and qualifications

Advanced analytical methods are essential for the investigation of crystalline materials and the understanding of the correlation between material properties and technology. The analytical methods are an important part of this curriculum. The module includes spectroscopic and diffraction methods covering a broad range of characterization tools from basic knowledge to advanced data analysis. The module refers to the knowledge gained in the others modules of Crystal Growth.

The students will be competent in choosing analytical methods techniques for characterization of crystaline materials. The students will be able to analyse and evaluate experimental data and identify different classes of crystalline materials.

The individual qualifications and skills of the module are specified below:

In this module students select and employ principles of common analytic methods used in materials science. They examine a variety of spectroscopic and analytical techniques for characterization of crystalline materials. They differentiate the interaction between crystal-line material with probe beams like X-rays, ionized particles and photons. They interpret the outcome of these interactions for mass spectroscopy, surface analysis and the meaning of the scattering vector and the structure factor.

### Syllabus

a) The course provides tools for the characterization of crystalline materials, especially the type and site of atoms as well as their first sphere surroundings. This includes UV-VIS and

IR spectroscopy. Surface analysis methods using X-ray Photon Spectroscopy (XPS), Secondary Ion Mass Spectroscopy (SIMS), Auger Spectroscopy (AGS), LEED and RHEED are introduced and compared. To analyze the local geometry, the chemical state and coordination spheres of atoms X-ray Absorption Spectroscopy (XAS), Extended Absorption Fine Structure (EXAFS), and X-ray Absorption Near Edge Structure (XANES) will be presented; this part includes an introduction into synchrotron technology. To find the oxidation state of atoms (e.g., $Fe^{2+}$, $Fe^{3+}$) Mössbauer Spectroscopy will be explained. Other high-resolution methods discussed are: Raman spectroscopy, STM and AFM microscopy, TEM microscopy.

b) Methods which make use of the diffraction of X-rays (or neutrons) by crystals yield much more detailed and precise knowledge on the arrangement of atoms in matter than any other methods. This course teaches the principles of X-ray diffraction starting from two point scatterers and ending at a (ideally infinite) crystal structure and its "structure factors". The geometrical relationships between crystallographic lattice planes on one side, incident and diffracted beams on the other, are explained by means of the reciprocal lattice and the Ewald construction.

## Teaching form

a) 3D multimedia introduction into the various methods, supported by solving problems and discussion of results.

b) Lecture + Practice: Students receive a multimedia introduction into the basics of X-ray diffraction by single crystals, overview of various diffraction methods.

## Examination form

Achievement of learning goals (unmarked): a) Analysis of experimental data; b) solution of exercises

Examination: one written exam

## Prerequisites for attending

a) None

b) Space Groups and Crystal Structures

## Usage of the module

M.Sc. Sustainable Materials

a) B.Sc. Physics and B.Sc. Chemistry

## Recommended reading


a) Schroder, D.K. (2006), Semiconductor Material and Device Characterization, 3rd Edition, Wiley, USA

Skoog, D.A., Holler, F. J., Crouch, S. R. (2007): Principles of Instrumental analysis, 2nd ed.. Thomson Brooks/Cole, Belmont.

Fultz, B. & Howe, J.M. (2001): Transmission Electron microscopy and diffractometry of materials. Springer, Berlin.

Cohen,S. H. &Lightbody, M. L. (1997-1999): Foundation for advances in medicine and science – atomic force microscopy/scanning tunnelling microscopy 1-3. Springer, Berlin.

b) Clegg, W., Blake,A. J., Gould, R. O., Main, P.(2001): Crystal Structure Analysis, Principles and Practice. Oxford University Press, USA.

Massa, W. (2004): Crystal Structure Determination, Springer,Berlin,210.


## Lecture notes

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## 3.7 Applied Materials I

| **Lecturer(s)** | | | | | |
|---|---|---|---|---|---|
| a) NN<br>b) Prof. Dr. M. Fiederle | | | | | |
| **Responsibility** | **Workload** | **Credits** | **Term** | **Cycle** | **Duration** |
| Fiederle | 180 h | 6 ECTS | SS | annual | 1 term |
| **Course /Course Name** | | **Presence** | **Private study** | | **Participants** |
| a) Crystal Physics<br>b) Semiconductors | | a) 2 wh / 30 h<br>b) 2 wh / 30 h | a) 60 h<br>b) 60 h | | a) 15<br>b) 15 |

### Learning goals and qualifications

The module covers the basic theories of Crystal and Semiconductor Physics and introduces the technology and characterization of semiconductor devices by electrical and optical methods. Using the fundamental knowledge from physics the module explains the complexity of solid-state materials. The content of the first part of this module is essential for the module Defects.

The students will be able to understand the structure of solid-state materials and to calculate the correlations between structural and electronic properties. They will be able to understand the function and processing of semiconductor devices.

The individual qualifications and skills of the module are specified below:

a) Students discover the physical properties of crystalline materials and the relation with material properties. They examine the crystal anisotropy and differentiate between the effects of piezoelectricity, ferroelectricity and ferroelastivity. They calculate with the basic tools of tensors and practice the tensor theory for describing the material properties of crystalline materials like nonlinear optics, piezoelectricity, ferroelectricity, ferroelasticity.

b) In this module students discover the basics of semiconductor physics. They apply the theory of solid-state physics and understand the principle of semiconductors and their functionality. They practice the basics of semiconductor materials and understand the principles of semiconductor devices as well as semiconductor technology.

### Syllabus

a) The course introduces technologically important physical properties of crystals based on their anisotropy, such as nonlinear optics, piezoelectricity, ferroelectricity, ferroelasticity. The basic tools for describing these properties (tensors) as well as some technical applications of these crystals are presented and applied to the calculation of material properties.

b) The course introduces the physics of semiconductors regarding the electronic structure and the consequences for the material properties. The effect of impurities, dopants and defects are taught for the semiconductors silicon, GaAs, GaN, ZnO and ternary compounds. The electrical, structural and optical characteristics are compared to the performance of semiconductor devices.

## Teaching form

a) Lecture + Practice: Multimedia lecture with practical demonstrations and discussion of all participants.

b) Lecture + Practice: e-book content with interactive tests for individual learning and multimedia content in the lecture.

## Examination form

Achievement of learning goals (unmarked): a) completed homework assignments; b) completed homework assignments

Examination: one written exam

## Prerequisites for attending

a) None

b) None

## Usage of the module

M.Sc. Sustainable Materials

## Recommended reading

a) Haussühl, S. (2007): Physical properties of crystals (chapter 1). Wiley-VCH, Weinheim, 439.

Nye, J.F. (1985): Physical properties of crystals. Oxford University Press, USA, 352.

b) Sze, S.M. (2002): Semiconductor Devices Physics and Technology, Wiley, 568.

Kittel, C. (2004): Introduction to Solid State Physics, Wiley, 704.

## Lecture notes

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## 3.8 Applied Materials II

| **Lecturer(s)** | | | | | |
|---|---|---|---|---|---|
| a) Prof. Dr. M. Fiederle<br>b) Prof. Dr. M. Fiederle | | | | | |
| **Responsibility** | **Workload** | **Credits** | **Term** | **Cycle** | **Duration** |
| Fiederle | 180 h | 6 ECTS | WS | annual | 1 term |

| **Course /Course Name** | **Presence** | **Private study** | **Participants** |
|---|---|---|---|
| a) Semiconductor Technology | a) 2 wh / 30 h | a) 60 h | a) 15 |
| b) Electrical Characterization of Crystals and Devices | b) 2 wh / 30 h | b) 60 h | b) 15 |

### Learning goals and qualifications

The module covers the basic theories of Crystal and Semiconductor Physics and introduces the technology and characterization of semiconductor devices by electrical and optical methods. Using the fundamental knowledge from physics the module explains the complexity of solid-state materials. The content of the first part of this module is essential for the module Defects.

The students will be able to understand the structure of solid-state materials and to calculate the correlations between structural and electronic properties. They will be able to understand the function and processing of semiconductor devices.

The individual qualifications and skills of the module are specified below:

a) Students classify the technology of semiconductor processing. They examine the principle of electronic and optical device production. With this knowledge they differentiate between various types of semiconductor planar technology for Charge Coupled Devices CCD, Complementary Metal Oxide Semiconductor FET and Bipolar Junction FET.

b) In this practical course students apply the analytic methods of electrical and optical characterization. They operate with semiconductor equipment and crystals for material analysis. They transfer the theory of the lectures to the laboratory work.

### Syllabus

a) The topic of this course is the planar technology for fabrication of semiconductor devices. The methods of planar technology are described starting from photolithography and continuing with etching technologies, doping by diffusion and ion implantation. The principles of CMOS and Bipolar Transistors devices are presented using the device processing of the planar technology. A detailed overview of state of the art of semiconductor devices like CCD, LED and DRAM concludes the course.

b) Laboratory experiments on the measurement of resistivity, piezoelectric, pyroelectric, and ferroelectric constants in crystals will be carried out. The principles of photolithography and structured contacts are carried out for a simple device structure. The performance of this structure is measured by I-V characteristics. Conventional semiconductor devices will be tested by I-V, C-V and optical methods.

## Teaching form

a) Lecture + Practice: e-book content with interactive tests for individual learning and multimedia content in the lecture

b) Practice: Lab course with discussion and experimental exercises

## Examination form

Achievement of learning goals (unmarked): a) completed homework assignments; b) participation in group discussions

Examination: one written exam

## Prerequisites for attending

a) Course b)

b) Course b)

## Usage of the module

M.Sc. Sustainable Materials

## Recommended reading

a) Sze, S.M. (2002): Semiconductor Devices Physics and Technology, Wiley, 568.

Kittel, C. (2004): Introduction to Solid State Physics, Wiley, 704.

b) Haussühl, S. (2007): Physical properties of crystals (chapter 1). Wiley-VCH, Weinheim, 439.

Nye, J.F. (1985): Physical properties of crystals. Oxford University Press, USA, 352.

Schroder, D.K. (2006): Semiconductor Material and Device Characterization 3rd Edition, Wiley, 800.

## Lecture notes

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| 3.9 X-Ray Methods | | | | | |
|---|---|---|---|---|---|
| **Lecturer(s)**<br>a) NN<br>b) Prof. Dr. A. Danilewsky | | | | | |
| **Responsibility**<br>Danilewsky | **Workload**<br>180 h | **Credits**<br>6 ECTS | **Term**<br>WS | **Cycle**<br>annual | **Duration**<br>1 term |
| **Course /Course Name**<br>a) Structure Analysis by X-Ray Diffraction<br>b) Defect Analysis by Diffraction | | **Presence**<br>a) 2 wh / 30 h<br>b) 2 wh / 30 h | **Private study**<br>a) 60 h<br>b) 60 h | | **Participants**<br>a) 15<br>b) 15 |

## Learning goals and qualifications

This module uses x-ray diffraction methods to analyze the ideal and real crystal structures of single crystals by using two different physical and mathematical approaches.

The student recognizes the key competence of a crystallographer, which is the structure analysis by X-ray diffraction.

The individual qualifications and skills of the module are specified below:

a) Students explain the Fourier synthesis of the electron density of a crystal and the different methods to overcome the famous “phase problem”. They identify the information obtained from an X-ray structure analysis and apply this for the characterization of different crystal structures.

b) The students gain advanced knowledge about X-ray diffraction, dynamical theory, and the use of synchrotron light for advanced defect characterization. They recognize the use of X-ray methods for industrial production and characterization of semiconductor materials.

## Syllabus

a) After the relationships between measured X-ray diffraction intensities and the electron density function of a crystal have been established, the course deals with different ways to solve the structure (i.e., to determine with high precision the atomic arrangement in the crystal). In a final part, methods to solve and refine crystal structures from powder diffraction patterns are treated.

b) Position and intensity of a Bragg reflection are used for structure analysis of a crystal. In addition, the fine structure of such a reflection contains information about the real structure of this crystal. In terms of dynamical diffraction theory defects are characterized using high-resolution diffractometry. Rocking curves and reciprocal space maps are demonstrated to give insight into the crystal quality. X-ray topography will be discussed as a useful imaging method for strain fields around extended defects.

## Teaching form

a) 3D, multimedia presentation supported by solution and discussion of problems

b) 3D, multimedia presentation supported by solution and discussion of problems

## Examination form

Achievement of learning goals (unmarked): a) solution of exercises; b) solution of exercises

Examination: one written exam

## Prerequisites for attending

a) X-Ray Diffraction by Crystals

b) X-Ray Diffraction by Crystals

## Usage of the module

M.Sc. Sustainable Materials

a) B.Sc. Physics and B.Sc. Chemistry

## Recommended reading

a) Clegg, W., Blake, A. J., Gould, R. O., Main, P. (2001): Crystal Structure Analysis, Principles and Practice. Oxford University Press, USA.

   Massa, W. (2004): Crystal Structure Determination, Springer, Berlin, 210.

b) Bowen, D. K. & Tanner, B. K. (1998): High Resolution X-Ray Diffractometry and Topography, Taylor & Francis, 264.

## Lecture notes

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| 3.10 Technical and Applied Mineralogy | | | | | |
|---|---|---|---|---|---|
| **Lecturer(s)**<br>a) Prof. Dr. U. Vogt<br>b) Dr. T. Sorgenfrei | | | | | |
| **Responsibility**<br>Sorgenfrei | **Workload**<br>180 h | **Credits**<br>6 ECTS | **Term**<br>WS | **Cycle**<br>annual | **Duration**<br>2 terms |
| **Course / Course Name**<br>a) Modern Ceramics, Cements, and Glasses<br>b) Thermal Analysis | | **Presence**<br>a) 3 wh / 45 h<br>b) 2 wh / 30 h | **Private study**<br>a) 75 h<br>b) 30 h | | **Participants**<br>a) 15<br>b) 15 |

## Learning goals and qualifications

The module complements the crystal growth modules by expanding the student knowledge to the most important non-crystalline and polycrystalline material groups as well as providing the students with an important tool to determine phase relationships.

The students become competent in determining, understanding, and using phase relationships. They gain a thorough understanding of the basics and the production methods of glasses and ceramics.

The individual qualifications and skills of the module are specified below:

a) Students recall the basic properties, requirements and production methods of glasses, cements, and ceramics, including modern optical materials and materials for fuel cells. They recognize limitations, advantages and disadvantages of the presented methods and relate them to each other.

b) After examination of the underlying thermodynamics students familiarize themselves with several techniques of thermal analysis including Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), and Thermal Gravimetry (TG). They collect experience in operating the machines and interpret data they have gathered.

## Syllabus

a) Polycrystalline and amorphous materials play a major role in modern technology. The course will cover the production methods of technical ceramics, cements, and glasses, as well as their applications, including optical materials and glass ceramics.

b) After a short introduction of the underlying thermodynamics the course deals with the principles of Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), and Thermal Gravimetry (TG). A phase diagram is constructed based on DTA and X-ray powder diffraction measurements. The exact chemical composition of a substance is determined by the results of TG measurements.

## Teaching form

a) Lecture + Practice: Multimedia presentation including practical demonstrations of the materials at hand and homework.

b) Lab course: Students receive an introduction into different methods of thermal analysis by doing real analysis with the instruments including the interpretation

## Examination form

Achievement of learning goals (unmarked): a) participation at group discussions; b) report

Examination: one written exam

## Prerequisites for attending

a) none

b) none

## Usage of the module

M.Sc. Sustainable Materials

M. Sc. Geology

a) B.Sc. Physics and B.Sc. Chemistry

## Recommended reading

a) Askeland, D.R., Phulé, P.P. (2002): The Science and Engineering of Materials. Thomson Brooks, Cole, 1032.

Bansal, N. P. (2005): Handbook of Ceramic Composites (2005). Kluwer Academic Publishers / Springer, New York, 554.

Chiang, Y.M., Birnie, D.P. & Kingery, W.D. (1996): Physical Ceramics: Principles for Ceramics Science and Engineering. Wiley, New York, 544.

Doremus, R.H. (1994): Glass Science. Wiley, New York, 352.

Lee, B.I., Pope, E.J.A. (1994): Chemical processing of ceramics. Marcel Dekker Inc., New

York, Basel, Hong Kong, 572.

Shelby, J.E. (2005): Introduction to glass science and technology. Royal Society of Chemistry, Cambridge, 308.

Weimer, A. W. (2011): Carbide, Nitride and Boride Synthesis and Processing. Chapman & Hall, London, 696.

b) Brown, M. E. (2001): Introduction to Thermal Analysis: Techniques and Applications, Kluwer Academic Publishers, 280.

Hemminger, W. F. & Cammenga, H. K. (1989): Methoden der Thermischen Analyse, Springer, Berlin, 300.

## Lecture notes

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## 3.11 Field Trips and Seminars

**Lecturer(s)**

a) Dr. A. Remhof, NN

b) Prof. Dr. M. Fiederle; Prof. Dr. A. Danilewsky

c) Dr. A. Simonov; Prof. Dr. A. Danilewsky, Prof. Dr. M. Fiederle, Dr. T. Sorgenfrei

| Responsibility | Workload | Credits | Term | Cycle | Duration |
|---|---|---|---|---|---|
| Danilewsky | 180 h | 6 ECTS | WS/SS | annual | 1 – 2 terms |

| Course /Course Name | Presence | Private study | Participants |
|---|---|---|---|
| a) Seminar: Recent Publications<br>b) Advanced Seminar on In-House Research<br>c) Field Trips to Industrial Facilities | a) 2 wh / 30 h<br>b) 1 wh / 15 h<br>c) 4 days / 40 h | a) 60 h<br>b) 15 h<br>c) 20 h | a) 15<br>b) 15<br>c) 15 |

### Learning goals and qualifications

The module allows the students to apply the knowledge gained in the other modules to current topics in crystalline materials.

The students become competent in presenting and analyzing research results; they gain firsthand knowledge of and familiarize themselves with production environments in industry and of large research facilities.

The individual qualifications and skills of the module are specified below:

a) The students understand, analyze, and present research results in the field competently. They identify the latest publications and the actual topics in applied research. They recognize the reading and writing of scientific articles.

b) The students participating in the research seminar improve their abilities of presenting scientific topics. They defend their results in scientific discussions. They identify possible flaws, misinterpretations or inconsistencies in their own work and in those of other lecturers. Students critically dispute scientific topics and use the correct scientific terminology.

c) The students visit industrial facilities and get in contact with the commercial world. They identify the difference between scientific and industrial production of crystalline materials. They discuss with former colleagues the possibilities of an employment in industry.

## Syllabus

a) Seminar on current trends in crystal growth, characterization, and applications of crystalline materials. Articles of the most relevant scientific journals are the topics of this seminar.

b) Seminar on current research projects in the institute.

c) Excursion to industries working in the fields of ceramics, semiconductors, optics, solar energy, glass, etc.

## Teaching form

a) Seminar: the students participate in the seminar by doing one presentation and by actively contributing to the discussion on the other presentations.

b) Seminar: the students participate in the seminar by doing one presentation on their own master thesis and by actively contributing to the discussion on the other presentations.

c) Excursion: The students visit producing companies and large research facilities, and discuss with the staff.

## Examination form

Achievement of learning goals (unmarked): a) successful presentation; b) successful presentation; c) active participation

Examination: none

## Prerequisites for attending

a) None

b) None

c) None

## Usage of the module

M.Sc. Sustainable Materials

## Recommended reading

a) Current issues of: 1. J. Cryst. Growth, 2. Cryst. Res. Technol., Cryst. Growth and Design, Z. Krist., Acta Crystallographica, J. Appl. Phys. etc.

b) None

c) None

## Lecture notes

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# a) Methods and Concepts (Elective Module)

**Lecturer(s)**

a) Prof. Dr. A. Danilewsky
b) Prof. Dr. M. Fiederle
c) Prof. Dr. S. Hergarten
d) Prof. Dr. D. Dolejš
e) Prof. Dr. A. Danilewsky
f) Dr. L. Kirste
g) Prof. Dr. A. Danilewsky
h) Prof. Dr. A. Danilewsky
i) Variable
j) Variable
k) Variable
l) Prof. Dr. A. Danilewsky
m) Variable
n) Variable

| Responsibility | Workload | Credits | Term | Duration |
|---|---|---|---|---|
| Danilewsky | 540 h | 18 ECTS | WS/SS | 3 terms |

| Course /Course Name | Presence | Private study | ECTS | Participants |
|---|---|---|---|---|
| a) Purification and Doping Methods | a) 2 wh / 30 h | a) 60 h | a) 3 ECTS | a) 15 |
| b) Semiconductor Devices | b) 2 wh / 30 h | b) 60 h | b) 3 ECTS | b) 15 |
| c) Computing in Geosciences | c) 3 wh / 45 h | c) 105 h | c) 5 ECTS | c) 16 |
| d) Thermodynamics of Geo-logical and Technical Mate-rials | d) 2 wh / 30 h | d) 60 h | d) 3 ECTS | d) 25 |
| e) Electron Back Scatter Dif-fraction | e) 2 wh / 30 h | e) 60 h | e) 3 ECTS | e) 15 |
| f) Theory and Applications of X-Ray Diffractometry | f) 2 wh / 30 h | f) 60 h | f) 3 ECTS | f) 15 |
| g) Advanced Analytics with Synchrotron Radiation I: Physics and Technology, | g) 2 wh / 30 h | g) 30 h | g) 2 ECTS | g) 15 |
| | h) 2 wh / 30 h | h) 30 h | h) 2 ECTS | h) 15 |
| | i) Variable | i) Variable | i) varia-ble | i) Variable |
| | j) Variable | j) Variable | j) varia-ble | j) Variable |
| | k) Variable | k) Variable | | k) Variable |

| | | | | |
|---|---|---|---|---|
| Imaging, Lithography<br>h) Advanced Analytics with Synchrotron Radiation II: Diffraction, Absorption and Spectroscopy<br>i) Special Topics in Functional Materials<br>j) Special Topics in Chemistry<br>k) Special Topics in Geology<br>l) Industrial Internship<br>m) External Module<br>n) Language Course | l) 160 h<br>m) Variable<br>n) Variable | l) 20 h<br>m) Variable<br>n) Variable | k) varia-ble<br>l) 6 ECTS<br>m) varia-ble<br>n) varia-ble | l) n/a<br>m) Variable<br>n) Variable |

## Learning goals and qualifications

a) Students identify the needs and requirements of vacuum and cleanroom technology of the production of semiconductors. They calculate the different levels of vacuum and classify concentration of particles in relation to the clean room class. They differentiate the methods of purification and doping. They apply this knowledge to compute the level of shallow impurities in different semiconductor materials.

b) After the basics of semiconductor physics students apply this knowledge for prediction of semiconductor devices. Students identify the designs of p-n junctions, Bipolar Junction Transistors and Complementary Metal Oxide Semiconductor Field Transistors. They develop simple devices like Charge Coupled Devices up to sophisticated devices like Memory and Complex Computer Chips.

c) Numerical data analysis, visualization, and process modeling have become essential parts of quantitative geosciences. Deepening the knowledge on data analysis and visualization and introducing methods of process modeling, this course provides the basics of quantitative methods used in several other courses. Going beyond technical aspects of computing, data analysis, and visualization, the students learn how to transfer conceptual models into equations and implement solutions in a high-level programming language (MATLAB) using the widespread Finite Difference Methods. As a major qualification, the students shall be able to assess which method is suitable for a given problem and be aware of potential pitfalls.

d) This module concentrates on physico-chemical principles that underlie structure-property relations of inorganic matter. These relations include feedback between occurrence and stability of minerals, silicate melts, aqueous fluids, their synthetic analogues including inorganic materials and atomic structure and its changes with temperature and pressure. Thermodynamic modeling of phase equilibria, construction of phase diagrams and prediction of element partitioning is a backbone of interpretation of pressure-temperature paths of metamorphic rocks, differentiation mechanisms of magmas as well as design and optimization of numerous technological processes such as crystallization, smelting, combustion, fluid extraction etc. Syntheses of inorganic materials and inovative material properties are increasingly predicted and designed with the aid of thermodynamic and phase equilibrium calculations.

e) The students are expected to develop a solid understanding of geological and materials thermodynamics, to become familiar with structure and use of thermodynamic datasets and are able to design solutions to phase equilibrium problems in petrology, crystallography, materials science or inorganic and physical chemistry.The elective course "Electron Back Scatter Diffraction" comprises a bundle of important modern state-of-the art techniques in crystallography that allow to determine the crystallographic orientation and composition of natural geo-materials and technical products. Crystallographic preferred orientations (CPO) of rock forming minerals are indicative for deformation mechanisms active during ductile flow at mid-to lower crustal levels. Likewise CPOs are important in material science as they influence the physical properties of materials. EBSD is a state-of-the-art technology to investigate the crystallographic orientation and textures in a sample. Students outline the underlying principles of EBSD, they prepare polished samples for EBSD analysis, examine the use of the Scanning electron microscope to which EBSD is attached. They collect data and interpret the diffraction pattern and index certain crystal orientations. Finally they discuss the underlying mechanisms (e.g. slip systems) that caused the CPO.

f) The elective course "Theory and Applications of X-Ray Diffractometry" introduces into the structural metrology of thin film based devices by interferometric methods of high-resolution X-ray diffraction (HRXRD) and X-ray reflectivity (XRR). Depending on the deposition processes (e.g. sputtering or epitaxial techniques), the structural properties of thin film material can be very different. The students will become familiar with X-ray measurement techniques to determine typical parameters of thin films like film thickness, composition, strain and relaxation, crystallinity, mosaic spread, crystallite size, surface and interface roughness and density. They will be able to select the appropriate X-ray metrology for certain structural issues. The students will be able to interpret X-ray measurements and understand the nano- and micro-structural properties of thin films and thin film based devices. This knowledge, offers the students the possibility of establishing a context of thin film deposition techniques, crystalline properties and device characteristics.

g) Actual cutting edge research needs high resolution characterization methods behind the limits of laboratory based instruments. Within this module, the students will plunge into the fascinating world of large scale research facilities providing high brilliant synchrotron X-ray radiation. After understanding the physics of particle accelerators and X-ray optics, the students will understand in the 1st part of the lecture the application of X-ray imaging methods..

h) The 2nd part deals with diffraction, absorption and fluorescence methods and their application in material sciences. The course will be completed by an excursion of the synchrotron light source ANKA at KIT, Karlsruhe. The course deepens and enhances the analytical skills of the students. They will become competent to choose adequate methods at large-scale facilities, which are not possible in the laboratory, to solve analytical challenges arising in materials research. Students apply their knowledge about the physics of electromagnetic waves to the wide fields of high resolution diffraction, imaging, advanced spectroscopic methods in absorption and fluorescence. Students will also identify adequate approaches for high resolution, in-situ and real time analysis and differentiate far and near order in beyond the capabilities of actual laboratory set-ups.

i) Within this module students can broaden their knowledge in the area of functional materials according to their personal professional wishes and goals with regard to the M.Sc. program as a whole. By choosing specific courses individual strength can be expanded and weaknesses can be specifically eliminated. Any combination of courses from the curriculum M.Sc. Sustainable Materials-specialized Functional Materials can be chosen, as long as the students fulfill any prerequisites of those courses and are not identical with the mandatory courses of the Crystalline Materials master.

j) Within this module students can broaden their knowledge in the area of chemistry according to their personal professional wishes and goals with regard to the M.Sc. program as a whole. By choosing specific courses individual strength can be expanded and weaknesses can be specifically eliminated. Any combination of courses from the B.Sc. or M.Sc. in Chemistry can be chosen, as long as the students fulfill any prerequisites of those courses, and are not identical with the mandatory courses of the Crystalline Materials master or the mandatory courses for a preceding BSc.

k) Within this module students can broaden their knowledge in the area of geomaterials according to their personal professional wishes and goals with regard to the M.Sc. program as a whole. By choosing specific courses individual strength can be expanded and weaknesses can be specifically eliminated. Any combination of courses from the BSc or M.Sc. in Geology can be chosen, as long as the students fulfill any prerequisites of those courses, and are not identical with the mandatory courses of the Crystalline Materials master or the mandatory courses for a preceding BSc.

l) The internship, at minimum 4 full work weeks exposes the student to an environment where he has to actively use and apply his skills and knowledge in materials. The internship gives good insight to real industrial applications and application processes of scientific matters. It enables the students to find out which scientific specification is most interesting for the individual career choice. The students can establish first industrial contacts, which could be very helpful for their later employment and/ or for choosing an appropriate master thesis in the applied sector of their scientific education.

m) Within this module students can broaden their knowledge outside the subject according to their personal professional wishes and goals with regard to the M.Sc. program as a whole. By choosing specific courses in Physics, Microsystems Engineering or a language module individual strength can be expanded and weaknesses can be specifically eliminated.

n) variable

## Syllabus

a) The course teaches the fundamentals of semiconductor purification and doping techniques. It describes the technologies of vacuum and clean room facilities and their importance for successful semiconductor production. It follows the major methods for purification of materials (rectification, sublimation, crystallization). An overview of doping methods will be given for scientific and industrial semiconductor production.

b) The course covers the wide field of semiconductor devices. The basic of semiconductor physics are applied to introduce and discover the design of different types of electronic devices. The course starts with the simple device structures of p-n junctions for diodes and leads to the principle of transistors. The complex design of Bipolar Junction Transistors and Metal Oxide Semiconductor Field Effect Transistors are discussed in relation to Planar Technology. Single device are shown for optical detectors and X-ray detectors.

c) The class starts with an introduction to process modeling using simple population models based on ordinary differential equations und their implementation using explicit and implicit Euler schemes. The following main part of the module comprises the basic equations behind the models widely used for modeling mass and heat transport processes, solid mechanics, groundwater flow, and landform evolution based on partial differential equations. After discussing the respective equations, the underlying principles, and their mathematical properties, the simplest numerical techniques in the field of partial differential equations (finite differences, upstream schemes) are discussed. Theory is accompanied by a step-by-step introduction to the MATLAB programming environment and exercises focusing on implementating the models in MATLAB and analyzing the results.

d) The course builds on basic physical chemistry, introduces equations of state for solid and liquid materials, proceeds from simple phases to multicomponent mixtures, and closes with a review of predictive methods: atomistic simulations of thermodynamic properties and numerical algorithms for computation of phase diagrams.
   1. Thermodynamic laws, mechanical and thermal processes
   2. Thermodynamic state functions and stability criteria
   3. Equations of state for gas and other fluids
   3. Equations of state for condensed phases
   4. Thermodynamics of mixing, partial properties of solutions
   5. Link between thermodynamic properties and phase diagrams

e) Calculation and construction of phase diagramsThe elective course “Electron Back Scatter Diffration” is designed to introduce the theory, applications, and operation Scanning Electron Microscopy (SEM) together with Electron Back Scatter Diffraction (EBSD). Topics are: field emission scanning electron microscopy, preparation and adjustment of samples for EBSD mode, calibration of EBSD system, orientation analysis, orientation mapping, documentation, interpretation. Introduction into textures of natural rocks and polycrystalline materials (e.g. solar cells).

f) The elective course “Theory and Applications of X-Ray Diffractometry” is intended to provide an introduction to practical high-resolution X-ray diffractometry and X-ray reflectivity as used in thin film semiconductor research and industry. We begin with the description of the structural properties of the objects to be investigated. Then we outline how these structural properties appear in reciprocal space. Using the Ewald construction, solutions are provided on how to tackle problems using X-ray diffraction and reflectivity systems. Following these explanations, typical problems for semiconductor thin film heterostructures are presented. The evaluation of 1-dimensional angle scans (e.g. rocking curves, specular scans, azimuthal scans) are described, as well as 2-dimensional scans (e.g. reciprocal space maps, pole figures). The reliability of these techniques and comparability to other analytical methods are discussed.

g) The elective course "Advanced Analytics with Synchrotron Radiation I + II" introduces into the basic physics of particle accelerators and the optics of high brilliant X-ray radiation. Analytical methods, which are not possible at laboratory X-ray sources will be explained by various examples for material research. Whereas the first part deals with the basics and imaging methods, the second part ist dedicated to diffraction, absorption and fluorescence methods. As a highlight the synchrotron light source ANKA at KIT Karlsruhe will be visited.

   This course is intended to provide an introduction to advanced analytical methods using intense X-ray radiation provided by synchrotron light sources. Physics and technology of particle accelerators for the use of the wide spectrum of electromagnetic waves as well as special features related to the work at large-scale facilities and research centers worldwide are explained in detail. An important part about imaging covers radiographic, tomographic as well as diffraction based topographic methods in 2D and 3D. Also actual research on ultra high speed 4D methods is included. A second part deals with the application of diffraction methods for in-situ and time resolved applications especially under non-ambient conditions. Analytics based on absorption, fluorescence and spectroscopy, also of the near order in molecules and building units in crystals or amorphous materials, will be presented in the second part. Namely X-ray absorption spectroscopy (XAS), Extended x-ray absorption fine structure (EXAFS), x-ray absorption near edge fine structure (XANES) as well as X-ray fluorescence analysis (XRF), x-ray fluorescence microprobe (µ-XRF) and the applications are addressed in this course. The reliability of these techniques and the merits compared to the laboratory based analytical methods are discussed using examples from actual research on crystalline and functional materials. A one day's excursion the synchrotron light source ANKA at Karlsruhe Institute of Technology will intensify the understanding of the complex methods.

h) Variable
i) The syllabus depends on the chosen elective courses
j) The syllabus depends on the chosen elective courses
k) The syllabus depends on the chosen elective courses
l) The internship provides the student with firsthand experience and knowledge of the demands in a production and/or research environment.
m) The syllabus depends on the chosen elective courses
n) Variable

## Teaching form

a) Multimedia lecture with lab visits demonstrating different processes, discussion of all participants
b) Multimedia lecture with demonstrating of semiconductor devices, discussion of all participants
c) Lecture mixed with practical exercises and homework.
d) Lecture combined with practical assignments (2 hr), individual project

e) Lecture + Exercise at the Scanning electron microscope

f) Multimedia lecture supported by solution and discussion of problems

g) Multimedia lecture supported by solution and discussion of problems, multimedia lecture supported by solution and discussion of problems, 1 day excursion to the Synchrotron light source ANKA, KIT Karlsruhe

h) TBA

i) Variable

j) Variable

k) Variable

l) Internship in a company doing production and research in the field, in a non-university research institute, or in a university institute if the activity is not part of the regular M.Sc. Crystalline Materials curriculum; it is required that the students participate in current research projects of the institution.

m) Variable

n) Variable

## Examination form

Achievement of learning goals (unmarked):

a) Active participation

b) Active participation

c) homework, active participation in the class, and a short written test at the end of the semester

d) attendance of lectures, completion of assignments, written test

e) Active participation, one written report

f) Active participation

g) Active participation, one written report, exercises, participation at group discussions

h) Variable

i) Variable

j) Variable

k) Variable

l) Positive employer’s reference letter after finishing the internship

m) Variable

n) Variable

## Prerequisites for attending

a) None

b) None

c) Basic knowledge in mathematics and computing, e.g., on the level of "Quantitative Methoden in der Geologie" or “Modellierung und Datenanalyse” from the B.Sc. Geowissenschaften

d) None

e) None

f) X-Ray Diffraction by Crystals

g) X-Ray Diffraction by Crystals

h) Variable

i) Variable

j) Variable

k) Variable

l) None

m) Variable

n) None

## Usage of the module

M.Sc. Sustainable Materials

## Recommended reading

a) Hoffmann, D.M., Singh, B., Thomas, J.H. (1998): Handbook of vacuum science and technology. Academic Press, San Diego, 835.

   Ullmann’s Encyclopedia on industrial chemistry (selected sections) 7th ed. (2010): Wiley-VCH, Weinheim.

b) Sze, S.M. (2006): Physics of Semiconductor Devices. Wiley, 832.

c) Gerya, T. (2009): Introduction to Numerical Geodynamic Modelling. Cambridge University Press, Cambridge, 358.

d) Stølen, S. & Grande, T. (2008): Chemical Thermodynamics of Materials: Macroscopic and Microscopic Aspects. Wiley, Chichester, 395.

Fegley, B. (2013): Practical Chemical Thermodynamics for Geoscientists. Elsevier, Amsterdam, 674.

Ganguly, J. (2008): Thermodynamics in the Earth and Planetary Sciences. Springer, Berlin/Heidelberg, 490.

e) Patiño Douce, A.E. (2011): Thermodynamics of the Earth and Planets. Cambridge University Press, Cambridge, 722.Hawkes, P.W. (ed.) & Reimer, L. (2010): Scanning Electron Microscopy. Springer Series in Optical Sciences 45, 527.

f) Bowen D.K., Tanner, B.K. (2006): X-ray metrology in semiconductor manufacturing, Taylor & Francis Group, USA.

Birkholz M. (2006): Thin Film Analysis by X-Ray Scattering, Wiley-VCH, Germany.

g) Settimio Mobilio, Federico Boscherini (Eds.) (2015): Synchrotron Radiation: Basics, Methods and Applications, Springer

Willmott, P., An Introduction to Synchrotron Radiation: Techniques and Applications John Wiley & Sons; 1. Auflage 2011.

h) Variable

i) Variable

j) Variable

k) Variable

l) Variable

m) Variable

n) Variable

## Lecture notes

https://ilias.uni-freiburg.de/login.php

http://www.krist.uni-freiburg.de/service/edv.php