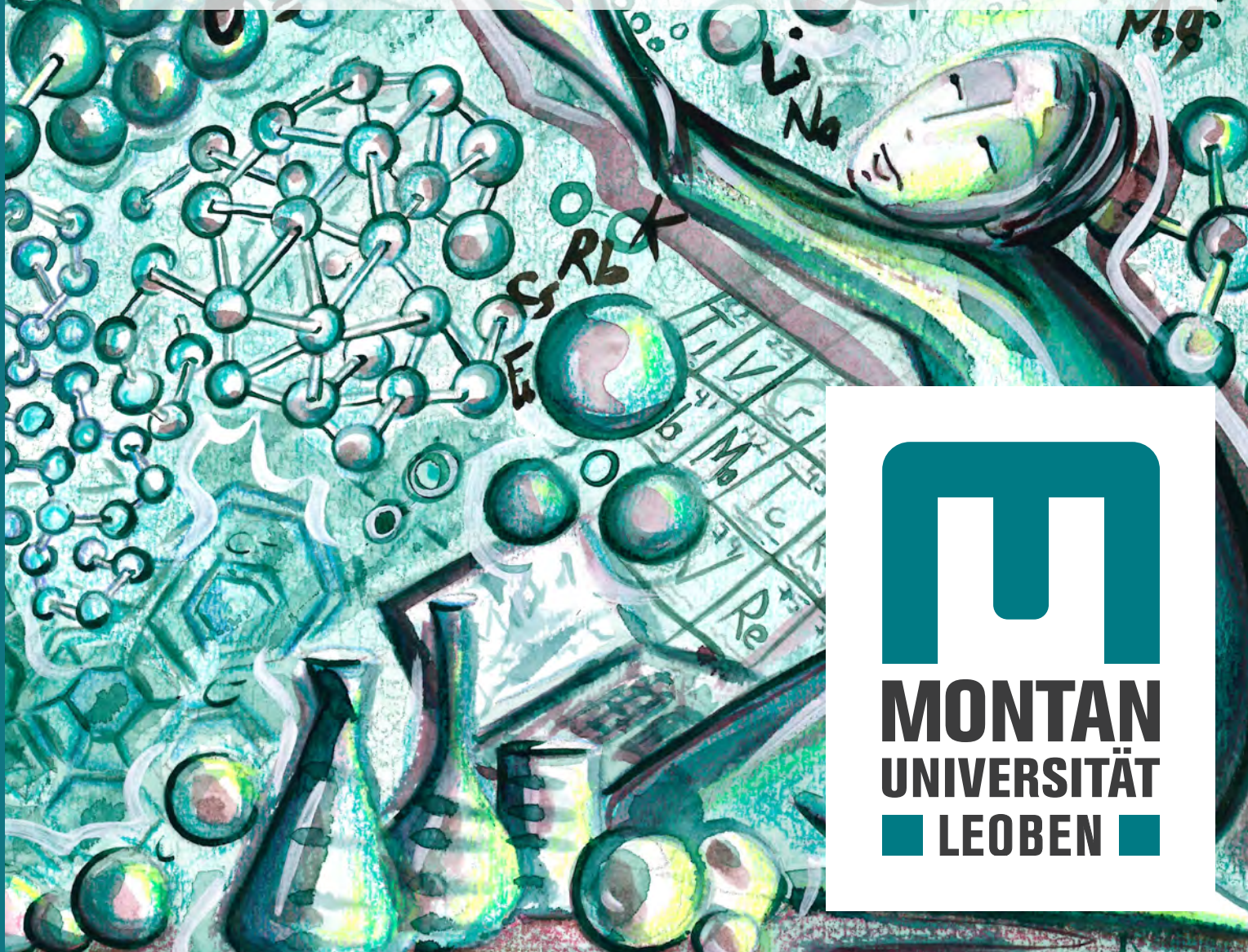
Materials Science

Department Materials Science

Annual report 2020



MONTAN UNIVERSITÄT LEOBEN

Preface

Dear Partners of the Department of Materials Science!

2020 was definitely a very demanding year, testing the resilience of all of us. When the pandemic outbreak of Covid-19 hit Austria, we immediately had to implement new ways of working in research and teaching, with the new concepts continuously adapted and further developed during the year. Needless to say, the health of our staff and all our students has always been the highest priority.

As with any crisis, we also had our positive learnings, for instance implementing and successfully handling distance learning methods and remote work. In addition, we were faced with increased administrative burden to cope with the new situation. We are proud to state that, due to a strict safety concept and the mandatory in-house virus testing before exams or lab courses, none of our colleagues and students have been infected during their work at the Department. Despite these demanding conditions, the scientific output could be kept at a high level. This is manifested, for example, by the almost unaffected number of articles published in some of the most prestigious journals in materials science.

Particularly important for the future development of the Department was the nomination of Lorenz Romaner as Professor for Computational Materials Science in December 2020. In addition to the activities of David Holec, this will enable an extended focus on interface modelling and boost the field of atomistic modeling and machine learning at the Department. We also established the Advanced Micro- and Nanostructure Characterization Group – a research group jointly operated by the Chairs within the Department, with the goal to foster synergies from the unique portfolio of characterization techniques available. Despite the Corona crisis, the year 2020 was intense in terms of investments into new equipment for materials characterization, such as new scanning electron and confocal laser microscopes, and materials processing, e.g. gas atomizer, 3D printer and tape caster were acquired and are being installed or already operational.

Finally, we are grateful to our staff and students for all their efforts which helped to master the last year. Furthermore, we appreciate the continuing support of our partners during these challenging times!

We hope you enjoy reading the following pages, which are intended to provide an overview of our activities in the last year.

Prof. Dr. Raul Bermejo Prof. Dr. Helmut Clemens Prof. Dr. Jürgen Eckert

Prof. Dr. Christian Mitterer Prof. Dr. Ronald Schnitzer

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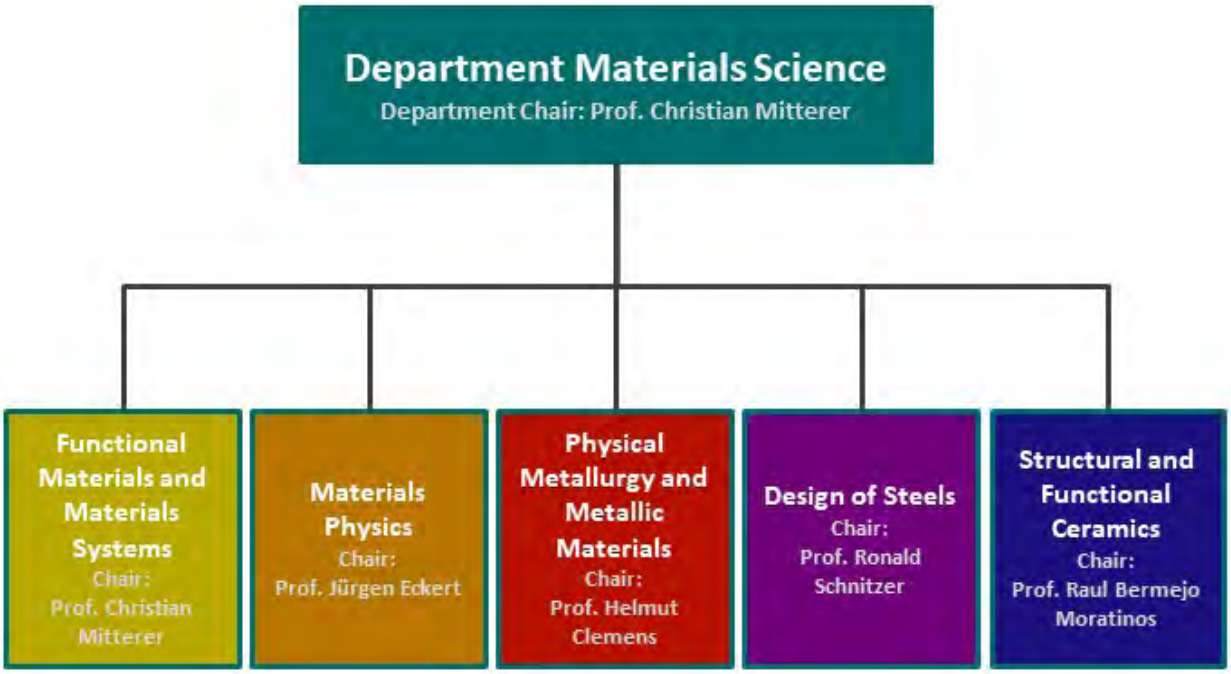
Organigram


Department Materials Science
Department Chair: Prof. Christian Mitterer
Functional Materials and Materials Systems
Chair:
Prof. Christian Mitterer
Materials Physics
Chair:
Prof. Jürgen Eckert
Physical Metallurgy and Metallic Materials
Chair:
Prof. Helmut Clemens
Design of Steels
Chair:
Prof. Ronald Schnitzer
Structural and Functional Ceramics
Chair:
Prof. Raul Bermejo Moratinos

Personnel

Personnel

In 2020, 173 people were employed at the Department Materials Science. The expenses for 43.5 employees were covered by federal funds, 129.5 employees were financed by third-party projects.

Head of department

Univ.-Prof. Dr.
Christian Mitterer

Chair/Deputy

Univ.-Prof. Dr.
Raul Bermejo Moratinos

Univ.-Prof. Dr.
Helmut Clemens

Univ.-Prof. Dr.
Jürgen Eckert

Univ.-Prof. Dr.
Ronald Schnitzer

Chair of Functional Materials and Materials Systems

Chair

Univ.-Prof. Dr.
Christian Mitterer

Deputy chair

Assoz. Prof. Dr.
Rostislav Daniel
Group leader

Group leader

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Robert Franz

Dr.
Nina Schalk

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Regina Kranz
Study administrations
Personnel management

Reinhilde Stopar
Study administrations
Personnel management
Financial management

Susanne Strasak, Bakk.phil.
Study administrations
Personnel management

Angelika Tremmel, MA
Accounting
Controlling
Public relations

Technicians

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Ing.
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Electrical engineering

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Graduate student

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MSc.
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PhD student

MSc.
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PhD student

Dipl.-Ing.
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PhD student

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PostDoc

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Student staff

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PostDoc

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Mag.
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Michael Tkadletz
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Dipl.-Ing.
Ao Xia
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Chair of Physical Metallurgy and Metallic Materials

Chair

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Group leader

Group leader

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David Holec

Priv.-Doz. Dr.
Verena Maier-Kiener

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Francisca Mendez Martin

Dr.
Boryana Rashkova

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Lorenz Romaner

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Bruno Krajnc
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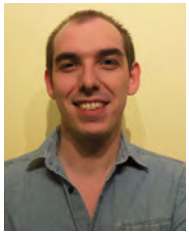
Thomas Leiner
Graduate student

Dipl.-Ing.
Lukas Löfler
PhD student



Thomas Lukas
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Graduate student

Fabian Pürstl
Graduate student

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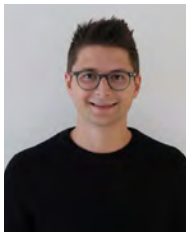

Philipp Schwendenwein
Student staff

Dipl.-Ing.
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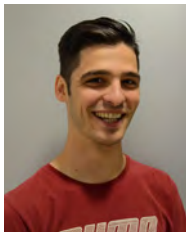
PhD student



Michael Sommerauer
Graduate student

Sebastian Teusl
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Dipl.-Ing.
Reinhold Wartbichler
PhD student

Dipl.-Ing.
David Wimler
PhD student

Dip.-Ing.
Stefan Zeisl
PhD student

Chair of Materials Physics

Chair

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Jozef. Keckes

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Ing.
Herwig Felber
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Manuela Karner
Cleaning

Silke Kaufmann
Metallography
(maternity leave)

Vanessa Topler
Metallography

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Dipl.-Ing.
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Dipl.-Ing.
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Mgr.
Jitka Holcova
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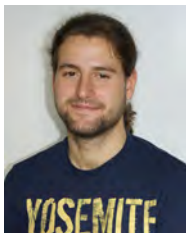
Dipl.-Ing.
Simon Pillmeier
PhD student



Dr.
Julian Rosalie
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Jakub Zalesak
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Tobias Ziegelwanger
Graduate student

Dr.
Mingue Zhao
PostDoc

Endowed Professorship and Chair of Design of Steels – BMK Professorship for Industry

Chair

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Deputy Chair

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Patrick Lebernegg
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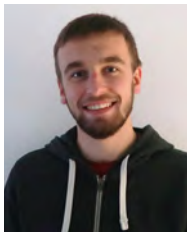

Dipl.-Ing.
Jan Platl
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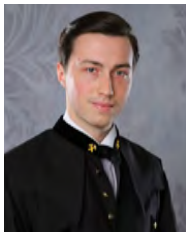
Personnel

Magdalena Pölzgutter
Graduate student

Armin Proyer
Graduate student



Daniel Rainer
Student staff

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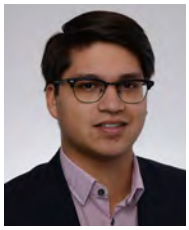

Dipl.-Ing.
Hannah Schönmaier
PhD student

Dipl.-Ing.
Manfred Stadler
PhD student

Alexander Wen
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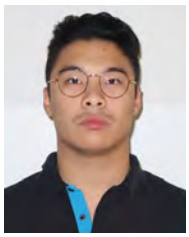

Theresia Zeitlhofer
Student staff

Chair of Structural and Functional Ceramics

Chair

Univ.-Prof. Dr.
Raul Bermejo Moratinos

Deputy Chair

Ass.-Prof. Dr.
Tanja Lube

University lecturer

Ao.Univ.-Prof. Dr.
Peter Supancic

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Financial management

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Ing.
Ronald Binder
Workshop

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Dr.
Manuel Gruber
Senior Scientist

Viktor Haipl
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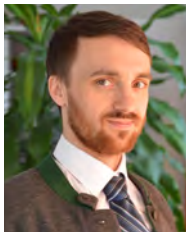
Walter Harrer
Senior Scientist

Dipl.-Ing.
Anna Katharina-Hofer
PhD student

BSc.
Abdullah Jabr
Graduate student

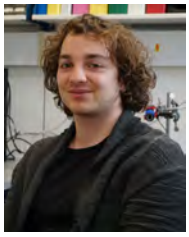
MSc.
Benjamin Kaufmann
PhD student



Dipl. -Ing
Irina Kraleva
Senior Scientist

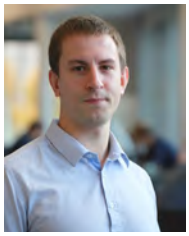
Dr.
Josef Kreith
Senior Scientist

Maximilian Munz
Student staff



Johannes Neumüller
Graduate student

Ing.
Roman Papsik
PhD student

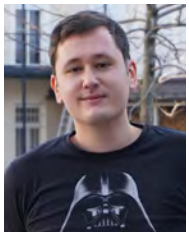


Elija Ribul
Student staff

Dipl. Ing.
Josef Schlachter
PhD student

Dipl. Ing.
Maximilian Staudacher
PhD student

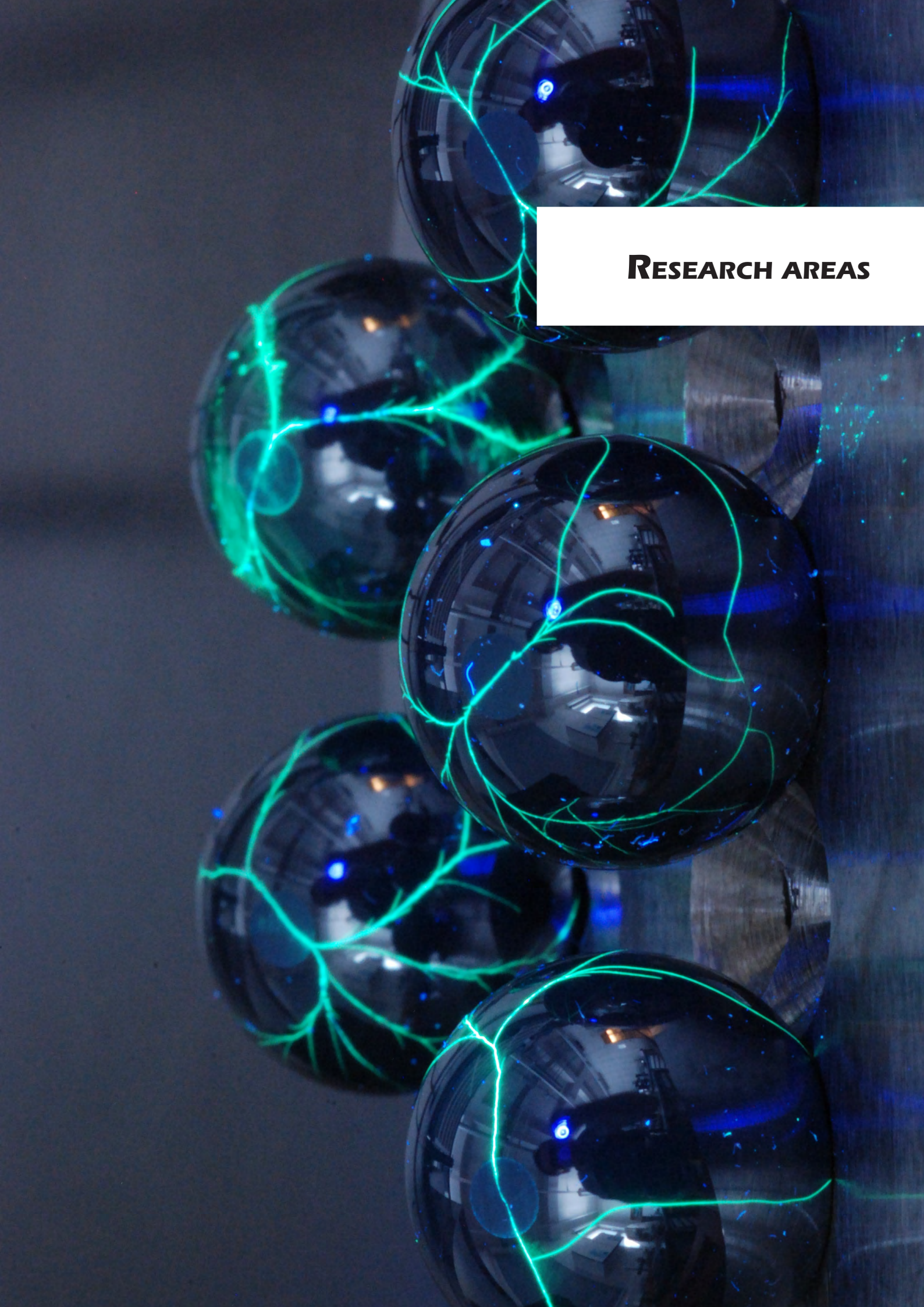
Andreas Vratanar
Student staff



Retired/ emeritus University professors

o.Univ.-Prof. Dr.
Robert Danzer

Univ.-Prof.i.R. Dr.
Albert Kneißl



Research areas

Mission statement

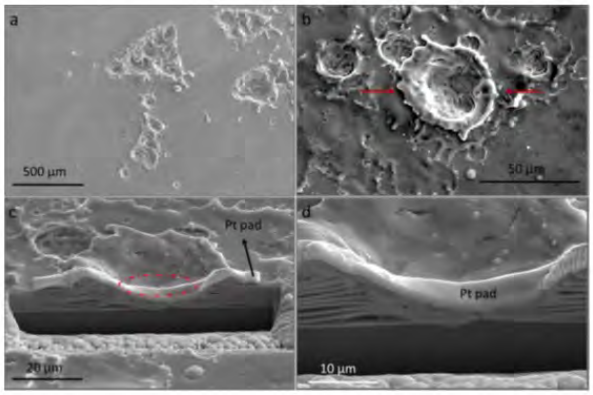
Within the Department of Materials Science, research is done at the highest international level, to achieve a detailed understanding of the structure and the properties of materials and material systems. In teaching, students are integrated as early as possible in research activities, to gain new insights by joint research of supervisors and students. The obtained findings are transferred to the society via publications, to establish a solid knowledge basis for future applications. International visibility of the Materials Science area at Montanuniversität Leoben stems from a supercritical size, which necessitates the completeness in methods available to us and in the materials classes covered.

Chair of Functional Materials and Materials Systems

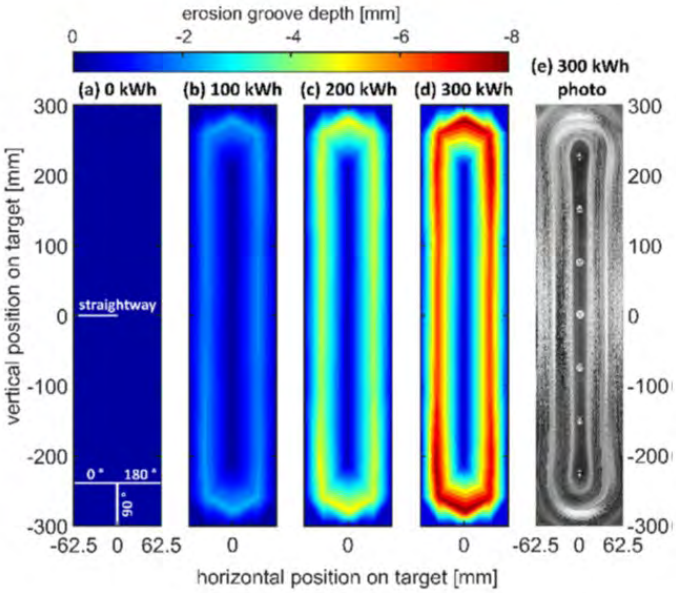
At the Chair of Functional Materials and Materials Systems, the following working groups with their group leaders added in parenthesis are established: Plasma and Surface Engineering (Robert Franz), Multifunctional Thin Films (Nina Schalk), Design and Architecture of Functional Materials Systems (Rostislav Daniel), and Advanced Micro- and Nanostructure Characterization (Michael Tkadletz, group operated jointly by the Chairs of Functional Materials and Materials Systems, Physical Metallurgy and Metallic Materials, and Steel Design).

Research at the Chair focuses on the functionalization of surfaces by coatings, thin films and nanoparticles. For material synthesis, plasma-assisted vapor deposition techniques are used. The Chair operates a unique portfolio of vapor deposition systems, ranging from lab- to industrial scale, including sputter deposition (DC, pulsed DC, HiPIMS), cathodic arc evaporation, and – presently being installed – magnetron sputter inert gas condensation of nanoparticles. This portfolio for the synthesis of functional materials is complemented by facilities for the investigation of microstructure and mechanical/tribological properties. Further support is provided by various simulation tools for deposition processes and for materials design. Additional methods for materials characterization and modelling are used in collaboration within the Department of Materials Science and other Chairs and Institutes within Montanuniversität Leoben. Application-oriented research is done for tribological coatings for tools and components for automotive and aerospace application, for thin films for functional devices for microelectronics and displays, and for the functionalization of surfaces for energy conversion and storage.

Special emphasis of research is laid on plasma-material interaction, as required for sputtering and arc evaporation of vapor sources, and its effect on film growth conditions. To fulfil the increasing demand for multifunctional thin films, multi-component vapor sources are used. In a recent approach, the modification of a dual-element cathode exposed to a cathodic arc was studied using a novel multilayer cathode design, where site-specific electron microscopy characterization techniques provided insights into crater formation and material intermixing below the crater surface. For sputter deposition processes, the effect of the ongoing evolution of the target erosion groove was shown to influence the magnetic field strength measured in front of the target surface, which significantly affects the homogeneity of thickness, microstructure, residual stress and electrical resistivity of molybdenum thin films.



Scanning electron microscopy images of craters formed on a multilayer Mo/Al cathode eroded by cathodic arc evaporation.



Evolution of the erosion groove on a planar molybdenum target over its lifetime expressed in kWh.

Chair of Physical Metallurgy and Metallic Materials

The chair is divided into the following research areas: 'High-resolution materials analysis' (Francisca Mendez-Martin and Boryana Rashkova), 'Mechanical properties and high-performance materials' (Verena Maier-Kiener), 'Phase transformations and high-temperature materials' (Svea Mayer), 'Material behavior under process and application conditions' (Petra Spörk-Erdely), 'Computational Materials Science' (David Holec and Lorenz Romaner (since December 2020)) and 'Materials testing' (Verena Maier-Kiener).

In the area of 'Mechanical Properties and High-Performance Materials', the interaction of mechanical deformation behavior with the microstructure from room temperature to application-relevant conditions is investigated. For this purpose, local, high-resolution characterization methods are mainly used in order to gain basic knowledge of material behavior, which can then be used specifically for further alloy design.

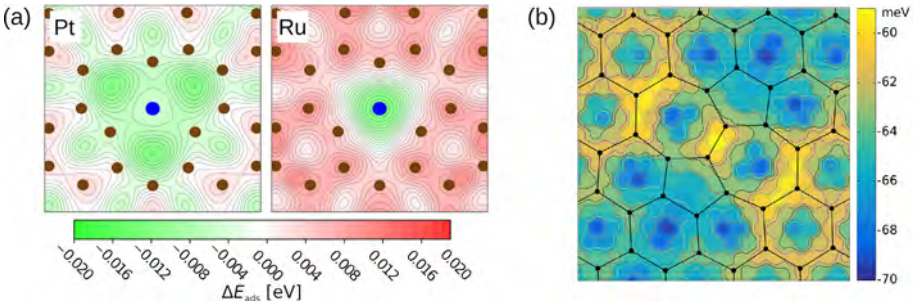
Intermetallic titanium aluminides and titanium alloys are used as structural materials in the next generation of aircraft engines and internal combustion engines. Through thermodynamic modeling and the use of the latest investigation and analysis methods, new alloy systems, e.g. for additive manufacturing, are developed together with industrial partners.

The focus of the computer-aided material modeling has been widened by extensive combination of atomistic techniques (including application of machine-learned potentials) in addition to the quantum mechanical approaches. Hybrid methods combining quantum mechanical and molecular dynamics simulations allowing for calculations of extended defects (such as grain boundaries) and impact of alloying elements have been developed. The research topics included mechanical properties of superlattice coatings, phase transformation in TiAl alloys, understanding of 2D materials or exploring H storage capabilities of carbon (see Figure) to name a few. The capabilities in the calculation of atomic-scale materials properties, including in particular crystallographic defects such as dislocations and grain boundaries, have been reinforced with the integration of Lorenz Romaner into the chair at the end of the year.

High-resolution characterization methods such as atom probe tomography and/or transmission electron microscopy are used to obtain qualitative and quantitative information about the morphology, composition and distribution of phases. The unique selling point in Austria are the two three-dimensional atom probes. With this technique, the composition of the above-mentioned materials is analyzed down to the atomic level. In order to better understand the behavior of modern materials under process and application conditions, specific diffraction and scattering methods are used.

In-situ experiments using synchrotron radiation and neutrons allow e.g. the characterization of precipitation processes and phase changes in thermodynamic imbalance as well as the deformation behavior of materials on the level of the crystal lattice.

In the field of materials testing the focus is on the correlation of microstructure and mechanical properties.



Computer-aided design of carbon-based materials for H storage: (a) stronger adsorption of H near metal dopants quantified by the change of adsorption energy, ΔEads (negative values mean stronger attraction for H) and (b) weakened attraction of H due to a Stone-Wales defect (pristine graphene shows values of adsorption energy between -68 and -64 meV/H atom).

Chair of Materials Physics

The activities of the Chair of Materials Physics are closely linked to its partnering Erich Schmid Institute (ESI) of Materials Science of the Austrian Academy of Sciences. Currently, four research groups are active at each of the respective institutions.

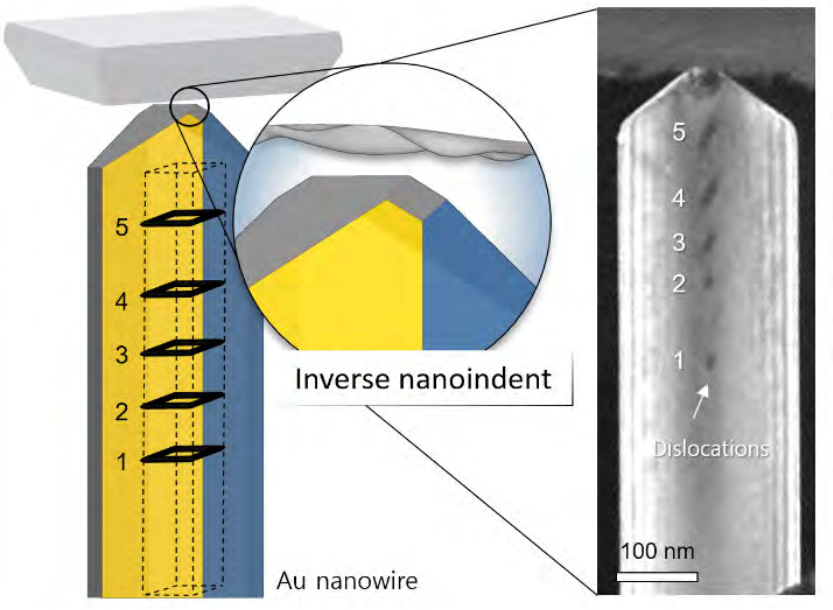
Research at the Chair of Materials Physics encompasses structural materials (e.g. steels, compositionally complex alloys, composites, as well as biological and bioinspired materials), miniaturized material applications for information technology (flexible metal-polymer systems, thin film structures, advanced metallization and functional ceramics for power electronics), materials for energy and high temperature applications (refractory metals, intermetallic alloys), as well as novel amorphous and nanocrystalline bulk materials (nanocomposites, magnetic nanomaterials, nanoporous metals) for use e.g. in hydrogen storage or medical applications.

During the last years, several research activities were initiated regarding interface properties of micro- and nanoscale multilayer systems for various material systems (organic, metallic, ceramic) for application in flexible electronics or hard metal coatings. In this aspect, due to their high hardness and good abrasion as well as corrosion resistance, metallic glasses can cover a previously inaccessible niche. Moreover, detailed tailoring of interface structures is an active research topic to improve strength, toughness and magnetic performance of nanomaterials to the application needs.

Furthermore, modern processing techniques such as additive manufacturing require high heating and cooling rates, and ideally isotropic material properties. The related thermodynamic properties, e.g. of suited metallic glasses, are being studied using fast calorimetry at synchrotron beamlines at ESRF in Grenoble and DESY in Hamburg, and correlated to locally resolved transmission electron microscopy.

To account for the ongoing trends in integration and miniaturization in conjunction with associated demands for detailed understanding of related material size effects, the respective structural and mechanical characterization capabilities at the Chair of Material Physics are at the international fore front. This allows for a scale bridging correlation between material microstructures and structural as well as functional properties from atomistic details to bulk components.

A current example regarding this is depicted below. Using in-situ nanomechanical testing in the transmission electron microscope in conjunction with atomistic simulations, the detailed dislocation nucleation and interaction processes giving rise to the nanohardness of a material were uncovered.

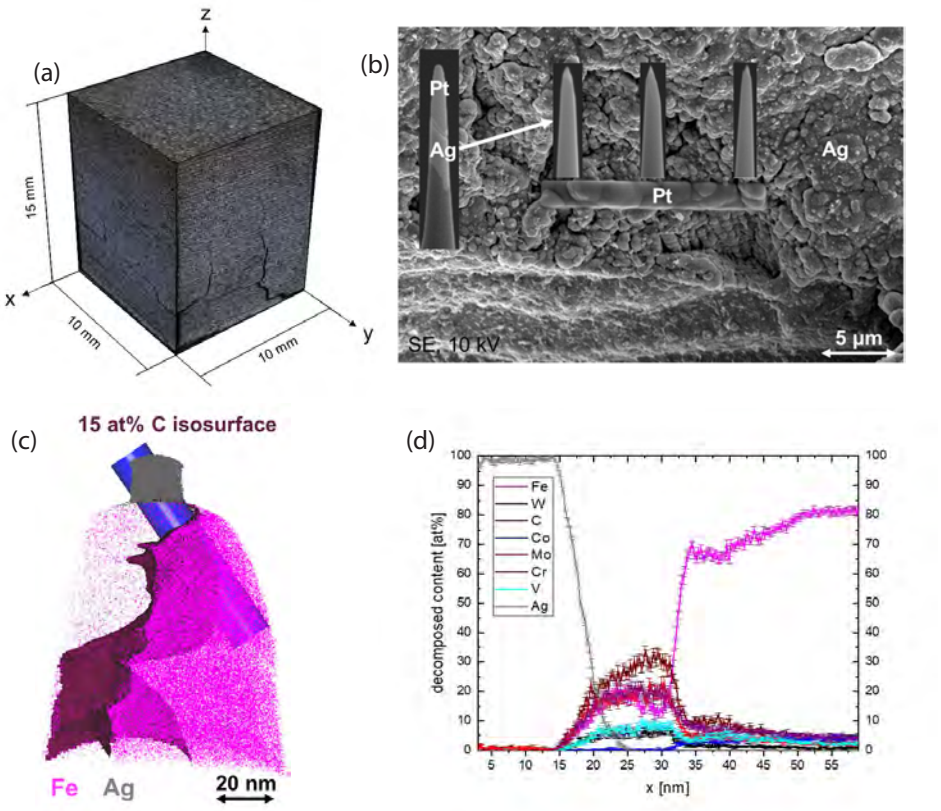


Schematic representation (left) and in-situ observation (right) of the initial deformation processes that occur during a nanohardness measurement, namely the nucleation and glide of prismatic dislocation loops (labelled 1-5).

Chair of Design of Steels - Endowed Professorship for Industry

At the beginning of 2016, the new chair for steel design was established at the Montanuniversität Leoben. The Chair was founded within the framework of the FFG initiative 'Production of the future' and focuses on applied basic research in the form of industry-related collaborations and research projects. The aim of the chair is the development of new and the optimization of existing high-performance steels. With around 1.8 billion tons a year produced worldwide, steel is still by far the most important construction material. Research and development of steels as a high-performance material will make a decisive contribution to the key issues of the 21st century, such as sustainability, reduction of CO_2 emissions, energy saving and recycling.

The research areas of the chair can be divided into three areas. The first includes low-alloyed high-strength steels, the second high-alloyed steels and the third area welding of steels. One particular research area deals with additive manufacturing of high-alloyed tool steels. These high carbon containing steels are prone to cracking during laser powder bed fusion, especially when preheating of the building platform is not available. In order to develop an optimized processing strategy and to enable improved alloy designs, an in-depth analysis of the predominant cracking mechanism was performed. Crack surfaces of macroscopic samples, as shown exemplarily in Fig. (a), were investigated by scanning electron microscopy. The results showed a clear correlation between crack propagation and solidification structure. To analyze the chemical composition in the immediate vicinity of the crack path, atom probe tomography tips were directly taken from the crack surface by the lift-out technique with a focused ion beam. Fig. (b) shows, that the crack surface was deposited with a silver layer in order to mark its exact position for subsequent atom probe investigations. Silver was also chosen due to its lower evaporation field compared to the steel matrix. The experiments revealed the presence of carbides directly underneath the Ag layer, see Fig. (c) and (d). These carbides might significantly contribute to cracking of the high alloyed tool steel samples during additive manufacturing.



(a) macroscopic cracks in an additively manufactured tool steel; (b) sample preparation by lift-out technique using focused ion beam from a silver coated crack surface; (c, d) atom probe investigation reveals carbides on the crack surfaces.

Chair of Structural and Functional Ceramics

The Chair of Structural and Functional Ceramics (ISFK) aims to provide engineering solutions to the ceramic industry with primary focus on structural and functional applications. The research fields cover ceramic processing, material and system characterization as well as process simulation, with special focus on electro-ceramics. Student engagement in (fundamental / applied) research projects at the Chair and participation in national and international conferences is also a key educational aspect of ISFK.

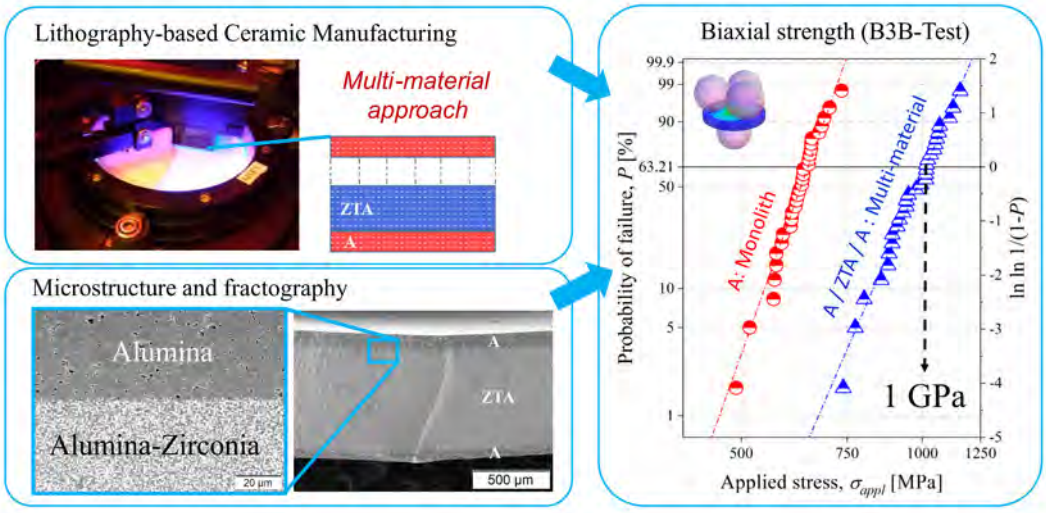
The work with industrial partners has evidenced the need for special testing techniques, e.g. for strength and toughness testing of thinner discs or plates, as well as small balls or cylinders (e.g. for roller bearings). A strong competence of the Chair is the development of testing methods for mechanical characterization of ceramics, which has led to several standards, today common practice in the ceramic industry. One example for such a special strength test is the ball-on-three-balls (B3B) test, which was developed at ISFK. This test enables the strength testing of particularly small and inexpensive samples.

The ISFK is also well known for its work on fracture statistics, lifetime prediction and reliability analysis. Failure analysis of ceramic materials and components is one of the main topics investigated at ISFK. This includes brittle fracture, subcritical crack growth and creep, but also more specific types of failure such as edge chipping and thermal shock. The knowledge obtained from failure analyses and fractography of specimens represents often the starting point for further work.

The chair's special methodological competencies also lay in the electro-mechanical characterization of electro-ceramic components due to thermo-electrical loads, with special focus on understanding and modelling the non-linear behaviour of many ceramic components and systems. Models on different size scales - from atomic to macroscopic scales- have been developed and integrated to describe the component behaviour. Especially the results of this work has led to a completely new knowledge, e.g. about the behaviour of strongly non-linear electrical resistances (e.g. Thermistors, Varistors).

A new research line at the ISFK has been encouraged by the ERC-Grant aiming to designing and manufacturing bio-inspired structures with high reliability. By the recent appointment of Prof. Bermejo, the working fields 'Design and Manufacturing' and 'Characterization of Multi-Material Systems' with a strong focus on microelectronics have been added to the research fields of the ISFK. Ongoing work in 3D-Printing from the fabrication to characterization is a new feature at the Chair, which is to be exploited in the future for the microstructural and architectural design of ceramic composites with enhanced properties (see Figure).

3D-printed alumina with 1 GPa strength



Investments

Investments

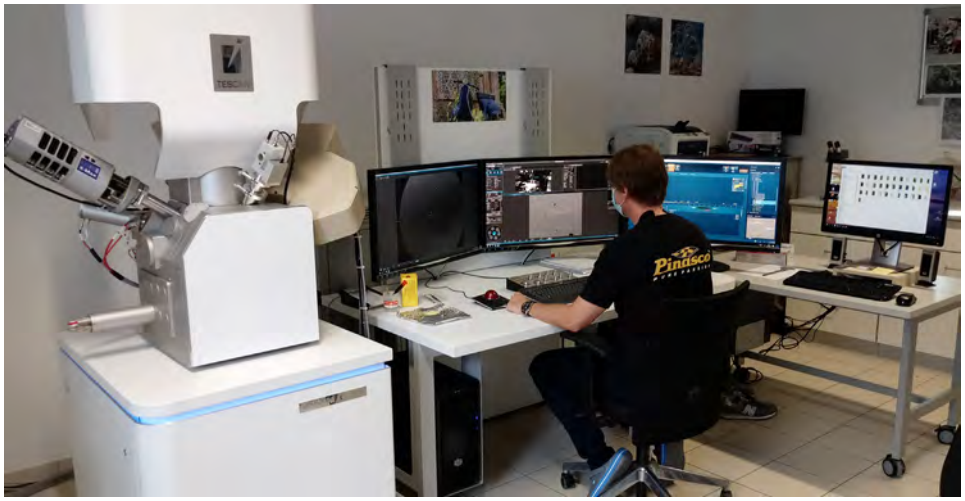
A 3D printer CeraFab 7500 (from Lithoz GmbH, together with the chair of Chemistry of Polymeric Materials) was acquired by the Chair of Structural and Functional Ceramics, which enables the production of complex, stable and high-resolution 3D objects of ceramics and composite materials. The acquisition of the device represents an essential unique selling point for the MUL. To date there is no 3D-printer for hybrid materials at an Austrian university.

To design innovative metallic powders for additive manufacturing purposes, the Chair of Materials Physics in 2020 also purchased an ATO Lab+ metal powder atomizer system. Utilizing a novel ultrasonic atomization technique, this instrument enables to process a wide range of conventional alloys, steels, and refractory alloys. Due to the incorporated vacuum system, even reactive materials such as aluminum or titanium can be handled.

Investments

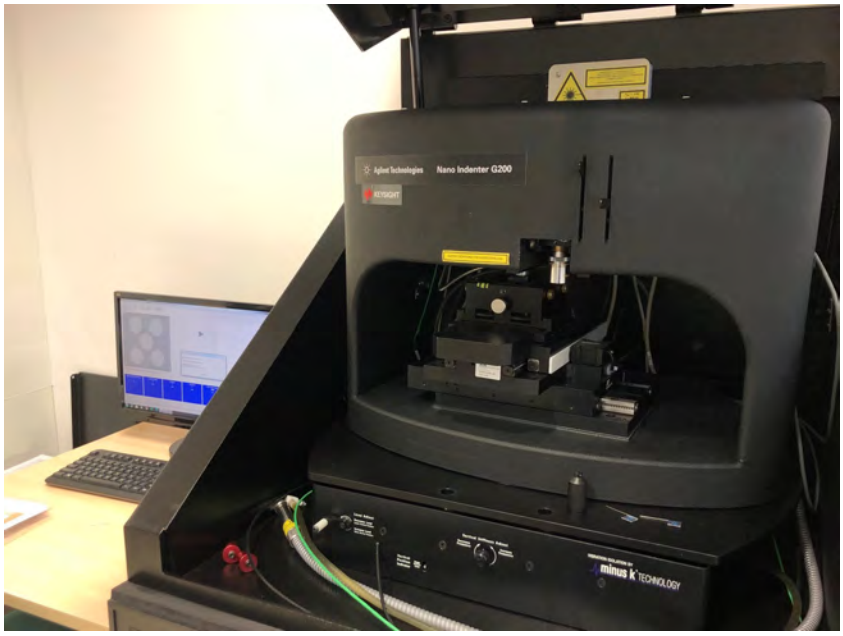
At the beginning of October 2020, a new confocal 3D laser scanning microscope from Keyence was installed at the Chair of Functional Materials and Materials Systems with the participation of the Chair of Structural and Functional Ceramics. The new microscope expands the possibilities for surface characterization by enabling the acquisition and analysis of three-dimensional surface topographies. It will be used, among other things, to analyze mechanically stressed surfaces, to measure three-dimensional structures of micro- and nanoelectronics, to determine the thickness of light-tight and transparent layers, and to determine surface roughness.

At the beginning of 2020, a new scanning electron microscope (SEM) was installed and put into operation at the Chair of Physical Metallurgy and Metallic Materials. The device was co-financed by the Chair of Petroleum Geology, which will result in intensive cooperation between the two chairs in the future. The new SEM is the Clara model from Tescan, a company based in Brno, Czech Republic. The new microscope features a Schottky field emission cathode, six different electron optics presets, and four different imaging detectors. This provides much better resolution than what was previously available on the existing instrument. In addition, the instrument also features charge compensation and a plasma cleaner. The EDX and WDX units were taken over from the existing instrument and adapted. Furthermore, the analysis software has been updated.



With the universal platform G200 from KLA-Tencor (formely Agilent/ Keysight), a new nanoindentation system was installed at the department, enabling nanomechanical testing with a large variety of special features. Additionally to the standard setup for measuring conventional hardness as well as Young's modulus from the nN/ µN regime up to high load regions of maximum 10 N, several advanced nanomechanical testing techniques can be applied and thermally activated deformation parameters can be studied in detail. Moreover, the system is equipped with a laser heating stage, which allows the independent heating of tip and sample up to 500°C in order to measure these thermally activated mechanical properties with an excellent thermal stability. All these nanomechanical possibilities can be further combined with a multitude of tip geometries and tip materials.

Furthermore, a unique electrochemical charging cell broadens the application range, by allowing for example investigations of the embrittling influence of hydrogen on technically relevant alloys, which play an important role for energy harvesting and storage. Recent studies demonstrate the applicability on the performance evaluation of fuel cell and battery materials during various charging cycles. This manifold combination of features in the G200 platform can thereby contribute to the scientific work regarding the development and improvement of materials, which are necessary for the upcoming energy revolution from fossil to renewable energy and green hydrogen.



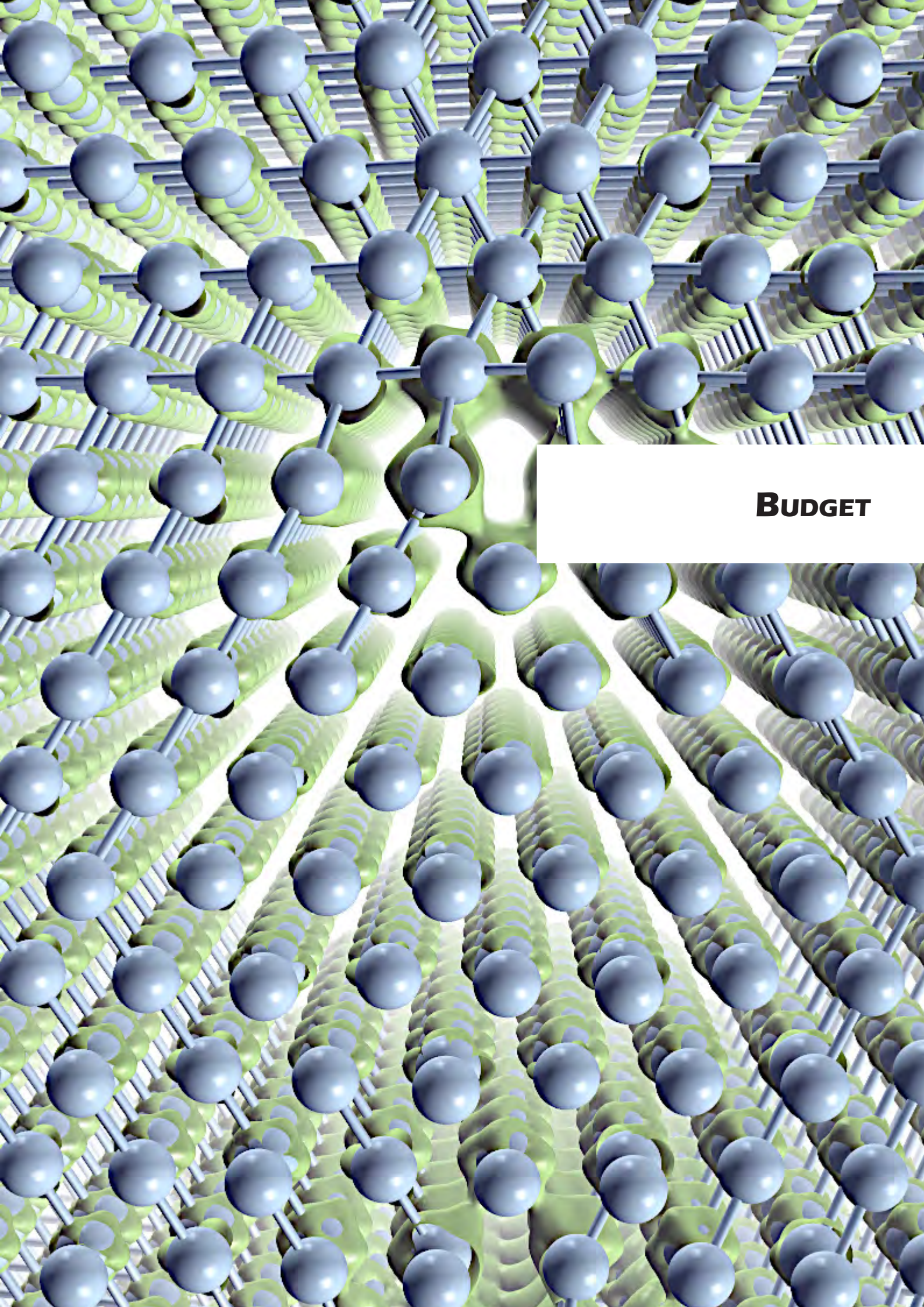
Investments

As part of the ERC grant from Prof. Bermejo a Tape Caster machine CAM-L252 (KEKO) and an Isostatic Laminator, model ILS – 66D (KEKO) were purchased at the ISFK for processing of ceramics. The Tape Caster is a carrier film based tape caster for the production of ceramic foils. The isostatic laminator is made for thermal pressing of foils/bars/substrates by isostatic pressure. Furthermore, two furnaces (Enviromental Furnace RHTH 80-300/18, from Nabertherm and Sintering Furnace HTL 10/17, from Thermconcept) for debinding and sintering of the green bodies were acquired.

Isostatic Laminator

Tape Caster

In 2020 the Chair of Materials Physics acquired a new wire-electro discharge machine, type Mitsubishi MV 1200S NewGen. In a nutshell, with this process conductive materials can be machined by spark erosion with a high degree of precision and a minimized impact on the material compared to processing based on abrasive wear. Regarding the specimen preparation for our large variety of investigated materials, such as nanocrystalline materials, refractory metals, titanium aluminides and bulk metallic glasses, this machine has become an indispensable tool for our research work.



Budget

Revenues

At Austrian universities, revenues are structured as follows:

1. global budget
2. third-party funds
    a. sponsored third-party funds
    b. contract research

Global budget

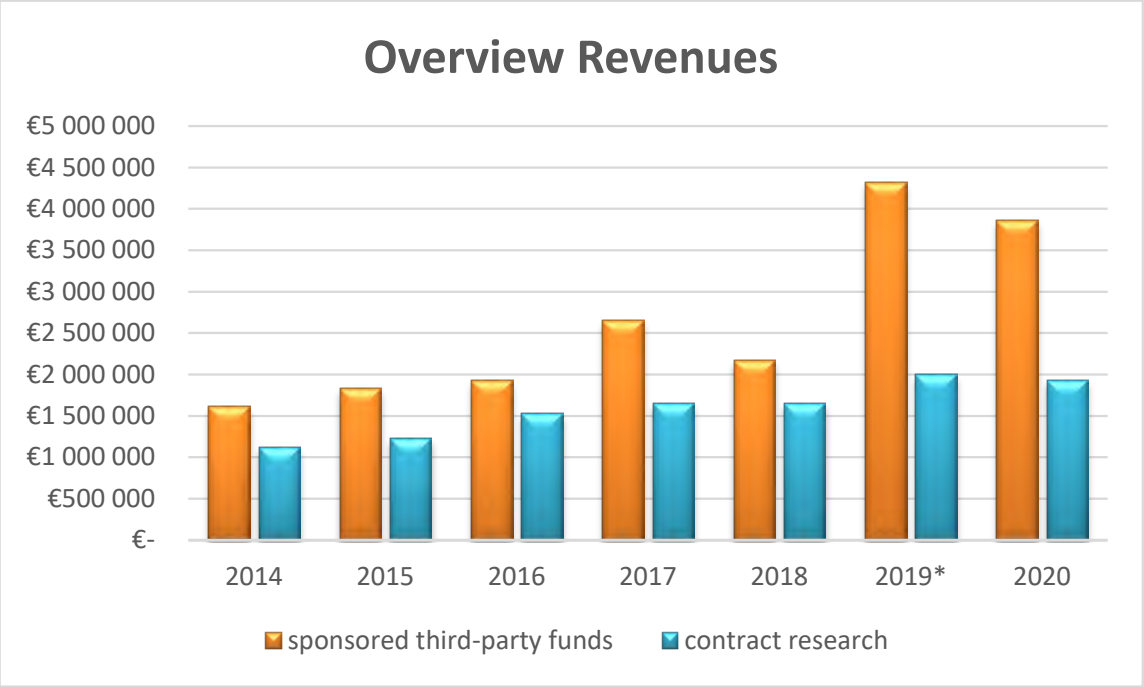
This endowment is to cover current operating expenses for research and teaching (incl. excursions, travel expenses, telephone, office supplies, copies for teaching and minor purchases for research operations; excl. university-funded positions)

Third-party funds

Due to extensive third-party funding activities, the Department managed to keep the revenue of the budget year 2020 at a high level compared to previous years.

The budget from funded projects amounted to: € 3.868.100,-.

The budget from contract research amounted to: € 1.934.000,-.



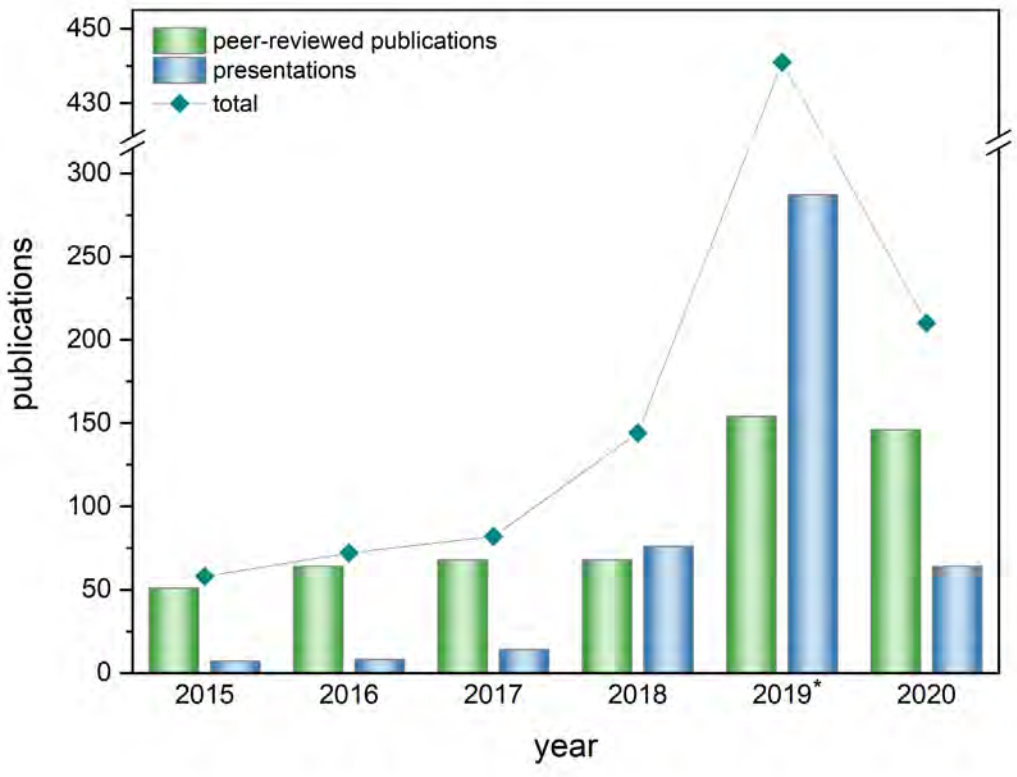
* Since the establishment of the Department of Materials Science in 2019, five chairs are included in this representation; prior to 2019, only three were included.

Publications
Final Theses

Publications and presentations

In line with the vision of the Department of Materials Science to conduct applied basic research of industrial relevance, it is a natural endeavor to publish the research results obtained in high-ranking journals and to present them at international conferences. In particular, this should also give young scientists the opportunity to present themselves to the international scientific community and to gain experience in publishing. Despite the Department's intensive cooperation with industrial partners, where often non-disclosure agreements are necessary, the research results obtained were made available to the public in 2020 in 146 articles in scientific journals and 64 presentations at scientific events. Not suprisingly, the Covid-19 pandemic with many conferences and workshops being cancelled or postponed caused a significant drop in oral and poster presentations. Even with this drop of presentation numbers, the Department contributes significantly to the publication activity and thus to making the research activities of the Montanuniversität Leoben visible.

The following figure shows the development of publications and conference contributions over the last 6 years.



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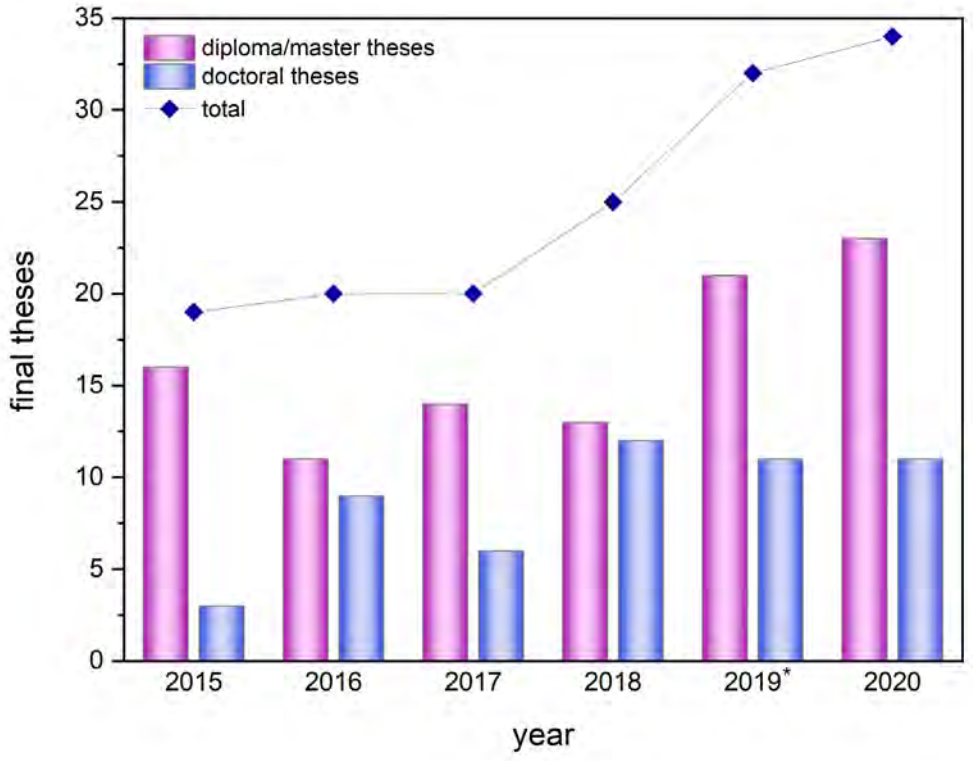
A detailed list of publications is available on the research portal of the Montanuniversität Leoben at 'https://pure.unileoben.ac.at/portal/de/'.

Master and doctoral theses

The following figure shows an overview of the completed diploma/master and doctoral theses of the last 6 years:



* Since the establishment of the Department of Materials Science in 2019, five chairs are included in this representation; prior to 2019, only three were included.

Master theses

In 2020, 23 students completed their master's thesis.

Billovits, Thomas
Piezotronic effect in Zinc oxide varistors

Erlacher, Georg
Tribological performance of different material pairings of exhaust valve and valve seat under impact-sliding conditions

Fabing, Carina
Influence of heat treatments on the mechanical and microstructural properties of PH 13-8 Mo maraging steel

Firneis, Daniel Ernst
Influence of microstructure on the R-curve behaviour and fracture toughness of tungsten

Gruber, Georg Christoph
Arc evaporated CrTa(B)N hard coatings for cutting tools

Haiden, Lukas Sebastian
Influence of polyimide substrate on electromechanical properties of sputter-deposited Mo and Cu thin films

Jop, Malina
Development and characterization of new low-cost intermetallic titanium aluminide alloys for advanced environmental-friendly propulsion systems

Jelinek, Alexander
Fracture behavior of a tough bulk metallic glass at micrometer dimensions

Krainer, Rudolf
Development and characterisation of 3D-stacks with porous metal layers

Lebernegg, Patrick
Selective laser sintering of an alloyed cold-work tool steel

Lechleitner, Julia
Thermochemical treatment of case hardening steel for the gear manufacturing

Lechner, Clemens Christoph
Development of a quench and temper steel for use in large diameter bearings for wind turbines

Loder, Bernd
Welding CCT diagrams of a low alloyed creep resistant 2.25Cr-1Mo-0.25V steel

Natter, Nikolas Rupert
Synthesis and characterization of novel carbon-based nanoporous materials for energy storage applications

Pillmeier, Simon
Influence of cold rolling on the fatigue crack growth behavior of tungsten

Pölzgutter, Magdalena
Development of a test method to investigate the damage behavior of resistance spot welded automotive steels

Preindl, Maximilian
Sputter deposited SnO_x films for gas sensors

Reich, René Herbert
Datafication of material mechanisms in nuclear environment

Rosenauer, Andreas
Reduction of fume emissions in shielded metal arc welding and gas metal arc welding

Sakic, Amin
Ab initio calculations of alloying impact on structural properties and stability of cementite

Schaffar, Gerald Josef Kamillo
An attempt to create amorphous intergranular films in nanocrystalline Cu-Zr using high-pressure torsion

Staudacher, Maximilian
Comparison of biaxial strength test methods for ceramics

Zeisl, Stefan
Development of a high entropy alloy for high temperature applications

Doctoral theses

In 2020, 11 doctoral students were awarded doctorates in montanistic sciences.

Hahn, Carola Elisabeth Katharina
Mechanical properties and deformation mechanisms of austenitic nitrogen steels under different loading conditions

He, Shuang
Theoretical study of hydrogen embrittlement in Ni-based alloys

Hofinger, Matthias
Thermomechanical fatigue resistant dual hardening steels

Jäger, Nikolaus
Novel multifunctional coatings for advanced tribological applications

Kainz, Christina Laura
Chemical vapor deposition of hard coatings in the system Ti-B-C-N

Kholtobina, Anastasiia
Ab-initio based modelling of hydrogen embrittlement in steel.

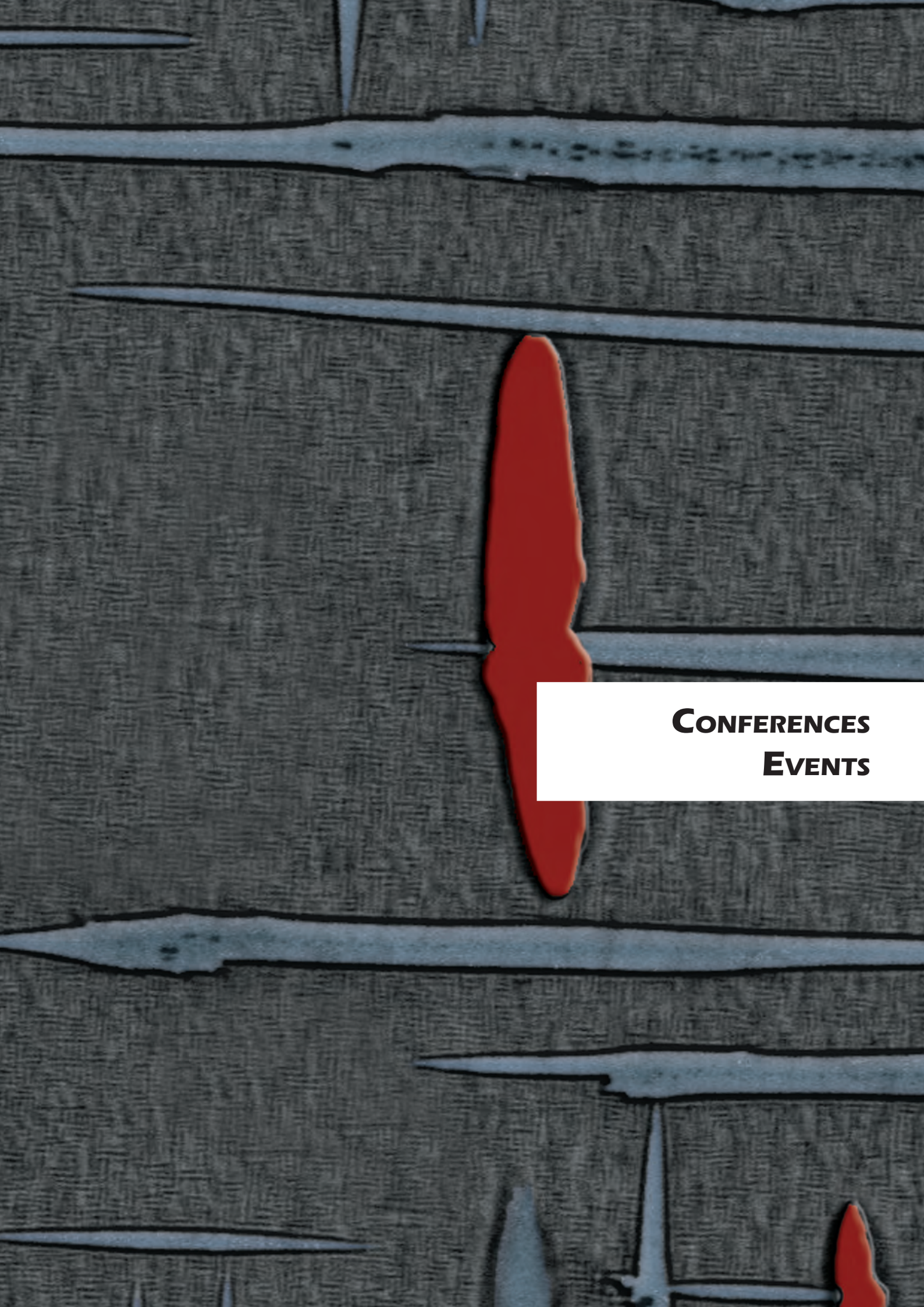
Kreiml, Patrice
Electro-mechanical behavior of flexible thin film systems

Meindlhumer, Michael
Cross-sectional and high-temperature structure-property relationships in nanocrystalline thin films

Pörnbacher, Josef
Chemical changes of TiC particles in a tool steel matrix alloy during hot isostatic pressing

Stylianou, Rafael Panayiotis
CVD TiCN/α-Al_2O_3 coated cemented carbide cutting tools

Xia, Ao
Synthesis, structure and properties of MoNbTaVW high entropy alloy thin films



Conferences
Events

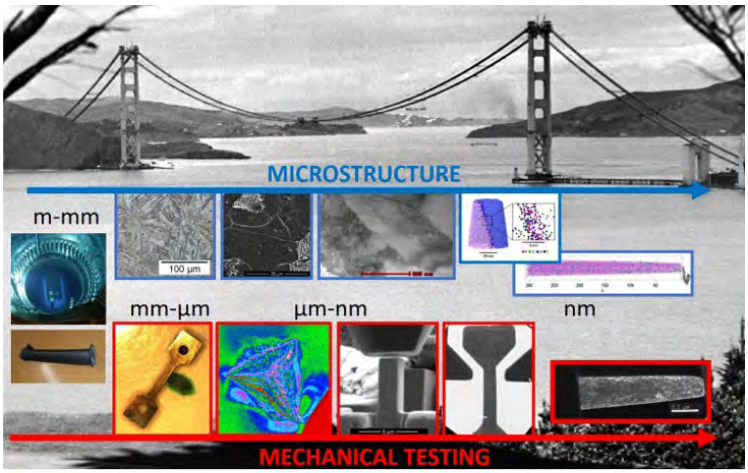
Conferences and events

Organization of conferences

Because of the outbreak of Covid-19 a lot of scientific events were cancelled. However, there were still some conferences, seminars and other events the Department and its staff were actively involved. The following is an overview of the activities carried out.

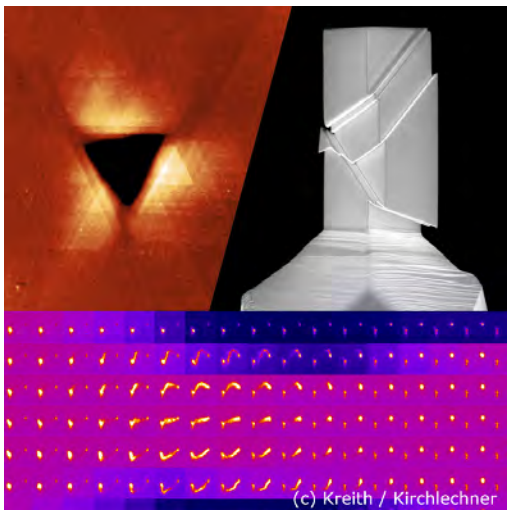
Berkeley – MUL Workshop on Small Scale Mechanical testing 2020 (2-3 March 2020, Berkeley, USA)

Small scale mechanical testing has become an integral part in materials science. The testing techniques available to researchers rapidly improved and became commercialized. This enables new frontiers, allowing to bridge the length scales as well as the gap between modeling and experiments. Especially the advances of materials evaluation in extreme environments such as radiation, temperature or hydrogen atmosphere are currently gaining interest. Early March 2020, just a week before the world wide Corona-Lockdown started, this second (2017, 2020: each coupled with materials science world congress TMS in San Diego) intense workshop organized by Montanuniversität Leoben (Dr. Verena Maier-Kiener) and University of California Berkeley (Prof. Peter Hosemann) brought together the newest advances made in scale bridging mechanical testing combined with complementary microstructural analysis and its applications to science and engineering. Many different contributions where presented by different researchers from the US, Kanada, Germany and Austria, and a friendly atmosphere supported this fruitful ongoing collaboration between Berkeley and Leoben.



Online Workshop 'AK Rasterkraftmikroskopie und nanomechnische Methoden' (8- 9 July 2020)

Due to the well-known Covid issues, the workshop 'AK Rasterkraftmikroskopie und nanomechanische Methoden' of the German Materials Society could not take place as planned in April and had to be adapted. On July 8/9 the event organized by C. Kirchlechner (Karlsruhe Institute of Technology) and D. Kiener (Montanuniversität Leoben) as 'local' host finally took place in virtual form and provided two days of interesting presentations, novel methodologies and scientific interaction. An invited talk by V. Maier-Kiener from the Chair of Physical Metallurgy and Metallic Materials, as well as several presentations from young researchers involving the Chairs of Materials Physics, Physical Metallurgy and Metallic Materials, Physics and the Polymer Competence Center Leoben highlighted the strong position of our university in this field.



MSE Materials Science and Engineering Congress 2020 online (22- 25 September 2020)

From September 22-25, 2020, the biannual 'Materials Science and Engineering Congress' (MSE) headed by the DGM (German Society for Material Science) with more than 1000 participants took place digitally due to corona-crisis. The Department of Materials Science was again represented with several contributions and an organized symposium. For the fourth time in a row, Verena Maier-Kiener organized an interesting symposium on the subject of 'Small scale and in-situ mechanical testing' together with Karsten Durst (TU Darmstadt) and Rebecca Janisch (Interdisciplinary Centre for Advanced Materials Simulation Bochum). An internationally diverse audience gathered for 4 days on the DGM's conference platform to listen to live lectures, present their own research results, look at posters or stroll through the virtual exhibition hall. Even if there was no face-to-face contact possible, the MSE still offered the opportunity for personal exchange via networking sessions and video chats - which everyone involved was happy to take advantage of.

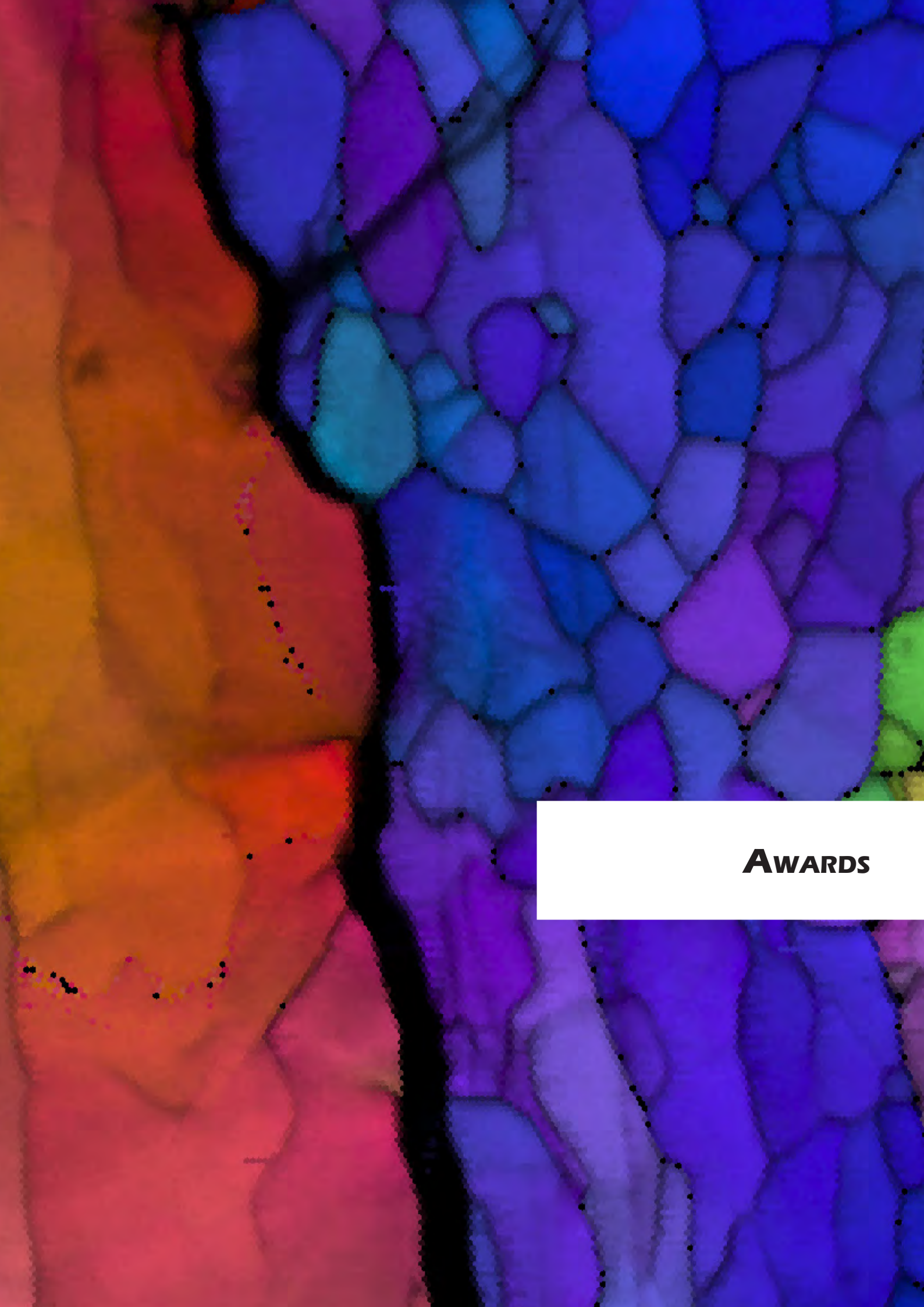
MSE YOUNG RESEARCHERS MEET PROFESSIONALS Experience · Competence · Knowledge Materials Science and Engineering

Symposium on Additive Manufacturing: Materials, Alloy Development, Microstructure and Properties, Materials Science & Technology 2020, (MS&T 2020) (2–6 November 2020, Pittsburgh, USA)

The 2020 Materials Science & Technology Technical Meeting and Exhibition (MS&T2020) organized by TMS, AIST and The American Ceramic Society took place in a virtual format instead of the initially planned on-site meeting in Pittsburgh. Together with K.G. Prashanth (Tallinn University of Technology), Z. Wang (South China University of Technology, Guangzhou) and F. Berto (Norwegian University of Science and Technology, Trondheim), J. Eckert organized a symposium on 'Additive Manufacturing: Materials, Alloy Development, Microstructure and Properties'. The symposium extended over four days and included invited presentations as well as contributed talks by international experts working on additive manufacturing of advanced high performance materials. The topics covered materials and alloy development, processing, properties and microstructure correlations for different additive manufacturing processes. Emphasis was placed on understanding the capabilities of the processes and the correlation between process conditions, process parameters, microstructure development and material properties, covering a broad range of materials spanning all the way from ferrous alloys including steels to Al-, Cu-, Co-, Mg-based alloys, high entropy alloys, intermetallics, metallic glasses, metal matrix composites including cermets and ODS alloys or precious metals-polymer composites. Although there was no possibility for on-site personal meetings and get-together, the exchange via networking sessions and video chats was very lively and contributed to the success of the symposium.

MRS Virtual Spring/Fall Meeting & Exhibit (27 November - 4 December 2020)

The 2020 MRS meeting took place as a combined online meeting of the annual MRS Spring and Fall conferences. Together with C. Brandl (Univ. Melbourne), D. Gianola (Univ. California at Santa Barbara), and S. Sandlöbes-Haut (RWTH Aachen), D. Kiener (Montanuniversität Leoben) organized a symposium entitled 'Defect-Dominated Plasticity and Chemistry in Metals and Alloys', which provided eleven sessions on various aspects regarding the topic in terms of on-demand pre-recorded contributions, a live session with invited speakers, and a live panel discussion involving esteemed experts in the field covering 15 time zones in real time (J. Cairney, Univ. Sydney; T. Zhu, Georgia Tech; T. Rupert, UC Irvine; S. Korte-Kerzel, RWTH Aachen) moderated by S. Sandlöbes-Haut & D. Kiener. While everyone missed the personal interaction, the experimental and computational insights and scientific debates at the symposium were at a very high level and underlined the importance of structural and chemical interface engineering for future material development.



Awards

Prizes and awards

The scientific work of the Department's employees met with a great response both nationally and internationally. It is gratifying to note that numerous younger employees in particular received awards for successful master's and doctoral theses. The following pages provide an overview of the awards received by members of the Department during the reporting period.

Helmut Clemens 'Head of the Year'

Helmut Clemens, Head of the Chair of Physical Metallurgy and Metallic Materials, was named Head of the Year in the 'Business and Research' category of the Kleine Zeitung newspaper. Born in Carinthia, he studied materials science at the Montanuniversität Leoben. After years in industry and at the universities of Stuttgart and Kiel, as well as at the Helmholtz Zentrum Geesthacht, he returned to the Montanuniversität Leoben in 2003 as professor of metallurgy and metallic materials. Clemens has already received very prestigious research awards for the development of intermetallic high-temperature materials. Now, based on a reader vote, he has been named Head of the Year of the Kleine Zeitung.

Photo: Jürgen Fuchs/Kleine Zeitung

Megan Cordill and Christian Mitterer - Houska Prize winners

Megan Cordill, researcher at the Erich Schmid Institute for Materials Science of the Austrian Academy of Sciences (ÖAW) is one of the new winners of the Houska Prize. She and her co-applicant, Christian Mitterer of the Chair of Functional Materials and Materials Systems were awarded the 2nd place in the category university research. Awarded by the B&C Private Foundation, the prize, which is endowed with a total of 500,000 euros for all winners, honors outstanding achievements in applied research.

LTR: Mariella Schurz (managing director of B&C Industrieholding), Megan Cordill, Christian Mitterer, Dr. Erich Hampel (Chief Executive Officer of B&C Industrieholding) (© B&C Privatstiftung)

Jürgen Eckert - Honorary Member Indian Institute of Metals

Jürgen Eckert has been appointed honorary member of the Indian Institute of Metals. This award represents the highest honor bestowed by the Indian Institute of Metals and is given to scientists who have made outstanding contributions to the advancement of science in the field of metallic materials, collaboration with Indian scientists, as well as the promotion of young scientists. Due to Covid-19 restrictions, the award was presented at the Indian Institute of Metals annual meeting via video conference.

Corresponding Member of the Technical Sciences Class of the Saxon Academy of Sciences in Leipzig

Jürgen Eckert was elected as a Corresponding Member of the Technical Sciences Class of the tradition-rich Saxon Academy of Sciences in Leipzig. Due to the pandemic situation, the presentation and introduction to the circle of academy members took place virtually via livestream in this case as well.

VSET VEBLEO Fellow Award

Jürgen Eckert has been honored as VST VEBLEO fellow for his significant contributions in metastable materials design and processing. Along this line he delivered a keynote talk on 'Phase formation and deformation behavior of complex metallic materials with hierarchical microstructures' during the VEBLEO webinar on Materials Science, Engineering and Technology held during September 17-20, 2020.

VEBLEO is an international organization specialized in organizing international conferences, webinars, workshops and exhibitions in the multidisciplinary field of science, engineering and technology across the globe. It provides a global platform for scientists, researchers and industries to discuss and promote recent trends in major subject areas like materials science, engineering and technology, nanomedicine, nanomaterials and nanotechnology, energy materials and technology, etc.

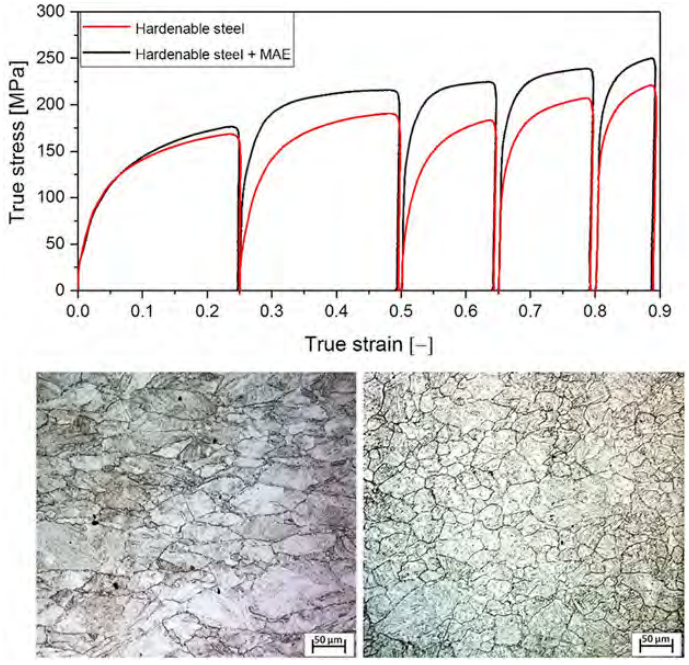
Theodor Körner Price for Sandra Ebner

Sandra Ebner was awarded the Theodor Körner Prize for her PhD thesis entitled 'Microstructural Evolution during Q&P Processing and Effects on the Mechanical Properties'. In her thesis, which Sandra Ebner carried out in the group of Christina Hofer at the Chair of Steel Design, she dealt with new types of third-generation Advanced High Strength Steels, which are used in automotive bodies to enable weight savings while at the same time increasing personal safety. The focus of the doctoral thesis was on in-situ diffraction experiments using high-energy X-rays, which can be used to investigate changes occurring in the material during heat treatment or mechanical loading in a time-resolved manner. The normally associated personal presentation by Federal President Dr. Alexander Van der Bellen unfortunately had to be cancelled this time due to the Corona pandemic.

LTR: Christina Hofer, Sandra Ebner, Ronald Schnitzer

Article by Raphael Esterl and Ronald Schnitzer selected for the 'Best of steel research international - 2020 edition'

The article by Raphael Esterl, Markus Sonnleitner and Ronald Schnitzer entitled 'Microstructural Analysis of the Recrystallization Behavior of Low Alloyed Steels' was selected for the special virtual edition 'Best of steel research international - 2020 edition.' This edition represents outstanding articles recently published in steel research international and are selected by the journal's editors.



Vice president ÖGV

At the General Assembly of the Austrian Society for Vacuum Technology (ÖGV) in January, Robert Franz from the Chair of Functional Materials and Materials Systems was elected Vice President for the functional period 2020-2021. The ÖGV aims to unite people, institutes and companies interested in the fields of vacuum generation, measurement and application as well as in the physics, chemistry and technology of thin films, including those interested in interfaces and surfaces, in order to promote research and development in the above-mentioned fields, in particular by issuing information, publications, commissioning research, organizing lectures and workshops, and conducting exchanges of experience and training courses.

AVS Dorothy M. and Earl S. Hoffmann Travel Grant

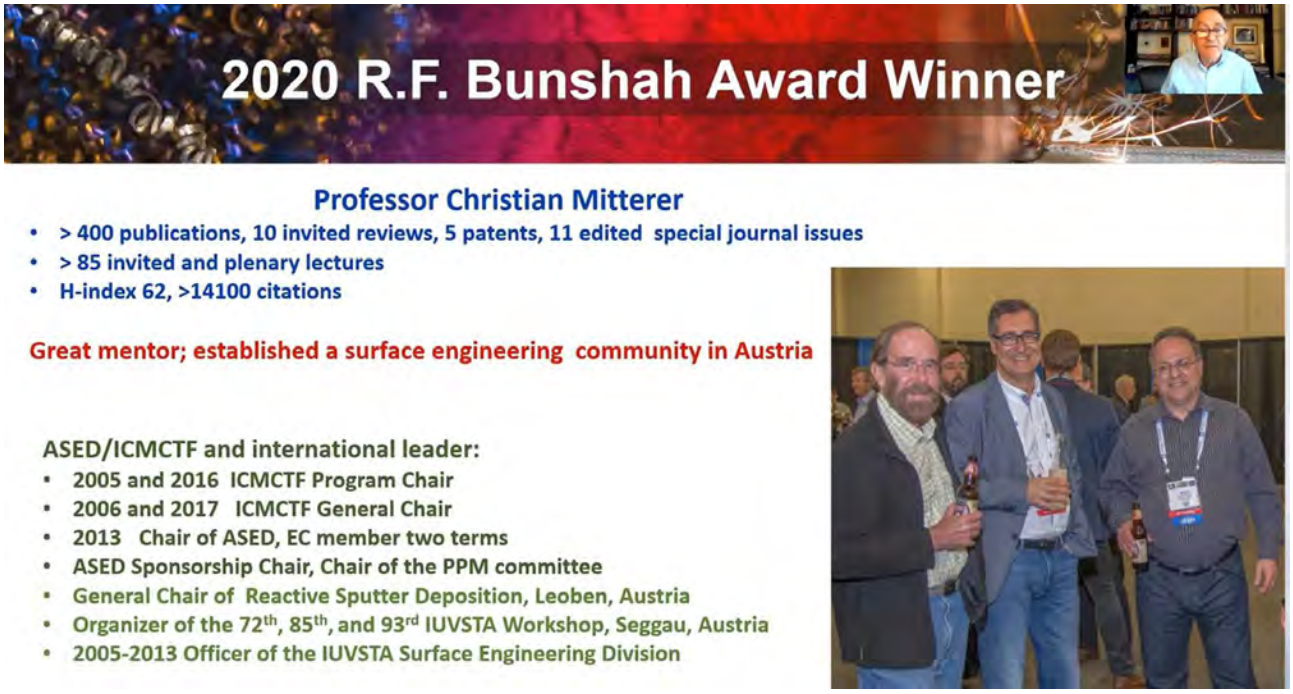
Mehran Golizadeh of the Chair of Functional Materials and Materials Systems received the AVS Dorothy M. and Earl S. Hoffman Travel Grant at AVS 66th International Symposium & Exhibition in Columbus, Ohio. With this award, the American Vacuum Society (AVS) recognizes and encourages excellent scientific and technological work by doctoral students in AVS subject areas. Mehran Golizadeh was recognized for his contribution to the characterization of the surface of eroded AlCr cathodes on which a modified layer is formed by the action of arc plasma. He did the work in Robert Franz's Plasma and Surface Engineering group as part of an FFG-funded project.

Master Thesis Award by the Austrian Ceramic Society

On the occasion of the 8th General Assembly of the Austrian Ceramic Society on 06 February 2020 in Graz, Ms. Anna-Katharina Hofer was awarded 1st prize in the category 'Master's Theses' for her work 'Processing and characterization of textured ceramic layered architectures'. The main topic of the awarded thesis was the fabrication and characterization of novel multilayered ceramic architectures with (bio-inspired) adjusted microstructure (texture). The work stems from a research collaboration with Pennsylvania State University, where Ms. Hofer herself spent a four-month stay at the American university.

R.F. Bunshah Award for Christian Mitterer

Christian Mitterer has been awarded the 2020 R.F. Bunshah Award from the Advanced Surface Engineering Division of the American Vacuum Society. This award represents the highest honor presented by the Division; it is typically given for the lifetime achievements of deserving scientists. The award was given for his 'seminal contributions to the materials science of coatings based on borides, nitrides carbonitrides, oxides and metal alloys.' Due to COVID-19 restrictions, the associated Honorary Lecture could not be presented at the annual International Conference on Metallurgical Coatings and Thin Films held in San Diego, California, in the spring, as is customary, but was delivered via video conference.



Josef Krainer-Promotion Award 2020 an Petra Erdely

In memory of the work of the Styrian governor Josef Krainer, the Styrian Commemorative Work has been awarding prizes in the categories of the Great Josef Krainer Prize, the Josef Krainer Appreciation Prize and the Josef Krainer Promotion Prize since 1993. The promotion prizes are intended to recognize the achievements of young scientists in particular and to encourage them to continue their scientific work. At this year's award ceremony, Petra Erdely, group leader of the Chair of Physical Metallurgy and Metallic Materials, was awarded one of the Josef Krainer Promotion Prizes 2020 in recognition of her research achievements in the field of materials science. In her doctoral thesis, which was awarded the prize, Petra Erdely focused on the development and characterization of intermetallic titanium aluminide alloys using diffraction and scattering techniques.

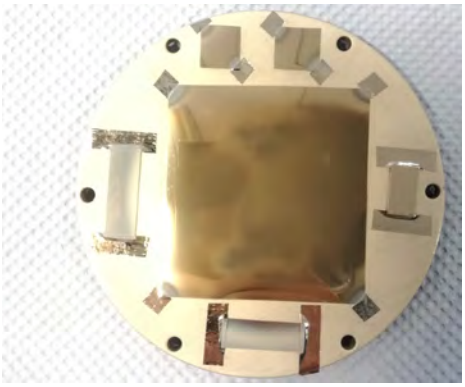
Sub Auspiciis PhD Promotion Petra Spörk-Erdely

It was not until 681 days after her PhD examination that Dipl.-Ing. Dr. mont. Petra Spörk-Erdely had her PhD Promotion. The long wait had several reasons: first the 'Ibiza scandal', then the Corona crisis. But on 22 October 2020 Petra Spörk-Erdely became the first woman in the history of the University of Leoben to receive her doctorate 'sub auspiciis Praesidentis rei publicae'. She did her doctoral thesis at the Chair of Physical Metallurgy and Metallic Materials. The main focus was the investigation of intermetallic titanium aluminides using modern X-ray diffraction and scattering methods at the German Electron Synchrotron (DESY), with additional complementary high-resolution characterization methods. Ms. Spörk-Erdely has already been awarded several prizes for her scientific work. Currently she is building up her own research group at the chair. Due to the current pandemic, the President of the Federal Republic of Germany was unable to attend the graduation ceremony in person. As a substitute, the president of the state parliament, Manuela Khom, held the ceremonial address.

LTR: Maximilian Jäger 1st. Vice Mayor from Leoben, Wilfried Eichelseder Rector, Petra Spörk-Erdely, Manuela Khom, president of the state parliament, Helmut Clemens (Photo: Freisinger)

ECSEL award for Lisa-Marie Weniger

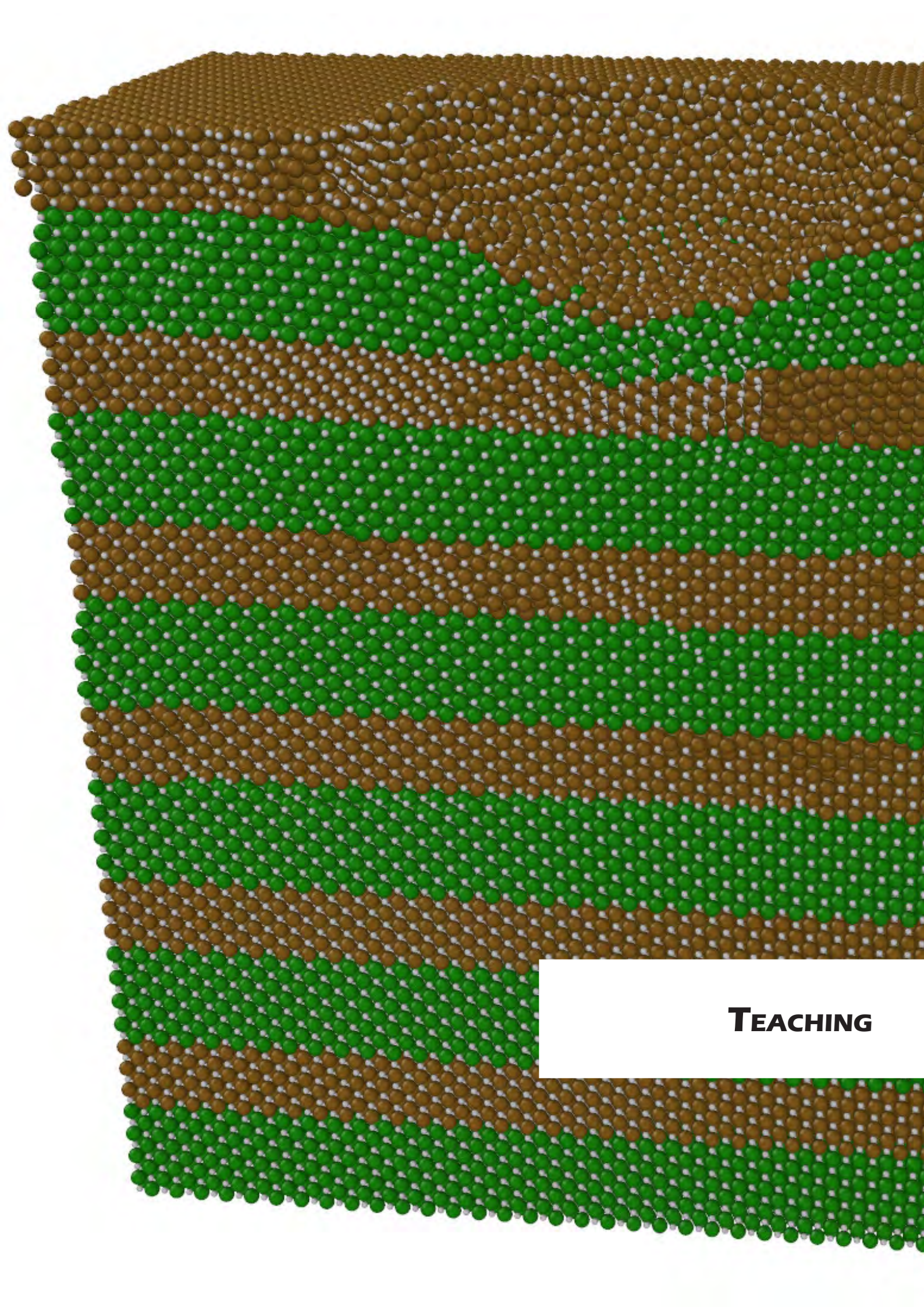
Lisa-Marie Weniger has got an award from ECSEL (Electronic Components and Systems for European Leadership) Austria for her master thesis research in the area of thin film metallic glasses based on noble metals which is conducted in collaboration with the Chair of Functional Materials and Materials Systems. Novel Gold-Silver-Silicon amorphous alloys, which were sputter deposited on polymer substrates, possess attractive combination of properties including corrosion resistance, biocompatibility, mechanical robustness and partial optical transparency. In her Master thesis Lisa Marie Weniger is uncovering the fundamental electrical and mechanical properties of novel alloys and examines their potential applications as ultrathin flexible electrodes.



TACT 2019 Silver Student Award

Ao Xia of the Chair of Functional Materials and Materials Systems received the Silver Student Award at last year's TACT 2019 (International Thin Films Conference in Taipei), Taiwan, hosted by the Taiwan Association for Coating and Thin Film Technology (TACT), for his contribution to the characterization of the structure and properties of MoNbTaVW high entropy alloy coatings. The coatings were prepared using a variety of physical vapor deposition (PVD) methods, including varying the coating angle as well as depositing nitride layers by adding nitrogen as a process gas. Other aspects addressed by Ao Xia as part of his PHD thesis in Robert Franz's Plasma and Surface Engineering group are the thermal stability and electromechanical properties of these coatings.

LTR: Babak Bakhit, Jui-Che Chang, Ao Xia, Prof. Jia-Hong Huang



Teaching

Teaching

In addition to research, teaching is an important task of the university. It is the basis for the high quality education of our graduates, who will later not only contribute to the sustainable development of Austria as a location for industry and research, but will also successfully gain a foothold internationally.

Semester Hours (Hrs)
Winter- and summer semester

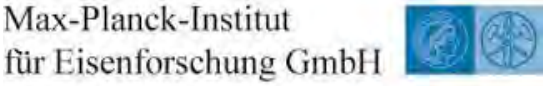
Chair	Compulsory subject (Hrs)	Elective subject (Hrs)	Free subject (Hrs)
Chair of Functional Materials and Materials Systems	15	4	32
Chair of Physical Metallurgy and Metallic Materials	50	15	30
Chair of Materials Physics	24,8	20	47
Chair of Design of Steels	14	2	16
Chair of Structural and Functional Ceramics	23	12	23

Exams

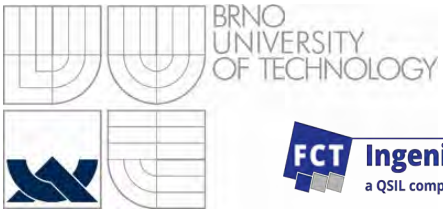
Chair	Number of exams
Chair of Functional Materials and Materials Systems	369
Chair of Physical Metallurgy and Metallic Materials	1112
Chair of Materials Physics	448
Chair of Design of Steels	126
Chair of Structural and Functional Ceramics	354

Cooperations

Cooperations

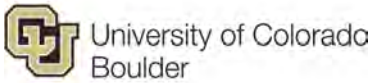


Universität für Bodenkultur Wien



EXCELENCIA
MARÍA
DE MAEZTU

Technische Universität München



THE UNIVERSITY
of EDINBURGH

Outlook

In the last year, we had to learn fast how to adapt to previously unknown external threads such as a pandemic outbreak that globally affects education and research. Guaranteeing safe education and research environments for students and scientific staff has become highest priority at our Department, culminating in the establishment of new working protocols, incorporating flexible working hours and locations. Several new digital tools have been incorporated into our teaching habits and shall play a vital role to enhance our classroom and laboratory activities in the years to come.

Our mission to foster international recognition in teaching and research has, for example, encouraged the Department to join an Erasmus Mundus Program, namely 'Advanced Materials Science and Engineering' (AMASE), together with five other European Universities, and we are expecting the first international students in Fall 2021. Furthermore, a new International Master will start in October 2021, which will offer specialization modules based on metallic alloys, functional materials, polymers and composites, as well as related manufacturing processes, in a multicultural environment. We will continue to promote these efforts towards student mobility and exchange of research competences between international partners to further increase the visibility of our Department and strengthen our research areas.

With the nomination of Dr. Lorenz Romaner as Professor for Computational Materials Science, a new area focusing on interface modelling and virtual materials design shall complement the existing teaching and research activities concerning atomistic modelling at our Department and provide valuable opportunities to connect experiments and modeling across all length scales.

Several new pieces of equipment for manufacturing (nano-lithography system, stereolithographic 3D-printer, nanoparticle deposition system, plasma surface modification system, femtosecond laser ablation unit) and characterization (high temperature and laser scanning confocal microscopes, Raman microscope, environmental testing chamber) just arrived or are in the acquisition process. Of particular notion is the approval for funding of a state-of-the-art atom probe tomography system for approx. 2.5 Mio€. These unique new capabilities will open completely new possibilities for designing new materials, and we will put them to good use to contribute with our skills and knowledge to the big challenges our society faces today, such as sustainable energy production, global warming and resource efficiency.

Specially in these challenging times, we are confident that by providing higher education in materials science to our students and offering multidisciplinary research competences to our industry partners, we are in a top position to address the societal needs of the 21st century.

We look forward to a successful cooperation in the year 2021!

Imprint

Montanuniversität Leoben
Department Materials Science

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