Amtliche Bekanntmachungen
der TU Bergakademie Freiberg

Nr. 15, Heft 2 vom 24. Juni 2011

Modulhandbuch

für den

Internationalen Masterstudiengang

Computational Materials Science

<u>INHALTSVERZEICHNIS</u>

Anpassung von Modulbeschreibungen

Zur Anpassung an geänderte Bedingungen können folgende Bestandteile der Modulbeschreibungen vom Modulverantwortlichen mit Zustimmung des Dekans geändert werden:

1. „Code/Daten“
2. „Verantwortlich“
3. „Dozent(en)“
4. „Institut(e)“
5. „Qualifikationsziele/Kompetenzen“
6. „Inhalte“, sofern sie über die notwendige Beschreibung des Prüfungsgegenstandes hinausgehen
7. „Typische Fachliteratur“
8. „Voraussetzungen für die Teilnahme“, sofern hier nur Empfehlungen enthalten sind (also nicht zwingend erfüllt sein müssen)
9. „Verwendbarkeit des Moduls“
10. „Arbeitsaufwand“

Die geänderten Modulbeschreibungen sind zu Semesterbeginn durch Aushang bekannt zu machen.

Code/Dates	KOTM MA.Nr.3120	Version: 02.12.10	Start: SS 2012
Name	Continuum Mechanics		
Responsible	**Last Name** Kuna **First Name** Meinhard **Title** Prof. Dr.		
Lecturer(s)	**Last Name** Kuna **First Name** Meinhard **Title** Prof. Dr.		
Institute(s)	Mechanics and Fluid-Dynamics		
Duration	1 semester		
Competencies	Students will get familiar with the fundamentals of continuum mechanics of three-dimensional bodies under large deformations.		
Contents	Most important ingredients are: tensor algebra and analysis, Eulerian and Lagrangian description, kinematics of continua in large deformations, definition of various measures of stretch and strain, dynamics of continua, generalizes stress tensors, balance laws (mass, momentum, energy, entropy), material theory		
Literature	P. Haupt: Continuum Mechanics and Theory of Materials, Springer, 2000		
Types of Teaching	Lecture (2 SWS); Exercise (1 SWS). Lectures will be given in English.		
Pre-requisites	Basic knowledge in theoretical mechanics		
Applicability	All programs that require sound knowledge of continuum mechanics, such as Mechanical Engineering, Geo-Engineering, Vehicle Construction and Materials Technology.		
Frequency	Every summer semester.		
Requirements for Credit Points	Oral exam (45 minutes)		
Credit Points	The course has a value of 4 credit points.		
Grade	The corresponding mark is the result of the oral examination.		
Workload	The course requires 120 hours split into 45 hours of personal attendance and 75 hours of private study.		

Code/Dates	DFT. MA .Nr. 3205	Version: 02.12.10	Start: SS 2012
Name	Density functional theory for materials science		
Responsible	**Last Name** Kortus **First Name** Jens **Title** Prof. Dr. rer. Nat. habil.		
Lecturer(s)	**Last Name** Kortus **First Name** Jens **Title** Prof. Dr. rer. Nat. habil.		
Institute(s)	Theoretical Physics		
Duration	1 semester		
Competencies	This course uses the theory and application of atomistic computer simulations based on quantum mechanics to model, understand, and predict the properties of real materials.		
Contents	Specific topics include: density functional theory and the total-energy pseudopotential method; errors and accuracy of quantitative predictions and free energy and phase transitions. The course employs case studies from applications of advanced materials to nanotechnology. Several laboratories will give students direct experience with simulations of electronic-structure approaches		
Literature	Martin, R. *Electronic Structure: Basic Theory and Practical Methods*. Cambridge, UK: Cambridge University Press.		
Types of Teaching	Lecture (2 SWS); Exercise (1 SWS); Practical Exercise (1 SWS). Lectures will be given in English		
Pre-requisites	It is recommended to pass Quantum Theory I		
Applicability	For students interested in atomistic simulations of materials.		
Frequency	Every summer semester		
Requirements for Credit Points	The exam will be oral (duration 30 min) in case of less than 12 students. Otherwise it will be a written exam (duration 120 min). Precondition of the exam will be a certificate from the exercises.		
Credit Points	The course has a value of 6 credit points.		
Grade	The corresponding mark is the result of the examination.		
Workload	The course requires 180 hours split into 60 hours of personal attendance and 120 hours of private study including preparation for lessons and exam.		

<table>
<tr><td>Code/Dates</td><td>DisTheo. MA .Nr. 3206</td><td>Version: 02.12.10</td><td>Start: WS 2012</td></tr>
<tr><td>Name</td><td colspan="3">Dislocation Theory and Discrete Element Method</td></tr>
<tr><td>Responsible</td><td colspan="3">Last Name Groh First Name Sebastien Title Prof. Dr.</td></tr>
<tr><td>Lecturer(s)</td><td colspan="3">Last Name Groh First Name Sebastien Title Prof. Dr.
Last Name Konietzky First Name Heinz Title Prof. Dr.-Ing. habil.</td></tr>
<tr><td>Institute(s)</td><td colspan="3">Mechanics and Fluid-Dynamics
Geotechnical</td></tr>
<tr><td>Duration</td><td colspan="3">1 semester</td></tr>
<tr><td>Competencies</td><td colspan="3">The student will get familiar with:
• dislocation theory and numerical methods available to model individual and collective properties of dislocations.
• different techniques based on discrete elements to perform and evaluate corresponding simulations</td></tr>
<tr><td>Contents</td><td colspan="3">Most important ingredients are:
• Elastic properties of dislocations, Thermal properties of dislocations; Nucleation and Multiplication of Dislocations; Dislocation properties in different crystal structures; Mechanisms of motion; Interaction and reactions between dislocations; Link between dislocation plasticity and crystal plasticity. Modeling dislocation properties in an elastic continuum.
• modeling strategy (conceptual and numerical model); classification of DEM; contact detection; constitutive laws; discontinuum versus continuum; modelling of granular material; simulation of damage and fracture; practical hints; applications; practical exercises in 2d and 3d.</td></tr>
<tr><td>Literature</td><td colspan="3"><u>Dislocation Theory:</u>
Theory of Dislocations: Hirth and Lothe
Strengthening Mechanisms in Crystal Plasticity (Oxford Series on Materials Modelling): Ali S. Argon
<u>Discrete Element Method:</u>
Pöschel, T. & Schwager, T. (2005): Computational Granular Dynamics, Springer, 322 p.
Jing, L & Stephansson, O. (2007): Fundamentals of Discrete Element Methods for Rock Engineering, Elsevier, 545 p.
Darve, F. & Ollivier, J.-P. (2008): Discrete Modelling of Geomaterials, European J. Env. Civil Eng., 12(2008)7-8, 253 p.
UDEC/3DEC-Manuals (2010), Itasca Consulting Group
PFC/PFC3D-Manuals (2010), Itasca Consulting Group</td></tr>
<tr><td>Types of Teaching</td><td colspan="3"><u>Dislocation Theory:</u>
Lecture (2 SWS) Exercise (1 SWS) Practical Exercise (1SWS).
<u>Discrete Element Method:</u>
Lecture (3 x 1,5 h); Exercise (3 x 1,5 h).
Lectures are given in English.</td></tr>
<tr><td>Pre-requisites</td><td colspan="3">Knowledge in the fields of metals; Introduction to Scientific Programming and Fundamental of Microstructures. Fundamentals in mechanics</td></tr>
<tr><td>Applicability</td><td colspan="3">Students of Master in Computational Materials Science or other students as minor subject. Students of Materials Science and Materials Engineering.</td></tr>
<tr><td>Frequency</td><td colspan="3">Every winter semester.</td></tr>
<tr><td>Requirements for Credit Points</td><td colspan="3"><u>Dislocation Theory:</u>
Oral examination if less than 5 students. Written examination</td></tr>
</table>

	otherwise. 2 weeks before the examination, a research article will be given to the students. It will give them enough time to analyze the paper (re-demonstrate formula, how the presented data play a role in a multiscale modelling framework, weaknesses of the method…) **If oral exam:** The student will have 30 minutes to present the research article. **If written exam:** 120 minutes to answer questions related to the research paper. Programming project Discrete Element Method: Report about programming task performed during private study
Credit Points	The course has a value of 7 credit points.
Grade	The corresponding mark is the result of the average between the oral/written examination, the programming project and the DEM report programming task weighted with coefficient 3, 3 and 1, respectively.
Workload	Dislocation Theory: The course required 174 hours split in 60 hours of personal attendance and 114 hours of personal work. The amount of time needed for the preparation and reworking of lectures and exercises is rather large due to the complexity of the topics treated within this course and because of the programming exercises involved. Discrete Element Method: The course requires 36 hours split into 9 hours of personal attendance and 27 hours of private study including the generation of the documentation about the programming task.

Code/Daten	ENWWT1 BA.Nr. 091	Stand: 14.7.09	Start: WS 2009/2010
Modulname	Einführung in die Fachsprache Englisch für Ingenieurwissenschaften (Werkstoffwissenschaft, Technologiemanagement, Fahrzeugbau: Werkstoffe und Komponenten, Gießereitechnik)		
Verantwortlich	**Name** Fijas **Vorname** Liane **Titel** Dr.		
Dozent(en)	**Name** Fijas **Vorname** Liane **Titel** Dr.		
Institut(e)	Fachsprachenzentrum		
Dauer Modul	2 Semester		
Qualifikationsziele/ Kompetenzen	Der Teilnehmer erwirbt grundlegende Fertigkeiten der schriftlichen und mündlichen Kommunikation in der Fachsprache, einschließlich eines allgemeinwissenschaftlichen und fachspezifischen Wortschatzes sowie fachsprachlicher Grundstrukturen und translatorischer Fertigkeiten.		
Inhalte	Materials Science and Engineering, Numbers and Measuring Units, Elements and Compounds, Metals, Properties and Behaviour of Metals, Stress-Strain Diagram, Extracting Metals/Blast Furnace, Steel Production, Materials for Computers and Communication/Silicon, III-V Compounds, Copper, Ceramics, Synthetic Materials, Composite Materials		
Typische Fachliteratur	English for Materials Science and Materials Technology, 1st and 2nd semester,TU Bergakademie Freiberg, 2001		
Lehrformen	Übung (4 SWS, Nutzung des Sprachlabors)		
Voraussetzung für die Teilnahme	Kenntnisse der gymnasialen Oberstufe bzw. der Stufe UNIcert II		
Verwendbarkeit des Moduls	Voraussetzung für Modul UNIcert III - Englisch für Werkstoff-wissenschaften		
Häufigkeit des Angebotes	Beginn jährlich zum Wintersemester.		
Voraussetzung für Vergabe von Leistungspunkten	erfolgreiche Teilnahme am Unterricht (mind. 80%) bzw. adäquate Leistung. Leistungsnachweis durch eine Klausurarbeit (im SS) im Umfang von 90 Minuten		
Leistungspunkte	4		
Note	Die Modulnote ergibt sich aus der Note der Klausurarbeit.		
Arbeitsaufwand	Der Zeitaufwand beträgt 120 h und setzt sich zusammen aus 60 h Präsenzzeit und 60 h Selbststudium. Letzteres umfasst die Vor-und Nachbereitung der Lehrveranstaltung sowie die Klausurvorbereitung.		

Code/Dates	MechTest.MA.Nr. 3207	Version: 03.02.11	Start: WS 2012
Name	Experimental Methods		
Responsible	**Last Name** Krüger **First Name** Lutz **Title** Prof. Dr.-Ing.		
Lecturer(s)	**Last Name** Krüger **First Name** Lutz **Title** Prof. Dr.-Ing. **Last Name** Martin **First Name** Stefan **Title** Dipl.-Ing		
Institute(s)	Materials Engineering Materials Science		
Duration	1 semester		
Competencies	Students will get familiar with: • Experimental Methods to measure the flow stress-, deformation- and failure behavior in a wide range of loading rate, temperature and stress state. • Basic principles and examples of the methods for microstructure analysis (optical and scanning electron microscopy, X-ray diffraction).		
Contents	Most important ingredients are: **<u>Experimental Methods</u>:** hardness tests, methods to measure the flow stress-behavior under tensile, compressive, bending and shear loading, Charpy-impact test, drop weight tear test, Pellini-Test, Robertson test. effect of temperature and strain rate on mechanical properties, brittle and ductile failure, methods to determine fracture toughness properties under quasi-static, impact and cycling loading, fatigue testing (Wöhler test / SN-curve), multiaxial testing methods, high strain rate tests (drop weight test, split Hopkinson bar) **<u>Microstructural Analysis</u>:** Basic principles of scanning electron microscopy and X-ray diffraction; phase identification and quantitative phase analysis, determination of the grain, crystallite size and defect-induced microstrains, global and local preferred orientation of crystallites		
Literature	**<u>Experimental Methods</u>:** Dowling, Norman E.: Mechanical Behavior of Materials – Engineering Methods for Deformation, Fracture, and Fatigue, 2007, Pearson Prentice Hall Meyers, Marc A.: Dynamic Behavior of Materials, John Wiley & Sons, New York, 1994 **<u>Microstructural Analysis</u>:** V. Randle, O. Engler: Introduction to texture analysis, macrotexture, microtexture and orientation mapping, Gordon & Breach, Amsterdam, 2000. V. Randle: Microtexture determination and its applications, Institute of Materials, London, 1992. Klug, Harold P., Alexander, Leroy E.: X-ray diffraction procedures for polycrystalline and amorphous materials, New York, Wiley, 2nd edition 1974.		
Types of Teaching	Lecture (3 SWS); Exercise (0 SWS); Practical Exercise (0 SWS) Lectures are given in English.		
Pre-requisites	Profound knowledge of English, basics in materials science, mechanics, advanced mathematics, physics for scientists, crystallography.		
Applicability	Master students in Computational Materials Science, Materials Science and Materials Engineering		
Frequency	Every winter semester		

Requirements for Credit Points	Joint examination for both parts of the module (Mechanical Testing and Microstructure Analysis). Written exam (120 min) if more than 5 students are present. Otherwise oral examination of 30 min.
Credit Points	The course has a value of 4 credit points.
Grade	Grade: The corresponding mark is the result of the examination.
Workload	The course requires 120 hours split into 45 hours of personal attendance and 75 hours of private study and exam preparation.

Code/Dates	FMC. MA .Nr. 3208	Version: 02.12.10	Start: SS 2012
Name	Fracture Mechanics Computations		
Responsible	**Last Name** Kuna **First Name** Meinhard **Title** Prof. Dr.		
Lecturer(s)	**Last Name** Kuna **First Name** Meinhard **Title** Prof. Dr.		
Institute(s)	Mechanics and Fluid-Dynamics		
Duration	1 semester		
Competencies	Development of an understanding of the fracture of materials and structures from the point of view of a design engineer; students acquire knowledge about theoretical (numerical) stress analysis of cracked structures as well as fracture mechanics concepts of brittle, ductile and fatigue failure. Development of the ability to design fail-safe structures with defects, qualitatively assess the safety and durability as well as estimate the duration of life for subcritical crack growth under (random) in-service loads.		
Contents	Most important ingredients are: fundamentals of fracture mechanics, including fracture mechanics concepts and relevant load parameters for elastic and plastic materials under static as well as cyclic loading. Suitable Finite-Element techniques for the calculation of load parameters are introduced. The application of fracture mechanics concepts to the assessment of safety and durability of structures is demonstrated with the help of real-world examples.		
Literature	Ted L. Anderson: Fracture Mechanics: Fundamentals and Applications, CRC Press 2004 M. Kuna: Numerische Beanspruchungsanalyse von Rissen, FEM in der Bruchmechanik, Vieweg-Teubner 2010		
Types of Teaching	Lecture (2 SWS); Exercise (2 SWS). Lectures will be given in English.		
Pre-requisites	Basic knowledge in theoretical mechanics		
Applicability	All programs that require sound knowledge of the mechanics of materials, such as Vehicle Construction, Mechanical Engineering, Materials Science, and Materials Technology.		
Frequency	Every summer semester.		
Requirements for Credit Points	Written exam (120 minutes)		
Credit Points	The course has a value of 5 credit points.		
Grade	The corresponding mark is the result of the written examination.		
Workload	The course requires 150 hours split into 60 hours of personal attendance and 90 hours of private study.		

Code/Dates	FUNMICRO. MA .Nr. 3209	Version: 02.12.10	Start: WS 2011
Name	Fundamental of Microstructures		
Responsible	**Last Name** Groh **First Name** Sebastien **Title** Prof. Dr.		
Institute(s)	Mechanics and Fluid-Dynamics		
Duration	1 Semester		
Competencies	The students will get familiar with the microstructural elements that can be found in real crystalline materials.		
Contents	Most important ingredients are: Crystallography, Dislocations, Void and Void growth mechanisms, solute atoms and strengthening mechanisms, Inclusion and Eshelby solution, characteristic length scale associated to each elements.		
Literature	Introduction to dislocations: Hull and Bacon Crystal defects and microstructures: Modeling across length scale. Phillips Strengthening Mechanisms in Crystal Plasticity (Oxford Series on Materials Modelling): Ali S. Argon		
Types of Teaching	Lecture (2 SWS); Exercise (0 SWS); Practical Exercise (0 SWS). Lectures are given in English.		
Pre-requisites	None		
Applicability	Students from the Master of Computational Materials Science		
Frequency	Every winter semester		
Requirements for Credit Points	Oral exam. The students will have 30 minutes to prepare the examination (one question from the lecture notes and one exercise to discuss). They will then have 30 minutes to discuss the topic and present a solution for the exercice. If there are more than 5 students a written exami (120 minutes) will have to be taken.		
Credit Points	The course has a value of 3 credit points.		
Grade	The corresponding mark is the result of the oral examination.		
Workload	The course required 90 hours split in 30 hours of personal attendence and 60 hours of personal work.		

Code/Dates	GERBA1A .MA.Nr. 094	Version. 28.04.2010	Start: WT 2010/11
Name	German Basic Level I A		
Responsible	**Surname** Keßler **First name** Gisela **Academic Title**		
Lecturer(s)	**Surname** Paul **First name** Sandra **Academic Title** Diplom-Lehrerin		
Institute(s)	Fachsprachenzentrum		
Duration	1 Semester		
Competencies	Students are imparted the basics of phonetics, orthography, grammar and vocabulary. They acquire basic knowledge of the German language and listening, speaking, reading and writing skills in general language as well as regional and cultural studies.		
Contents	Communication in everyday life situations (get to know each other, shopping, restaurant, the course of the day, time expressions); grammar: e.g. question asking, numbers, conjugation of verbs, present and past tenses, amounts, plural forms of nouns, compositions		
Literature	Berliner Platz, volume 1 Langenscheidt		
Types of Teaching	Exercise (60 hours)		
Pre-requisites	No previous proficiency in German is required.		
Applicability	The course is particularly appropriate for exchange students and for international students. Prerequisite for the module German Basic Level 1 B		
Frequency	The course is taught in the winter term.		
Requirements for Credit Points	Successful participation in class (attendance of at least 80%) Passed written exam (90 minutes) at the end of the term.		
Credit Points	4		
Grade	The grade earned in the written exam determines the overall grade.		
Workload	The total time budgeted for the course is set at 120 hours, of which 60 hours (4 SWS) are spent in class and the remaining 60 hours are spent on self-studies. Self-studies include preparing before and after the lessons as well as preparing for examination.		

Code/Dates	IHPC. MA.Nr. 3210	Version: 02.12.10	Start: WS 2012
Name	Introduction to High Performance Computing and Optimization		
Responsible	**Last Name** Ernst **First Name** Oliver **Title** Prof. Dr.		
Lecturer(s)	**Last Name** Ernst **First Name** Oliver **Title** Prof. Dr. (every other year) **Last Name** Knuepfer **First Name** Andreas **Title** Dr. (TU DD)		
Institute(s)	Numerical Analysis and Optimization		
Duration	1 semester		
Competencies	The purpose of this course is to provide an introduction to parallel numerical algorithms and to parallel computing on shared and distributed memory multiprocessor systems.		
Contents	Most important ingredients are: Design and Analysis of Algorithms, Portable Parallel Programming with OpenMP and the MPI (Message Passing Interface), Code profiling and tracing (VAMPIRE) and optimization methods. BLAS (Basic Linear Algebra Subprograms), Parallel Equation Solution (dense/sparse systems), LU-Decomposition, Tridiagonal Solvers, Iterative Methods.		
Literature			
Types of Teaching	Lecture (2 SWS); Exercises (1 SWS). Lectures are given in English.		
Pre-requisites	Basics of numerical analysis and knowledge in scientific programming.		
Applicability	Master students of the Computational Materials Science program.		
Frequency	Every winter semester.		
Requirements for Credit Points	Written exam (120 min), if more than 20 students are present; alternative oral exam (30 minutes). Precondition of the exam will be a Programming Project.		
Credit Points	The course has a value of 4 credit points.		
Grade	The corresponding mark is the result of the exam.		
Workload	The work time needed is 120 hours, consisting of 45 hours of lectures, 75 hours self controlled study including exam preparations and 50 hours for the programming project including the consultations.		

Code/Dates	ISP. MA .Nr. 3211	Version: 07.02.11	Start: WS 2011
Name	Introduction to Scientific Programming		
Responsible	**Last Name** Steinbach **First Name** Bernd **Title** Prof. Dr.		
Institute(s)	Informatics		
Duration	1 Semester		
Competencies	Students will get familiar with the syntax and semantic of a procedural programming language, an object oriented programming language and the approach of interactive programming. Based on this knowledge, the students must be able to implement interactive programs having a graphical user interface that can be executed in the environment of several operating systems.		
Contents	Most important ingredients are: with regard to procedural programming: data types and variables, pointer and arrays, expressions, statements, operators, control structures, functions, structures, functions of a standard library, with regard to object oriented programming: objects and classes , encapsulation, access rights, inheritance, polymorphism, overloading of functions an operators, type casting, templates, functions of a standard library, and with regard to interactive programming: signal, slot, event, property, graphical user interface.		
Literature	Kernighan, Ritchie: The C Programming Language (2nd Edition) – ANSI C, ISBN 0131103628; Stroustrup: The C++ Programming Language: Special Edition, ISBN 0201700735; Blanchette, Summerfield: C++ GUI Programming with Qt 4 (2nd Edition) - The official C++/Qt book, ISBN 0132354160;		
Types of Teaching	Lecture (2 SWS); Exercise (2 SWS); Practical Exercise (0 SWS). Lectures are given in English.		
Pre-requisites	Basic knowledge in mathematics for an university study		
Applicability	Study courses that need a basic knowledge in programming		
Frequency	Every winter semester		
Requirements for Credit Points	Written exam (120 minutes) or programming projects.		
Credit Points	The course has a value of 6 credit points.		
Grade	The corresponding mark is the result of the written examination or the programming projects.		
Workload	The course requires 180 hours split into 60 hours of personal attendance and 120 hours of private study.		

Code/Dates	MasThesis.MA.Nr. 3212	Version: 02.12.10	Start: SS 2012
Name	Master Thesis Computational Science		
Responsible	All Professors from the CMS program		
Lecturer(s)	None		
Institute(s)	None		
Duration	1 semester		
Competencies	The objective of the master thesis is to give the students the opportunity to apply the knowledge acquired during their studies on a research project.		
Contents	Not Applicable		
Literature	Not Applicable		
Types of Teaching	Not Applicable		
Pre-requisites	all modules of the first and second semester except Research Seminar and Journal Club		
Applicability	Students from the Master of Computational Materials Science		
Frequency	Not Applicable		
Requirements for Credit Points	A written document, a defense of 20 minutes and 10 minutes of questions Approval of the examination committee of CMS that the master thesis is sufficient.		
Credit Points	The course has a value of 30 credit points.		
Grade	The corresponding mark is the result of the defence and the master thesis document weighted with coefficient 1 and 3, respectively.		
Workload	The total time budget for this module is set at 900 hours and is all spent as an intern a research group.		

Code/Dates	MatProp.MA.Nr. 3213	Version: 03.02.11	Start: WS 2011
Name	Material Properties		
Responsible	**Last Name** Biermann **First Name** Horst **Title** Prof. Dr.-Ing..		
Lecturer(s)	**Last Name** Weidner **First Name** Anja **Title** Dr.Ing. (Metals) **Last Name** Meyer **First Name** D.C. **Title** Prof. Dr. (Semiconductors)		
Institute(s)	Materials Engineering **(Metals)** Experimental Physics		
Duration	1 semester		
Competencies	Students will get familiar with: **(i) metallic materials** (ferrous materials, non-ferrous metals, light metals, high-temperature metals), their microstructure and mechanical properties as well as heat treatment. Focus is given to plastic deformation and failure. The module will enable the students to differentiate the different groups of metallic construction materials. **(ii) semiconductors** (processes within semiconductor devices and the quantitative description of these processes as well as the basis of application and design principles of semiconductor devices)		
Contents	Most important ingredients are: **Metallic Materials:** • Ferrous metals (plain carbon steels, high-alloyed steels, cast irons); • Non-ferrous metals (e.g. copper, nickel) • Light metals (aluminum, titanium, magnesium) • High-temperature alloys (superalloys, intermetallic alloys) **Semiconductors:** Density and transport of charge carriers in thermodynamic equilibrium, doping, effects of impurities like traps, recombination centers, life-time of carriers, diffusion length, p-n-junctions and applications, diodes, junction transistors, sensors, photovoltaic elements, metal-semiconductor contacts and applications; Schottky diodes, FET.		
Literature	**Metallic Materials:** M. F. Ahby, D.R.H. Jones, Engineering materials 2, 2nd ed., Butterworth-Heinemann, Oxford, 1998 James F. Shackelford, Introduction to Materials Science for Engineers, 7th ed. Addison Wesley., 2009 **Semiconductors:** Standard references of solid state physics for physicists, standard references of semiconductors devices for physicists (e. g. Ch. Kittel: Introduction to Solid State Physics, S.M.Sze: Semiconductor Devices)		
Types of Teaching	Lecture (4 SWS); Exercise (0 SWS); Practical Exercise (0 SWS) decomposed as follow: Metallic Materials: 2/0/0 Semiconductors: 2/0/0		
Pre-requisites	Basic fundamentals of physics, chemistry and solid materials		
Applicability	Students of Master in Computational Materials Science or other students as minor subject. Students of Materials Science and Materials Engineering.		
Frequency	Every winter semester		

Requirements for Credit Points	This module has 2 exams, one for each materials class. **Metallic Materials:** Written exam, 90 – 120 min, if more than 5 students are present. Otherwise oral exam of 30 min. **Semiconductors**: Oral exam (45-60 minutes, up to ten participants) or written exam (90-120 minutes).
Credit Points	The course has a value of 6 credit points.
Grade	The corresponding mark is the result of two examinations averaged with the weights 1/2 and 1/2.
Workload	The course requires 180 hours split into 60 hours of personal attendance and 120 hours of private study.

Code/Dates	WERKMEC .BA.Nr. 253	Version: 02.12.10	Start: WS 2011
Name	Mechanics of Materials		
Responsible	**Last Name** Kuna **First Name** Meinhard **Title** Prof. Dr.		
Lecturer(s)	**Last Name** Kuna **First Name** Meinhard **Title** Prof. Dr.		
Institute(s)	Mechanics and Fluid-Dynamics		
Duration	1 semester		
Competencies	Development of an understanding of the deformation and failure mechanisms of technological materials; students will get familiar with elastic, plastic, viscous, viscoelastic and viscoplastic behaviors of materials; development of the ability to assess the behavior of materials and to design structures accordingly.		
Contents	Most important ingredients are: continuum mechanics foundations of deformation and failure, rheological models for elastic, plastic, viscous, viscoelastic, and viscoplastic behavior; failure theories / criteria for multiaxial loading; introduction to fracture and damage mechanics		
Literature	J. Lemaitre and J.-L. Chaboche: Mechanics of Solid Materials, Cambridge University Press,2000		
Types of Teaching	Lecture (2 SWS); Exercise (2 SWS); Practical Exercise (0 SWS). Lectures are given in English		
Pre-requisites	Basic knowledge in theoretical mechanics		
Applicability	All programs that require sound knowledge of mechanics of materials, such as Materials Science, Materials Technology, Vehicle Construction and Mechanical Engineering.		
Frequency	Every winter semester		
Requirements for Credit Points	Written exam (120 minutes)		
Credit Points	The course has a value of 6 credit points.		
Grade	The corresponding mark is the result of the written examination.		
Workload	The course requires 180 hours split into 60 hours of personal attendance and 120 hours of private study.		

Code/Dates	NADE. MA .Nr. 3214	Version: 02.12.10	Start: SS 2012
Name	Numerical Analysis of Differential Equations		
Responsible	**Last Name** Ernst **First Name** Oliver **Title** Prof. Dr.		
Lecturer(s)	**Last Name** Ernst **First Name** Oliver **Title** Prof. Dr.		
Institute(s)	Numerical Analysis and Optimization		
Duration	1 semester		
Competencies	Students are introduced to fundamental techniques for the numerical solution of ordinary and partial differential equations.		
Contents	ODEs: Euler methods, Runge Rutta Methods, Linear Multistep Methods, Stability, Stiffness; PDEs: Finite Difference techniques, time stepping, von Neumann stability analysis.		
Literature	Finite Difference Methods for Ordinary and Partial Differential Equations von Randy Leveque, University of Washington		
Types of Teaching	Lecture (2 SWS); Exercise (1 SWS) Practical Exercise (0 SWS). Lectures are given in English		
Pre-requisites	Advanced mathematics course for scientists and engineers. Some familiarity with the theory or applications of differential equations is helpful		
Applicability	Students of all Engineering programs requiring numerical methods for differential equations..		
Frequency	Every summer semester.		
Requirements for Credit Points	Written exam (2 hours)		
Credit Points	The course has a value of 3 credit points.		
Grade	The corresponding mark is the result of the written examination		
Workload	The course requires 90 hours split into 45 hours of personal attendance and 45 hours of private study.		

Code/Dates	PP.MA.Nr. 3215	Version: 02.12.10	Start: WS 2012
Name	Personal Programming Project		
Responsible	**Last Name** Groh **First Name** Sebastien **Title** Prof. Dr.		
Lecturer(s)	**Last Name** Groh **First Name** Sebastien **Title** Prof. Dr. **Last Name** Kortus **First Name** Jens **Titel** Pr Dr **Last Name** Mühlich **First Name** Uwe **Titel** Dr		
Institute(s)	Mechanics and Fluid-Dynamics Theoretical Physics		
Duration	1 semester		
Competencies	The students will develop and document then own numerical tool (one out of the following three: Density Functional Theory, Molecular Dynamics, Finite Elements Method). Furthermore, they will use it to calculate one material property of their choice.		
Contents	Most important ingredients are: Developing the tool, commenting the source file, documentation and example to calculate mechanical behavior or physical properties.		
Literature	None		
Types of Teaching	By the end of the first semester, the students will have to decide on which numerical tool they want to work. Based on a first come first serve, 1/3 of the students will work on FEM, 1/3 on MD and the last 1/3 on DFT. A supervisor of the project will be assigned to the students. During the third semester, the students will have consultation meetings with their supervisor to discuss the roadblocks and the advancement of the project.		
Pre-requisites	None		
Applicability	Students from the Master of Computational Materials Science		
Frequency	Every winter semester		
Requirements for Credit Points	Two weeks before the end of the semester, the students will deliver the final product (source code, documentation, analysis of an example solved with their numerical tool). The project will be defended (20 minutes).		
Credit Points	The course has a value of 7 credit points.		
Grade	The corresponding mark is the result of the written documents and the defense.		
Workload	The course requires 210 hours of personal work.		

Code/Dates	PLAS. MA.Nr. 3216	Version: 02.12.10	Start: WS 2012
Name	Plasticity		
Responsible	**Last Name** Häusler **First Name** Christoph **Title** Dr.		
Lecturer(s)	**Last Name** Häusler **First Name** Christoph **Title** Dr.		
Institute(s)	Mechanics and Fluid-Dynamics		
Duration	1 semester		
Competencies	Students will get familiar with the principal formulation of in-elastic constitutive equations from the viewpoint of thermodynamics. Special emphasis is placed on the formulation of plastic and viscoplastic constitutive laws.		
Contents	Most important ingredients are: balance laws, thermodynamically motivated formulation of constitutive equations, plasticity, thermoplasticity, viscoplasticity		
Literature	Ottosen and Ristinmaa: ”The Mechanics of Constitutive Modeling” Khan and Huang: “Continuum Theory of Plasticity” Lemaitre and Chaboche: “Mechanics of Solid Materials”		
Types of Teaching	Lecture (2 SWS); Exercise (1 SWS); Practical Exercise (0 SWS). Lecture will be given in English.		
Pre-requisites	Contents of Continuum Mechanics		
Applicability	Master students in Computational Materials Science, Master students in mechanical Engineering		
Frequency	Every winter semester.		
Requirements for Credit Points	Written exam, 90 – 120 min, if more than 5 students are present. Otherwise oral examination of 30 min.		
Credit Points	The course has a value of 4 credit points.		
Grade	The corresponding mark is the result of the examination.		
Workload	The course requires 120 hours split into 45 hours of personal attendance and 75 hours of private study.		

Code/Dates	PHTHQ1.BA.Nr. 175	Version: 02.12.10	Start: WS 2011
Name	Quantum Theory I		
Responsible	**Last Name** Kortus **First Name** Jens **Title** Prof. Dr. rer. Nat. habil.		
Lecturer(s)	**Last Name** Kortus **First Name** Jens **Title** Prof. Dr. rer. Nat. habil.		
Institute(s)	Theoretical Physics		
Duration	1 semester		
Competencies	Students will get familiar with basic physical relationships in the context of quantum theory, and will be qualified to formulate these mathematically.		
Contents	Starting with experimental results giving evidences of the need quantum mechanics to model the microscopic world, a brief introduction containing the Schrödinger equation, the theory of Hilbert space, linear and Hermitian operators, particles with spin and many-body systems (bosons, fermions) is given. A qualitative understanding of the chemical bond is taught. The infinite potential well, the potential barrier (tunneling), the harmonic oscillator and the hydrogen atom will be discussed. The angular momentum operators will be defined and their properties discussed. Approximation methods (variational calculus, perturbation theory) will be tackled by example. During the practical courses, after a short introduction on the use of Mathematica, this software will be used to solve mathematical and physics related problems.		
Literature	Claude Cohen-Tannoudji: Quantum Mechanics Vol. 1		
Types of Teaching	Lecture (2 SWS); Exercise (2 SWS); Practical Exercise (2 SWS) Lectures are given in English		
Pre-requisites	Basic knowledge in theoretical mechanics and algebra.		
Applicability	Master degree in Computational Materials Science, Geoinformatics and Geophysics, Electronic- and Sensor Materials, Diploma in Applied Mathematics and Bachelor degree Applied Natural Science		
Frequency	Every winter semester		
Requirements for Credit Points	The exam will be oral (duration 30 min) in case of less than 12 students. Otherwise it will be a written exam (duration 120 min). Precondition of the exam will be a certificate from the exercises.		
Credit Points	The course has a value of 6 credit points.		
Grade	The corresponding mark is the result of the oral examination.		
Workload	The course requires 180 hours split into 90 hours of personal attendance and 90 hours of private study.		

Code/Dates	ResSem.MA.Nr. 3217	Version: 03.02.11	Start: WS 2011
Name	Research Seminar and Journal Club		
Responsible	**Last Name** Groh **First Name** Sebastien **Title** Prof. Dr.		
Lecturer(s)	None		
Institute(s)	Mechanics and Fluid-Dynamics		
Duration	4 semesters		
Competencies	The student will attend monthly research seminars.		
Contents	Most important ingredients are: Literature review on the seminar topic Attending the seminar Interacting with the speakers		
Literature	None		
Types of Teaching	One week before the seminar, the students will review the work carried by the speaker on seminar topic. A list of questions will be prepared. That should make the students confident, and it will help the shiest students to interact with the speakers.		
Pre-requisites	None		
Applicability	Students from the Master of Computational Materials Science		
Frequency	Every winter semester		
Requirements for Credit Points	Interaction with the speakers		
Credit Points	The course has a value of 3 credit points (1 credit point per semester). During the 4^{th} semester, students will attend research seminar in their master thesis' institute.		
Grade	The corresponding mark is the evaluation of the interaction with the speakers.		
Workload	Reading and analysing research paper, which will require approximately 90 hours.		

Code/Dates	STSSP Ma. Nr. 3218	Version: 02.12.10	Start: SS 2012
Name	Selected Topics of Solid State Physics		
Responsible	**Last Name** Rafaja **First Name** David **Title** Prof. Dr. rer. nat. habil.		
Lecturer(s)	**Last Name** Rafaja **First Name** David **Title** Prof. Dr. rer. nat. habil.		
Institute(s)	Materials Science		
Duration	1 semester		
Competencies	Basic principles of solid state physics, correlation between the crystal and real structure and the electronic, magnetic, optical and thermal properties of solids. Absolving the course, the students should be able to recognise the effect of the structure on materials properties and to apply their knowledge in materials design		
Contents	Drude model of electrical conductivity; temperature dependence of electrical resistivity in metals and semiconductors; Schottky contact; p-n contact; superconductivity (Landau theory); magnetic susceptibility; dia-, para-, ferro-, antiferro- and ferrimagnetism; optical properties of solids; complex index of refraction; dispersion curves for systems with free and bound electrons; Kramers-Kronig relationship; colour of metals; optical theory of reflection for multilayer systems; thermal expansion; specific heat (Einstein and Debye models); heat conductivity		
Literature	R.E. Hummel: Electronic properties of materials, Springer-Verlag C. Kittel: Introduction in solid state physics, Wiley		
Types of Teaching	Lectures (3 SWS). Lecture will be given in English.		
Pre-requisites	Knowledge in the fields of advanced mathematics, physics for scientists, general organic and inorganic chemistry, crystallography.		
Applicability			
Frequency	Every summer semester. This module corresponds to the second semester of the existing AFKP BA. Nr. 221 module starting every winter semester.		
Requirements for Credit Points	Oral exam (30 minutes)		
Credit Points	The course has a value of 5 credit points.		
Grade	The corresponding mark is the result of the oral examination.		
Workload	The course required 150 hours split in 45 hours of personal attendance and 105 hours of private study. The latter includes courses and exam preparation.		

Code/Dates	STFEM. MA .Nr. 3219	Version: 02.12.10	Start: SS 2012
Name	Selected Topics of the Finite Element Method		
Responsible	**Last Name** Mühlich **First Name** Uwe **Title** Dr		
Lecturer(s)	**Last Name** Mühlich **First Name** Uwe **Title** Dr		
Institute(s)	Mechanics and Fluid-Dynamics		
Duration	1 semester		
Competencies	Students will get familiar with the theoretical fundamentals of the FEM related to geometrically and physically nonlinear problems. They should be able to program Finite-Element-solutions for simple physically nonlinear applications. Based on the knowledge provided by the module, students should be able to select appropriate Finite-Element-tools for specific problems and to evaluate the numerical results properly.		
Contents	Most important ingredients are: Weak form of the equilibrium conditions, FEM for physically nonlinear problems, Coupled problems with FEM, FEM for linear dynamic problems, Programming of FEM-solutions with MATLB and optional: FEM for large deformations and specific structural elements.		
Literature	Wriggers: Nichtlineare Finite-Element-Methoden, Springer 2001 Bonet, Wood: Nonlinear continuum mechanics for finite element analysis		
Types of Teaching	Lecture (2 SWS); Exercise (1 SWS); Practical Exercise (1SWS). Lectures are given in English		
Pre-requisites	Basic knowledge in theoretical mechanics; Module Numerical Methods for Mechanics or Introductory Lecture FEM or comparable		
Applicability	Students of Master in Computational Materials Science		
Frequency	Every summer semester.		
Requirements for Credit Points	Oral exam (35-50 minutes) The successful preparation of a FEM solution with MATLAB is required to be examined.		
Credit Points	The course has a value of 6 credit points.		
Grade	The corresponding mark is the result of the oral examination.		
Workload	The course requires 180 hours split into 60 hours of personal attendance and 120 hours of private study. The amount of time needed for the preparation and reworking of lectures and exercises is rather large due to the complexity of the topics treated within this course and because of the programming exercises involved.		

Code/Dates	MD. MA .Nr. 3220	Version: 02.12.10	Start: SS 2012
Name	Selected Topics of the Molecular Dynamics Method		
Responsible	**Last Name** Groh **First Name** Sebastien **Title** Prof. Dr.		
Lecturer(s)	**Last Name** Groh **First Name** Sebastien **Title** Prof. Dr.		
Institute(s)	Mechanics and Fluid-Dynamics		
Duration	1 semester		
Competencies	The student will get familiar with Molecular Dynamics and interatomic potential (EAM, MEAM). By the end of the semester, they will be able to implement new functionality in existing MD codes and to develop interatomic potentials for diverse elements.		
Contents	Most important ingredients are: Newton's equation of motion, numerical integrator (Verlet, leap-frog), order of accuracy of the integrator, conservation laws of Hamiltonian systems, Interatomic interactions, Energy minimization (conjugate gradient, steepest descent method), Periodic boundary conditions, microcanonical ensemble, constant pressure method, Parrinello-Rahman's method, Nose-Hoover thermostat and others.		
Literature	Computer simulations of dislocations (Oxford Series on Materials Modelling): Bulatov and Cai Undestanding molecular simulation. From Algorithms to Applications (Acedemic Press): Frenkel and Smit		
Types of Teaching	Lecture (2 SWS) Exercise (1 SWS) Practical Exercise (1 SWS). Lectures are given in English.		
Pre-requisites	Knowledge in the fields of metals; Introduction to Scientific Programming and Fundamental of Microstructures, Quantum Mechanics		
Applicability	Master students in Computational Materials Science.		
Frequency	Every summer semester.		
Requirements for Credit Points	Oral examination if less than 5 students. Written examination otherwise. 2 weeks before the examination, a research article will be given to the students. It will give them enough time to analyze the paper (re-demonstrate formula, how the presented data play a role in a multiscale modelling, weaknesses of the model…) **If oral exam:** The student will have 30 minutes to present the research article. **If written exam:** 120 minutes to answer questions related to the research paper. Programming project		
Credit Points	The course has a value of 6 credit points.		
Grade	The corresponding mark is the result of the average between the oral/written examination and the programming project weighted with the coefficient 1 and 1, respectively. Both examinations will have to be passed.		
Workload	The course required 180 hours split in 60 hours of personal attendance and 120 hours of personal work. The amount of time needed for the preparation and reworking of lectures and exercises is rather large due to the complexity of the topics treated within this course and because of the programing exercises involved.		

Code/Dates	STOMATE. MA.Nr. 3221	Version: 02.12.10	Start: WS 2012
Name	Stochastic Methods for Materials Science		
Responsible	**Last Name** van den Boogaart **First Name** Gerald **Title** Prof. Dr.		
Lecturer(s)	**Last Name** van den Boogaart **First Name** Gerald **Title** Prof. Dr.		
Institute(s)	Stochastic		
Duration	2 semester		
Competencies	The student will understand the role of stochastic modelling and stochastic algorithms for computational material sciences. He/she will learn to select, implement and test stochastic algorithms and models in an applied context.		
Contents	The lecture introduces examples of stochastic methods of material modeling, analysis and simulations: e.q. models and algorithms for the simulation of random structures (random mosaics, random composites, packing, …) and random behavior (crack initiation, random loads, random fatigue, …), statistical and stereological analysis of structural data and EBSD-crystal orientation measurements, Monte-Carle algorithms for material simulation, Markov-Chain-Monte-Carlo/Metropolis-Hastings algorithms for parameter estimation and structure reconstruction.		
Literature	e.g. Stoyan, Kendall, Mecke: Stochastic geometry and its applications		
Types of Teaching	Lecture (2 SWS); 0.5 SWS consulting for the programming project, Lectures are given in English		
Pre-requisites	Basic knowledge of stochastic, statistic, geometry, continuum mechanics, computer programming, and either crystallography or basic group theory.		
Applicability	Master and postgraduate studies in mathematics, engineering or physics. The module is especially designed for the international master program in computational materials science and PhD students working in material modeling.		
Frequency	Every winter semester.		
Requirements for Credit Points	The examination of the module consists of a 30-minutes oral exam and a marked programming project. The project has to be finished in the semester following the lectures.		
Credit Points	The course has a value of 4 credit points.		
Grade	The mark is computed as the arithmetic average of the marks of the exam and the programming project. Both need to be passed.		
Workload	The work time needed is 120 hours, consisting of 30 hours of lectures, 40 hours self controlled study including exam preparations and 50 hours for the programming project including the consultations.		

Code/Dates	TM.MA.Nr.3222	Version: 02.12.10	Start: WS 2011
Name	Thermodynamics of Materials		
Responsible	**Surname** Masset **First Name** Patrick **Title** Dr. HDR		
Lecturer(s)	**Surname** Masset **First Name** Patrick **Title** Dr. HDR		
Institute(s)	Energy Process and Chemical Engineering		
Duration	1 semester		
Competencies	Students will get familiar with thermodynamic properties of materials and phase diagram calculation methods.		
Contents	Most important ingredients are: • Thermodynamic laws and quantities • Thermodynamic properties of materials • Calculation of complex equilibriums in multiphase and multi component systems • Optimization of phase diagrams		
Literature	Mats Hillert, “Phase equilibria, phase diagrams and phase transformations”, 2nd Ed., Cambridge (2009) Robert de Hoff, “Thermodynamics in Materials Science2, 2nd Ed., Taylor&Francis (2006) Hans Leo Lukas, Suzana Fries, Bo Sundman, “Computational Thermodynamics, the CALPHAD method”, Cambridge (2007).		
Type of Teaching	Lecture (2 SWS); Exercise (0 SWS); Practical Exercise (1 SWS). Lectures are given in English.		
Prerequisites	Background in physical chemistry and materials science		
Applocability	Students of Master in Computational Materials Science or other students as minor subject. Students of Materials Science and Materials Engineering.		
Frequency	Every winter semester		
Requirements for Credit Points	written exam (120 minutes) if more than 5 students. Oral exam (30 minutes) otherwise.		
Credit Points	The course has a value of 3 credit points. The corresponding mark is the result of the oral/written examination.		
Grade	The corresponding mark is the result of the oral/written examination.		
Workload	The course requires 90 hours split into 45 hours of personal attendance and 45 hours of private study.		

Freiberg, den 23.06.2011

gez.

Prof. Dr.-Ing. Bernd Meyer

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