Naterials Science

# Department Materials Science

# Annual report 2023



# Preface

### Preface

Dear colleagues and friends of the Department of Materials Science!

As we ushered this past year, envisioning the further development of our university propelled by the election of the new Rectorate, we are pleased to share the progress made in our endeavours. Our focus on internationalization, development of green technologies and responsible materials has shaped new strategies in research, teaching, and our third mission.

Within our department, we recognize the pivotal role of materials in both scientific research and educational programs. The successful launch of the new Bachelor Study program, "Materials Science and Technology", featuring innovative courses that engage students with materials specific content already from their first semesters, marks a significant milestone. This program lays the foundation for our participation in the European School of Materials (EEIGM), an initiative involving six materials science departments across Europe, aimed at inspiring students to tackle global challenges in materials science. The international master's program "Advanced Materials Science and Engineering - AMASE" has seen its inaugural graduations in the fall and became an integral part of our department's educational program.

A noteworthy addition to our department are two new Christian Doppler laboratories. The CD-Lab "Knowledge-based Design of Advanced Steels" focuses on studying the effects of increased scrap use and the resulting presence of undesirable tramp and trace elements on steel properties. The CD-Lab "Advanced Computational Design of Crystal Growth" develops computational methods to improve crystal growth processes with emphasis on silicon carbide.

Our department also expanded its capabilities with the acquisition of high-end equipment, including a novel Spark Plasma Sintering system for ultra-fast firing of 3D-printed ceramics, a cryo-nanoindenter for micro- and nanomechanical testing at cryogenic temperatures, and two small-scale testing devices enabling scale bridging fatigue testing at micro- and mesoscale.

The second Materials Science Colloquium in Lech am Arlberg focused on "Computational Materials Science," featuring international speakers from Germany and the USA. In Leoben we hosted the 7<sup>th</sup> conference on "Fractography of Advanced Ceramics", the 7<sup>th</sup> "Young Ceramists Additive Manufacturing" (yCAM), the 57<sup>th</sup> Metallography conference as well as the 20<sup>th</sup> "Symposium on Alloying Element effects on Migrating Interfaces". We also organized the 93<sup>rd</sup> IUVSTA Workshop in Seggau, addressing "Advances in the Characterization of Surface Engineering Structures, Coatings, and Thin Films".

We are proud of several conference awards received by our young graduate students and distinguished recognition for our researchers. The numerous publications in esteemed journals such as Materials Today Advances, Journal of Materials Chemistry A, Advanced Materials, Advanced Science, Nature Communications or Communications Materials, underscore the high quality of our department's research activities throughout 2023.

We extend sincere gratitude to our researchers, students, and industrial partners for their unwavering support and continuous motivation to collaboratively tackle future challenges. We invite you to enjoy the following pages, providing an overview of our department's activities in 2023.

Prof. Dr. Raul Bermejo

Prof. Dr. Jürgen Eckert

Prof. Dr. Christian Mitterer

Prof. Dr. Ronald Schnitzer

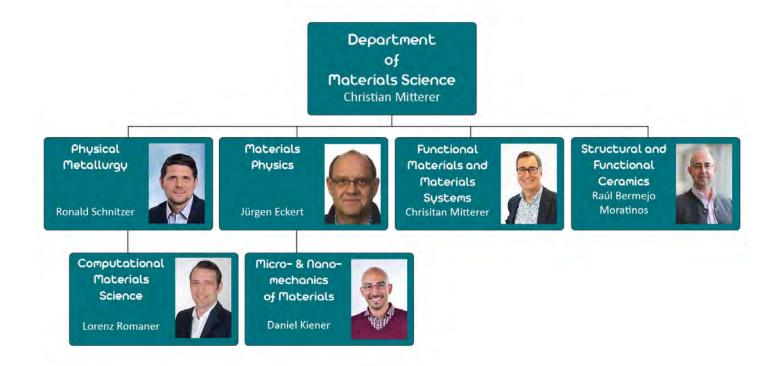
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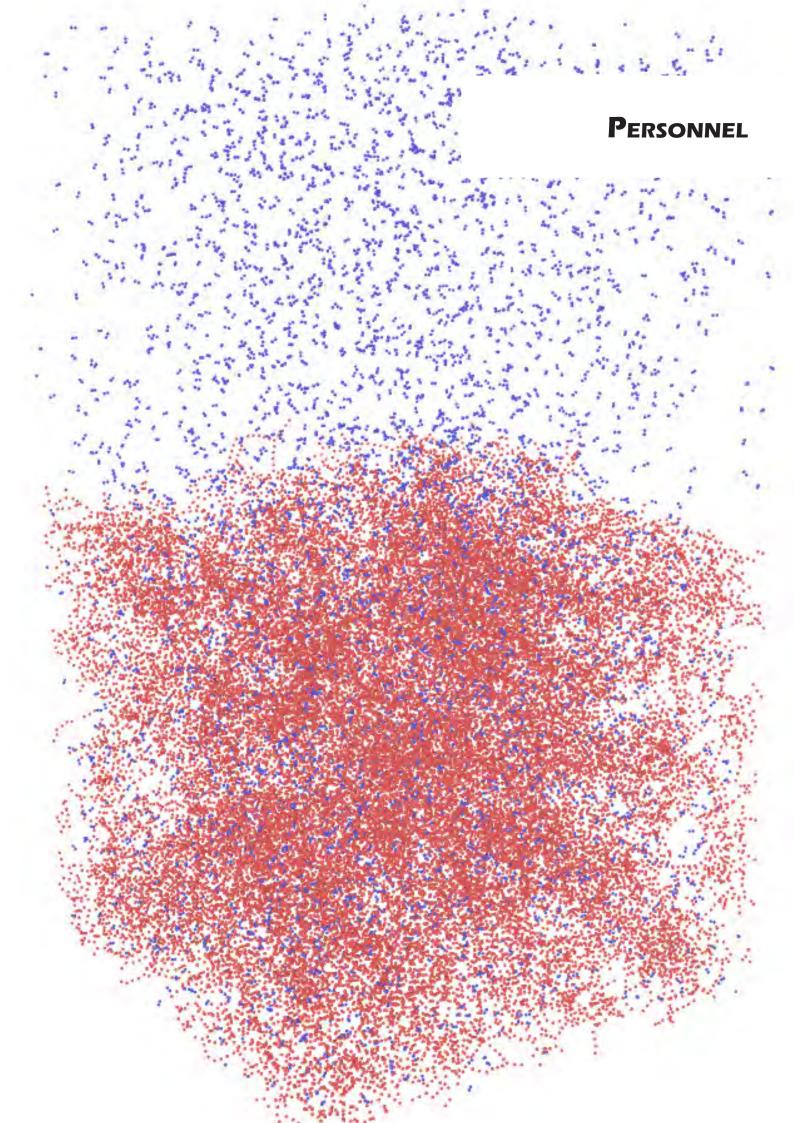
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# Organigram

### ORGANIGRAM





### Personnel

In 2023, 193 people were employed at the Department of Materials Science. The expenses for 90 employees were covered by federal funds, 103 employees were financed by third-party projects.

### **Head of department**

Univ.-Prof. Dr. **Christian Mitterer** *Chair of Functional Materials and Materials Systems* 



#### Chair

Univ.-Prof. Dr. **Raul Bermejo Moratinos** *Chair of Structural and Functional Ceramics* 



Univ.-Prof. Dr. **Christian Mitterer** *Chair of Functional Materials and Materials Systems* 



Univ.-Prof. Dr. Dr.h.c. **Jürgen Eckert** Chair of Materials Physics



Univ.-Prof. Dr. **Ronald Schnitzer** *Chair of Physical Metallurgy* 



### **Chair of Functional Materials and Materials Systems**

#### Chair

Univ.-Prof. Dr. **Christian Mitterer** 



#### **Group leader**

Assoz. Prof. Dr. **Rostislav Daniel** *Group leader* 



Dr. **Michael Tkadletz** Group leader



#### **Office management**

**Cornelia Schnedl** 



**Susanne Strasak,** Bakk.phil.



#### **Deputy chair**





Priv.-Doz. Dr. Verena Maier-Kiener Group leader





Angelika Tremmel, MA



#### Technicians

**Sabrina Hirn** *Surface engineering* 



Walter Kopper Materials testing



#### Scientific staff

**Wolfgang Archer** Student assistant



Dipl.-Ing. Alexander Blocher PhD student



**Daniel Gass** Student assistant



Dipl.-Ing. **Georg Gruber** PhD student











Dipl.-Ing. **Aydan Cicek** PhD student



Hannah Gottlieb Student assistant



**Christopher Heim** *Graduate student* 



Dr. Anna Hofer-Roblyek PostDoc



**Magdalena Kirchmair** *Graduate student* 



**Edyta Kobierska, inz.** *PhD student* 



Dr. **Fabian Konstantiniuk** *PostDoc* 



**Alexandra Lechner** Student assistant



Mahdieh Mehrabi Graduate student



MSc. **Saeideh Naghdali** PhD student



Dr. **Christina Kainz** *PostDoc* 



Dipl.-Ing. Florian Knabl PhD student



Dipl.-Ing. **Lukas Kölbl** PhD student



Dr. **Nikolaos Kostoglou** *PostDoc* 



Dipl.-Ing. **Lea Lumper** PhD student



MSc. **Nafsika-Maria Mouti** PhD student



MSc. Serena Naicker PhD student



Dr. Marisa Rebelo de Figueiredo PostDoc



BSc. **Leon Ruess** Graduate student



Maximilian Schiester Graduate student



Marco Straßburg Graduate student



Dr. **Bernhard Völker** PostDoc



**Susanne Wenger** Student assistant



Dr. **Michal Zitek** PostDoc



Dr. **Boryana Rashkova** PostDoc



Dipl.-Ing. **Gerald Schaffar** *PhD student* 



Dipl.-Ing. **Michael Sommerauer** PhD student



Mag. **Velislava Terziyska** Scientific staff



Dr. **Helene Waldl** PostDoc



Dipl.-Ing. **Stefan Zeiler** PhD student





### **Chair of Physical Metallurgy**

#### Chair

Univ.-Prof. Dr. **Ronald Schnitzer** 



#### **Group** leader





Anna Jelinek

Dr.

Dr. **Petra Spörk-Erdely** 



#### **Office management**

**Cornelia Schnedl** 



**Susanne Strasak,** Bakk.phil.



### **Materials** Science

#### **Deputy chair**

Univ.-Prof. Dr. **Lorenz Romaner** *Group leader* 







Dr. **Oliver Renk** 





Angelika Tremmel, MA



#### Technicians

Ing. **Thomas Fischer** *Thermomechanical characterization* 



**Gerhard Hawranek** Scanning electron microscopy



Ing. **Alfons Lontschar** IT administration



#### Scientific staff

**Wolfgang Archer** Student assistant



Kimberly Sophia Filzmoser Student assistant



Dipl.-Ing. **Marek Gocnik** PhD student



**Alfred Gajsek** Workshop



Ing. Bruno Krajnc Materials testing



**Silvia Pölzl** Metallography



Dipl.-Ing. Christoph Dösinger PhD student



Dr. **Dominik Gehringer** *PostDoc* 



BSc. **Armin Golesch** *Graduate student* 



Dr. **Gloria Graf** *PostDoc* 



**Johann Grillitsch** *Student assistant* 



Dipl.-Ing. Lukas Hatzenbichler PhD student



Matej Holec Scientific staff



**Jens Jarnot** Student assistant



Dipl.-Ing. **Stefan Kardos** *PhD student* 



Dipl.-Ing. **Nikolaus Kostwein** PhD student



BSc. **Maximilian Graf** *Graduate student* 



Dipl.-Ing. **Celine Halkali** *PhD student* 



BSc. **Christian Hofer** *Graduate student* 



Dipl.-Ing. **Georg Holub** PhD student



BSc. **Lorena Juarez-Perez** *Graduate student* 



BSc. **Matthias Karner** Graduate student



Klaus Krammer Student assistant



Dr.-Ing. **Andreas Landefeld** *PostDoc* 



BSc. **Thomas Luger** Graduate student



Ph.D. **Martin Matas** PostDoc



Dr. **Michael Musi** PostDoc



**Shafi Omer** Student assistant



**Stefan Pfundner** Student assistant



Dr. **Zaher Ramadan** PostDoc



Dipl.-Ing. **Thomas Leiner** PhD student



BSc. **David Marin Morales** *Graduate student* 



BSc. **Carlos Moya Merino** Graduate student



Dipl.-Ing. David Obersteiner PhD student



BSc. **Matthias Pferschy** *Graduate student* 



MSc. **Zahra Rajabzadeh** PhD student



BSc. **Andreas Rechberger** *Graduate student* 



Dipl.-Ing. Alexander Reichmann PhD student



Stephanie Ritter Intern



Dipl.-Ing. **Amin Sakic** PhD student



Dipl.-Ing. **Benjamin Seligmann** PhD student



Ph.D. **Kiranbabu Srikakulapu** *Postdoc* 



MSc. **Jing Tang** PhD student



BSc. **Hanna Teuschl** Graduate student



BSc. **Nicole Rinnhofer** *Graduate student* 



Dipl.-Ing. Andreas Rosenauer PhD student



Dipl.-Ing. **Daniel Schrittwieser** PhD student



Dipl.-Ing. **Tobias Spitaler** PhD student



Lucia-Maria Stockinger Student assistant



Dipl.-Ing. Lorenz Taucher PhD student



BSc. **Sebastian Teusl** *Graduate student* 



**Romina Troger** *Student assistant* 



BSc. **Luiz Vieira Corea** Graduate student



Anabel Wolfsberger Intern



BSc. **Keegan Zetterberger** *Graduate student* 



Dr. **Claus Trost** PostDoc



MSc. **Clement Vincely** PhD student





BSc. **Maximilian Ziegler** *Graduate student* 





#### **Chair of Materials Physics**

#### Chair

Dr.

Univ.-Prof. Dr. Dr.h.c. Jürgen Eckert



#### **Group leader**

Anton Hohenwarter

Deputy chair

Univ.-Prof. Dr. **Jozef. Keckes** Group leader



Univ.-Prof. Dr. Daniel Kiener



#### **Office management**

Sabine Wilfling



#### Technician/Non-scientific staff

Gabriele Felber TEM preparation



Manuela Karner Cleaning







Silke Kaufmann Metallography (maternity leave)



Melissa Suschetz Metallography



#### Scientific staff

**Eredem Akar** Student assistant



Dr. **Abdalaziz Aljabour** *PostDoc* 



Dr. **Sabine Bodner** PostDoc



Dr. **Michael Burtscher** PostDoc



**Paola Dorner** Student assistant



MSc. **Adam Elbataioui** PhD student



Dr. Markus Alfreider PostDoc



BSc. Atacan Asci Graduate student



Dipl.-Ing. Nadine Buchebner PhD student



MSc. **Fei-Fan Cai** PhD student



**Edmund Dürrer** Student assistant



**Felix Ferk** Student assistant



**Julia Gröger** Student assistant



Mgr. **Jitka Holcova** Scientific staff



**Nicole Käfer** Student assistant



Dipl.-Ing. Julius Keckes PhD student



Dipl.-Ing. **Hannah Lichtenegger** PhD student



**Paul Mayrhofer** Student assistant



Dipl.-Ing. Daniela Neumüller PhD student



Dipl.-Ing. Sepide Hadibeik Neishaboori PhD student



Dipl.-Ing. Alexander Jelinek PhD student



Dipl.-Ing. **Manoel Kasalo** PhD student



Dipl.-Ing. **Kevin Kutlesa** PhD student



Dipl.-Ing. Arthur Lintner PhD student



Dr. **Igor Moravcik** PostDoc



Dipl.-Ing. Simon Pillmeier PhD student



MSc. **Niklas Plutta** PhD student



Mag. Dr. **Lidija Rafailovic** PostDoc



Dipl.-Ing. Klemens Schmuck PhD student



Dr. **Florian Spieckermann** PostDoc



Dr. **Oleksandra Tolochyna** *PostDoc* 



**Sarah Wilding** Student assistant



Dipl.-Ing. **Tobias Ziegelwanger** PhD student



Dipl.-Ing. **Thomas Pogrielz** *PhD student* 



Dipl.-Ing. **Felix Römer** PhD student



Dipl.-Ing. Lukas Schweiger PhD student



**Robert Strauss** Student assistant



Dr. **Juraj Todt** PostDoc



Dipl.-Ing. Michael Wurmshuber PhD student



#### **Chair of Structural and Functional Ceramics**

#### Chair

Univ.-Prof. Dr. Raul Bermejo Moratinos



#### **Deputy Chair**

Ao.Univ.-Prof. Dr.

**Barbara Putz** 



#### **Group leader**





#### **Office management**

**Judith Sifkovits** Study administrations Personnel management Financial management



#### Technicians

Sarah Kohlbacher IT administration







#### Scientific staff

BSc. **Luisa Bastos-Mateus** Graduate student



BSc. **Andrea Gomez** Graduate student



Dipl.-Ing. **Dominik Gutnik** PhD student



Dr. **Walter Harrer** *PostDoc* 



Dipl.-Ing. **Abdullah Jabr** *PhD student* 



BSc. **Pia Kaplan** Graduate student



Dr. Josef Kreith Senior Scientist



**Ruven Bauer** Student assistant



Dr. **Manuel Gruber** PostDoc



**Viktor Haipl** Student assistant



Dipl.-Ing. Anna-Katharina Hofer PhD student



Mtech. **Arijit Jana** PhD student



Dipl. -Ing Irina Kraleva Senior Scientist



Christian Krug Student assistant



**Lukas Ladinger** *Student assistant* 



BSc. Johannes Neumüller Student assistant



BSc. **Michael Pasterk** Graduate student



**Clemens Proksch** *Graduate student* 



BSc. **Elija Ribul** Graduate student



Dipl.-Ing. Josef Schlacher PhD student



Bsc. Fabian Stücklberger Graduate student



BSc. **Maximilian Munz** Graduate student



Dipl.-Ing. **Roman Papsik** PhD student



BSc. **Thomas Priet** Graduate student



BSc. **Tobias Prötsch** Graduate student



Dr. Johanna Sänger PostDoc



Dipl.-Ing. **Maximilian Staudacher** *PhD student* 



Bsc. **Viktoria Waidbacher** *Graduate student* 



#### **Retired / emeritus university professors**

Univ.-Prof.i.R. Dr. **Helmut Clemens** 



Univ.-Prof.i.R. Dr. Albert Kneißl



#### Visiting scientists

Prof. Dr. **Ludvik Martinu** Polytechnique Montréal, Canada



Dr. **Clive Randall** *The Pennsylvania State University, USA* 



MSc. **Alessandro Togni** Università degli Studi di Modena, Italy



em. o.Univ.-Prof. Dr. **Robert Danzer** 







Prof. Dr. **Jolanta Sapieha** Polytechnique Montréal, Canada



MSc. **Donglan Zhang** Central South University, Changsha, China





### **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.

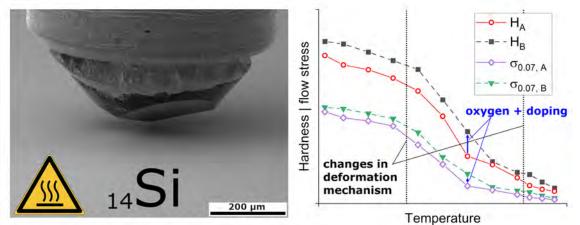


#### **Chair of Functional Materials and Materials Systems**

At the Chair of Functional Materials and Materials Systems, the following working groups with the respective group leaders are established: Advanced Surface Engineering (Nina Schalk), Materials for Microelectronics (Rostislav Daniel), Advanced Micro- and Nanostructure Characterization (Michael Tkadletz, group jointly operated with the Chair of Physical Metallurgy), and Scale Bridging Materials Testing under Extreme Conditions (Verena Maier-Kiener).

Research at the Chair focuses on the design and synthesis of advanced functional materials and surfaces by surface activation, modification, and deposition of coatings, thin films and nanoparticles using plasma-assisted vacuum techniques. The Chair operates a unique portfolio of lab- to industrial scale vapor deposition systems, including sputter deposition (DC, pulsed DC, HiPIMS) and cathodic arc deposition for the synthesis of coatings and thin films, magnetron sputter inert gas condensation for the synthesis of nanoparticles, as well as plasma surface modification systems. This portfolio to develop functional materials is complemented by facilities for the investigation of microstructure and mechanical/tribological properties. The Chair operates a comprehensive spectrum of materials testing devices, bridging the gap from macro-mechanical testing under different loading conditions and temperatures to a unique set of micro- and nanomechanical testing systems, including various in-situ and operando nanoindenters enabling micromechanical tests ranging from -150 to 1000°C as well as under controlled electrochemical conditions. Furthermore, we provide various simulation tools for deposition processes and materials design. Additional methods for characterization and modelling are used in collaboration within the Department of Materials Science and other Chairs within Montanuniversität. Active research examples include tribological coatings for tools and components for automotive and aerospace applications, thin films for functional devices for microelectronics and displays, functional surfaces for energy conversion and storage, as well as the development of advanced micromechanical testing methods for materials characterization under extreme conditions.

A highlight of the year 2023 was a paper in Materials & Design within a special issue on Nanomechanical Testing focusing on the exploration of high-temperature deformation of monocrystalline silicon by extreme nanoindentation. In this study, nanoindentation emerged as an overly potent tool for characterizing the deformation behavior of silicon between room temperature and 950°C. The investigation led to the identification of three distinct deformation regimes: a low-temperature region up to 400°C characterized by phase transformations, a mid-temperature range exhibiting dislocation plasticity with pronounced strain-rate sensitivity and moderate activation energies, and finally, above 800°C a high-temperature region where perfect dislocation plasticity prevailed. This contributes novel insights into the deformation behavior of silicon, relevant to high power microelectronics where silicon must operate reliably at elevated temperatures, as well as during deposition processes.



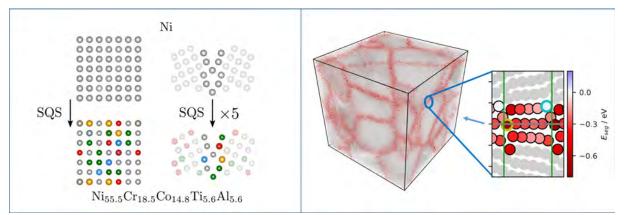
High-temperature deformation of monocrystalline silicon by extreme nanoindentation

#### **Chair of Physical Metallurgy**

Research on structural materials at the Chair of Physical Metallurgy comprises the investigation of the processing-structure-properties relationship of advanced steels, titanium alloys as well as titanium aluminides and Ni-based superalloys. 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 probe microscopes. 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.

Modern computational materials science methods are used to design and understand materials, as well as their processing methods. The group's expertise lies in combining quantum-mechanical simulations, molecular dynamics simulations, thermokinetic modeling and machine learning to predict physical properties of bulk crystal phases, their extended defects such as grain boundaries or dislocations, or nanostructures. Recent highlights include predictions of alloying impact in TiAl-based and Al-based alloys, discussing phenomena related to stability and bulk diffusion of high entropy alloys or prediction of SiC polytype stability. Aspects of tungsten oxide nanowhiskers' formation and photoluminescence of carbon quantum dots were also revealed. Segregation calculations were extended to treat complex chemical compositions and machine learning methods were applied to scale atomistic calculations to representative microstructural elements (see figure). The group also published an open-source implementation of a scale-bridging quantum-mechanics/molecular-mechanics method. Furthermore, large scale simulations of crystal growth facilities on the basis of the physical vapor transport method could be demonstrated in FEM simulations.



Left: Illustration of atomistic structures used for describing segregation in high-entropy alloys. Right: Predicting segregation energies in microstructural elements with machine learning methods.

#### **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, five research groups and one junior research group are active at both institutions.

Research at the Chair of Materials Physics concerns structural materials (e.g., steels, compositionally complex alloys, composites, as well as biological and bioinspired materials), miniaturized material systems 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 nanocrystalline and amorphous bulk materials (nanocomposites, magnetic nanomaterials, nanoporous metals) for use e.g. in hydrogen storage or medical applications.

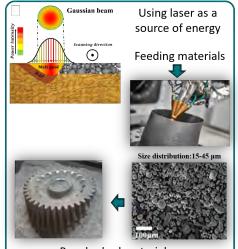
During the last year, the research activities focusing on interface properties of micro- and nanoscale (multilayered) materials in various systems (metallic, ceramic, organic) for application in flexible electronics or hard coatings were continued. Due to their high hardness and good abrasion as well as corrosion resistance, metallic glasses can cover a previously inaccessible niche. Moreover, detailed tailoring of nano- and microstructures is one of our most active research topic to improve strength or toughness, but also functional properties like magnetic performance or hydrogen generation and storage properties of nanomaterials to the application needs – with special focus on generating novel sustainable and "responsible" materials for "green technologies".

To account for the ongoing trends in integration and miniaturization in conjunction with associated demands for detailed understanding of related material size effects, we also consider scale-bridging correlation of material microstructures and structural, as well as functional properties from atomistic details to bulk components using state-of-the-art structural and mechanical in-situ characterization techniques.

Furthermore, modern processing techniques such as additive manufacturing require high heating and cooling rates for creating materials with unique properties. The related thermodynamic properties, e.g. of disordered metastable alloys, are studied using fast calorimetry at synchrotron beamlines at ESRF in Grenoble and DESY in Hamburg, correlated to locally resolved transmission electron microscopy, and backed-up by appropriate simulation and modelling. We also use additive manufacturing for creating and tailoring materials with unique structure and properties that cannot be generated by other processing techniques, thus exploiting this technology for property and mechanism-based materials design. A current example regarding this is depicted below. Tailoring materials specifically designed for additive manufacturing in combination with tuning process conditions for optimized non-equilibrium processing allows to derive new materials with unique microstructures and properties that can be additively manufactured into parts with complex

structures for high performance applications.

Additive manufacturing via laser powder bed fusion (LPBF) of metallic powders for generating advanced materials with unique microstructures and properties for design of high-performance materials and complex parts with outstanding properties.



Powder bed materials

#### **Chair of Structural and Functional Ceramics**

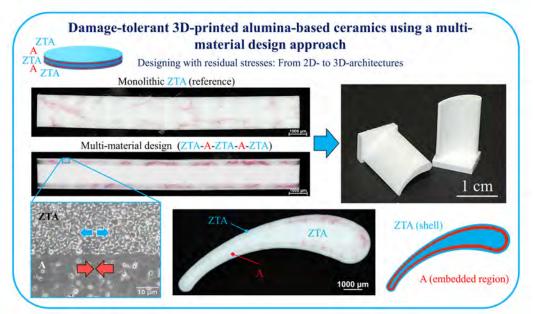
The Chair of Structural and Functional Ceramics (ISFK) aims to provide engineering solutions to the ceramic industry with primary focus on structural and functional applications. The research fields cover ceramic processing, material and system characterization, as well as process simulation, with special 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 analysis and fractography of specimens represents often the starting point for further work.

The chair's special methodological competences also lay in the electro-mechanical characterization of electro-ceramic components upon 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 resistance in functional ceramics.

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. The working fields "Design and Manufacturing" and "Characterization of Multi-Material Systems" with a strong focus on microelectronics have gained importance in the research landscape of the ISFK. Pioneer work in stereolithographic 3D-Printing of ceramics is a new feature at the Chair, which enables the fabrication of parts with tailored microstructure (see Figure) and opens new paths for the architectural design of ceramic composites with enhanced properties.





### **INVESTMENTS**

#### Acquisition of a new DSC

In July 2023, a new dynamic differential scanning calorimeter (DSC) was acquired at the Chair of Physical Metallurgy. A major improvement is the automatic sample changer, enabling fully automatic measurement series of up to 19 samples. Continuous temperatures of up to 1500°C at heating rates of 0.001 to 50K/min are possible with the TGA-DSC. The measuring atmospheres include argon, helium and synthetic air. Measurements under vacuum ( $10^{-2}$  mbar) are also possible. The resolution of the balance is 0.1µg, the resolution of the type S thermocouple is 1µW.

The measurement of the differential heat flow between reference and sample enables the analysis of phase transformations, precipitations and melting points. Oxidation and evaporation reactions can also be investigated using the balance, which has a capacity of 35g.

The new device complements the possibilities in thermomechanical characterization laboratory. The laboratory's equipment includes a quenching dilatometer with low-temperature extension, a quenching dilatometer with alpha measuring head, a tensile/compression deformation dilatometer, two DSC systems, four creep test machines and a high-temperature laser confocal microscope.



The new DSC in the thermomechanical characterization laboratory

#### New Cryo-Nanoindentation platform Alemnis

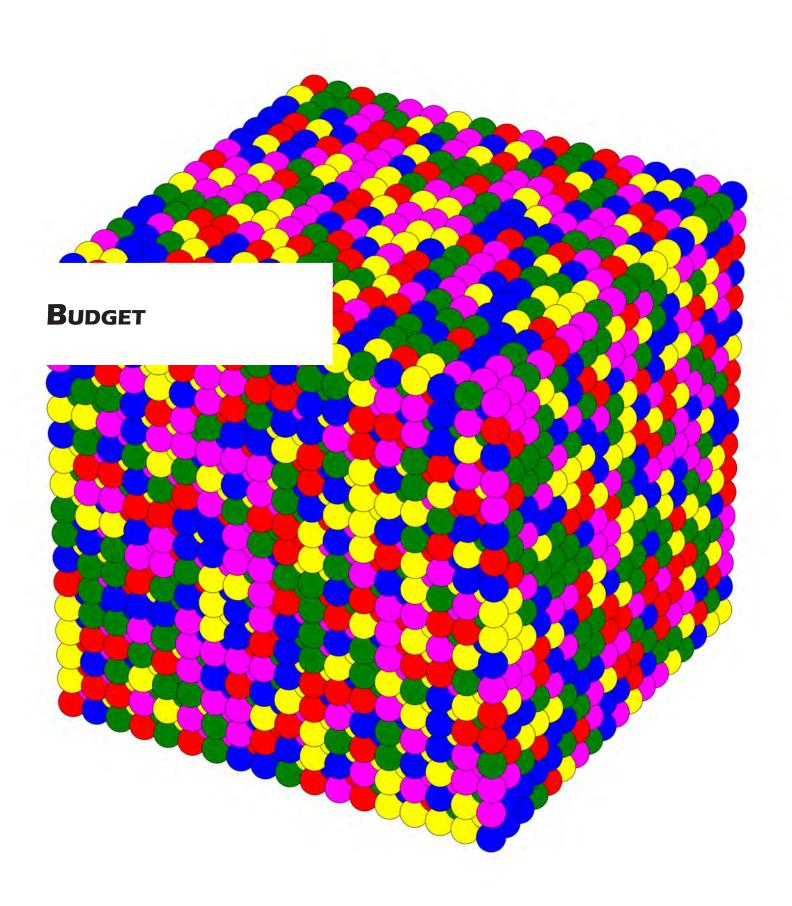
With the newly installed nanoindentation platform from Alemnis, the capabilities for micro- and nanomechanical testing available at the Department have been significantly extended. The modular design allows to use the Alemnis Standard Assembly (ASA) for in-situ and ex-situ experiments at room temperature, while the additional Low Temperature Module (LTM-CRYO) can be utilized to perform in-situ experiments at temperatures between -150 °C and 200 °C. In the ex-situ configuration, the ASA can be used as a stand-alone nanoindenter equipped with an optical microscope to navigate over the sample surface. For live observation of indentation or micromechanical experiments, the setup can be equipped to the available Tescan Vega scanning electron microscope. This in-situ configuration allows to use the LTM-CRYO module, where liquid nitrogen cooling enables controlled indentation experiments at cryogenic temperatures.

In addition to its capacity for conducting tests at cryogenic temperatures, the new indentation system distinguishes itself with its intrinsic displacement control mechanism. Unlike the load-controlled indentation systems existing at the Department, this feature enables superior control, particularly during micromechanical experiments.

Future application areas of the new cryo-indentation system are the evaluation of structural and functional materials for energy technology, with a strong focus on hydrogen production, transportation, storage and utilization. The new Alemnis device expands the palette of nanoindentation systems available at the Department, now enabling measurements under an extremely wide range of harsh conditions in the temperature range between -150 and 1000 °C.







# 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

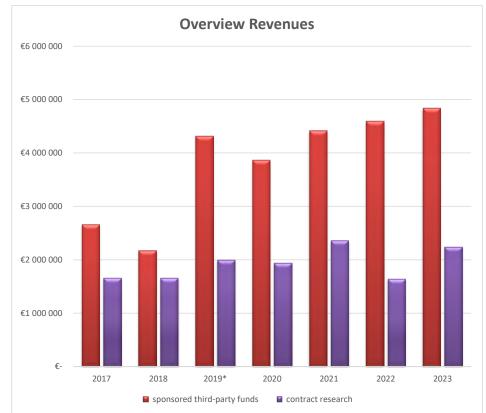
#### **Global budget**

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 2023 at a high level compared to previous years.

The budget from funded projects amounted to: € 4.837.200,-.



The budget from contract research amounted to: € 2.239.400,-.

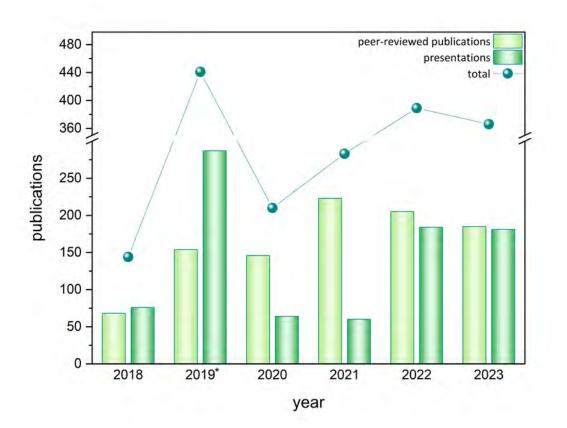
\* Since the establishment of the Department of Materials Science in 2019, four chairs are included in this representation; prior to 2019, only three were included.



## **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 2023 in 185 articles in scientific journals and 181 presentations at scientific events. With this, 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.



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

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

## **Materials** Science

## **Chair of Functional Materials and Materials Systems**

F. Frank, M. Tkadletz, C. Saringer, C. Czettl, M. Pohler, M. Burghammer, J. Todt, J. Zalesak, J. Keckes, N. Schalk, Investigation of the microstructure of a graded ZrN/Ti<sub>0.33</sub>Al<sub>0.67</sub>N multilayer coating using cross-sectional characterization methods, Surface & Coatings Technology 453 (2023) 129126.

R.-F. Guo, C.-Y. Hsu, N. Kostoglou, S. Hinder, M. Baker, C. Mitterer, C. Rebholz, C.-Y. Wang, Improved thermolytic dehydrogenation of LiBH<sub>4</sub> nanoconfined in few-layer graphene with different functionalities, Materials Today Sustainability 24 (2023) 100486.

D. Kiener, M. Wurmshuber, M. Alfreider, G.J.K. Schaffar, V. Maier-Kiener, Recent advances in nanomechanical and in situ testing techniques: Towards extreme conditions, Current Opinion in Solid State and Materials Science 27 (2023) 101108.

L. Kölbl, C. Mitterer, R. Franz, Synthesis of crystalline silver niobate thin films opening pathways for future process development, Vacuum 213 (2023) 112077.

Y. Moritz, C. Saringer, M. Tkadletz, A. Fian, C. Czettl, M. Pohler, N. Schalk, In-situ X-ray diffraction study of the oxidation behavior of arc-evaporated TiAlSiN coatings with low Al contents, Surface & Coatings Technology 475 (2023) 130161.

G.J.K. Schaffar, D. Tscharnuter, V. Maier–Kiener, Exploring the high-temperature deformation behavior of monocrystalline silicon – An advanced nanoindentation study, Materials & Design 233 (2023) 112198.

M. Tkadletz, H. Waldl, M. Schiester, A. Lechner, G. Schusser, M. Krause, N. Schalk, Efficient preparation of microtip arrays for atom probe tomography using fs-laser processing, Ultramicroscopy 246 (2023) 113672.

H. Waldl, M. Hans, M. Schiester, D. Primetzhofer, M. Burtscher, N. Schalk, M. Tkadletz, Decomposition of CrN induced by laser-assisted atom probe tomography, Ultramicroscopy 246 (2023) 113673.

L.-M. Weniger, C. Gammer, M. Niewczas, M. J. Cordill, F. Spieckermann, P. Djemia, D. Faurie, C.-H. Li, A. Lassnig, V. L. Terziyska, C. Mitterer, J. Eckert, O. Glushko, Precious metal amorphous AgAuSi: Alloy design by swapping gold for silver, Materials & Design 232 (2023) 112099.

C. Yan, B. Bor, A. Plunkett, B. Domènech, V. Maier-Kiener, D. Giuntini, Nanoindentation creep of supercrystalline nanocomposites, Materials & Design 231 (2023) 112000.

## **Chair of Physical Metallurgy**

A. Ahmadian, D. Scheiber, X. Zhou, B. Gault, L. Romaner, R.D. Kamachali, W. Ecker, G. Dehm, C.H. Liebscher, Interstitial segregation has the potential to mitigate liquid metal embrittlement in iron, Advanced Materials 35 (2023) 2211796.

D. Gehringer, M. Friák, D. Holec, Models of configurationally-complex alloys made simple, Computer Physics Communications 286 (2023) 108664.

G. Graf, M. Seyffertitz, P. Spoerk-Erdely, H. Clemens, A. Stark, L. Hatzenbichler, D. Holec, M. Burtscher, D. Kiener, X. Li, K. Liu, On the stability of Ti(Mn,Al)<sub>2</sub> C14 Laves phase in an intermetallic Ti–42Al–5Mn alloy, Intermetallics 161 (2023) 107962.

M. Musi, G. Graf, H. Clemens, P. Spoerk-Erdely, Alloying elements in intermetallic γ-TiAl based alloys – A review on their influence on phase equilibria and phase transformations, Advanced Engineering Materials (2023) 2300610.

G.K. Nayak, A. Kretschmer, P.H. Mayrhofer, D. Holec, On correlations between local chemistry, distortions and kinetics in high entropy nitrides: An ab initio study, Acta Materialia 255 (2023) 118951.

O. Renk, A. Hohenwarter, V. Maier-Kiener, R. Pippan, Exploring the anneal hardening phenomenon in nanocrystalline Pt-Ru alloys, Journal of Alloys and Compounds 935 (2023) 168005.

O. Renk, R. Pippan, Anneal hardening in single phase nanostructured metals, Materials Transactions 64 (2023) 1464-1473.

A. Rosenauer, D. Brandl, G. Ressel, S. Lukas, C. Gruber, M. Stockinger, R. Schnitzer, In situ observations of the microstructural evolution during heat treatment of a PH 13-8 Mo maraging steel, Advanced Engineering Materials (2023) 2300410.

D. Scheiber, M.N. Popov, L. Romaner, Temperature dependence of solute segregation energies at W GBs from first principles, Scripta Materialia 222 (2023) 115059.

D. Scheiber, J. Svoboda, F.D. Fischer, H.J. Böhm, L. Romaner, Fully coupled segregation and precipitation kinetics model with ab initio input for the Fe-Au system, Acta Materialia 244 (2023) 118577.

## **Chair of Materials Physics**

F.-F. Cai, A. Blanquer, M.B. Costa, L. Schweiger, B. Sarac, A.L. Greer, J. Schroers, C. Teichert, C. Nogués, F. Spieckermann, J. Eckert, Hierarchical surface pattern on Ni-free Ti-based bulk metallic glass to control cell interactions, Nano-Micro Small (2023) 202310364.

H. Chen, K. Kosiba, T. Lu, N. Yao, Y. Liu, Y. Wang, K.G. Prashanth, C. Suryanarayana, Hierarchical microstructures and strengthening mechanisms of nano-TiC reinforced CoCrFeMnNi high-entropy alloy composites prepared by laser powder bed fusion, Journal of Materials Science & Technology 136 (2023) 245-259.

Y. Dong, D. Wang, Q. Li, X. Luo, J. Zhang, K.G. Prashanth, P. Wang, J. Eckert, L. Mädler, I.V. Okulov, M. Yan, Strong and ductile titanium via additive manufacturing under a reactive atmosphere, Materials Today Advances 17 (2023) 100347.

S. Evertz, J. Zálešák, M. Hans, H.C. Jansen, J.F. Keckes, H. Sheng, J. Eckert, C. Gammer, J.M. Schneider, Mapping strain across Co<sub>80</sub>Ta<sub>7</sub>B<sub>13</sub> / Co<sub>62</sub>Ta<sub>6</sub>B<sub>32</sub> glassy interfaces, Materials & Design 234 (2023) 112327.

## **Materials** Science

S. Hadibeik, H. Ghasemi-Tabasi, A. Burn, S. Lani, F. Spieckermann, J. Eckert, Controlling the glassy state toward structural and mechanical enhancement: Additive manufacturing of bulk metallic glass using advanced laser beam shaping technology, Advanced functional materials (2023) 20231118.

A. Jelinek, S. Žák, M. J. Cordill, D. Kiener, M. Alfreider, Nanoscale printed tunable specimen geometry enables high-throughput miniaturized fracture testing. Materials and Design, 234(2023) 112329.

D. Kiener, M. Wurmshuber, M. Alfreider, G. J. K. Schaffar, V. Maier-Kiener, Recent advances in nanomechanical and in situ testing techniques: Towards extreme conditions, Current opinion in solid state & materials science 27 (2023) 101108.

D. Neumüller, L.D. Rafailović, A.Z. Jovanović, N.V. Skorodumova, I.A. Pašti, A. Lassnig, T. Griesser, C. Gammer, J. Eckert, Hydrogen evolution reaction on ultra-smooth sputtered nanocrystalline Ni thin films in alkaline media—from intrinsic activity to the effects of surface oxidation, Nanomaterials 13 (2023) 2085.

L. Schweiger, D. Kiener, M. Burtscher, E. Schafler, G. Mori, F. Spieckermann, J. Eckert, From unlikely pairings to functional nanocomposites: FeTi–Cu as a model system, Materials Today Advances 20 (2023) 100433.

G. Wu, S. Liu, Q. Wang, J. Rao, W. Xia, Y.-Q. Yan, J. Eckert, C. Liu, E. Ma, Z.-W. Shan, Substantially enhanced homogeneous plastic flow in hierarchically nanodomained amorphous alloys, Nature Communications 14 (2023) 3670.

## **Chair of Structural and Functional Ceramics**

A.-K. Hofer, I. Kraleva, T. Prötsch, A. Vratanar, M. Wratschko, R. Bermejo, Effect of second phase addition of zirconia on the mechanical response of textured alumina ceramics, Journal of the European Ceramic Society 43 (2023) 2935-2942.

A. Jabr, J. Fanghanel, Z. Fan, R. Bermejo, C. Randall, The effect of liquid phase chemistry on the densification and strength of cold sintered ZnO, Journal of the European Ceramic Society 43 (2023) 1531-1541.

A. Jabr, H.N. Jones, A.P. Arguelles, S. Trolier-McKinstry, C. Randall, R. Bermejo, Scaling up the cold sintering process of ceramics, Journal of the European Ceramic Society 43 (2023) 5319-5329.

R. Papšík, O. Ševeček, A.-K. Hofer, I. Kraleva, J. Kreith, R. Bermejo, Prediction of edge and tunnelling crack formation in layered ceramics using a stress-energy fracture criterion, Journal of the European Ceramic Society 43 (2023) 2928-2934.

R. Papšík, O. Ševeček, E. Martin, R. Bermejo, Prediction of ring crack initiation in ceramics and glasses using a stress-energy fracture criterion, Journal of the American Ceramic Society (2023) 4329–4342.

B. Putz, T.E.J. Edwards, E. Huszar, P.A. Gruber, K.P. Gradwohl, P. Kreiml, D.M. Többens, J. Michler, Electro-mechanical behaviour of Al/Al2O3 multilayers on flexible substrates: Insights from in situ film stress and resistance measurements, Advanced Engineering Materials 25 (2023).

J. Schlacher, Z. Chlup, A.-K. Hofer, R. Bermejo, High-temperature fracture behaviour of layered alumina ceramics with textured microstructure, Journal of the European Ceramic Society 43 (2023) 2917-2924.

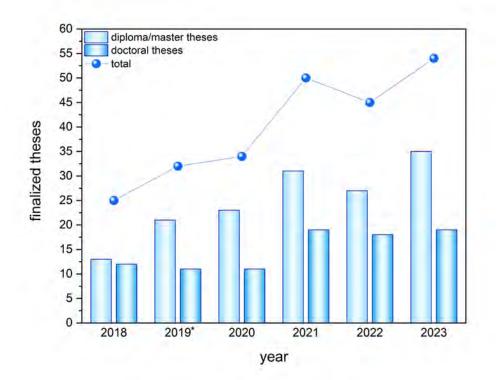
J. Schlacher, T. Csanádi, M. Vojtko, R. Papšík, R. Bermejo, Micro-scale fracture toughness of textured alumina ceramics, Journal of the European Ceramic Society 43 (2023) 2943-2950.

M. Staudacher, T. Lube, P. Supancic, The Ball-on-Three-Balls strength test for discs and plates: Extending and simplifying stress evaluation, Journal of the European Ceramic Society 43 (2023) 648-660.

M. Staudacher, P. Supancic, T. Lube, The Ball-on-Ring-test: Enhancing an analytical solution by numerical analysis for elastic deformation and small displacements, Journal of the European Ceramic Society 43 (2023).

## **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, four chairs are included in this representation; prior to 2019, only three were included.

### **Master theses**

In 2023, 35 students completed their theses.

#### **Bastos Mateus, Luisa**

Thermal shock behavior of 3D-printed alumina ceramics with spatially tailored porosity

#### Glettler, Jürgen

Testing of additiv manufactured specimens: Development of test rig, verification, investigation of strength as function of AM-printing direction

#### Gruber, Fabian Ingo

Thermal treatment of continuous alumina fibers

#### Gutnik, Dominik

Interface adhesion measurement of industrially processed layers on polyimide

# Final Theses

#### Holub, Georg

Simultaneously increasing strength and ductility of nano-crystalline Cu-Zn-alloys made from powderous raw materials

Job, Veronika Elisabeth Characterization of high alloyed steel composites under ballistic impact

Juarez Perez, Lorena Xiomara Precipitation evolution of  $\gamma^{\prime}$  hardened fcc Fe-Ni based alloys

Kapala, Joseph Munyika

Production of damage tolerant Ti-6Al-4V by laser powder bed fusion (L-PBF)

#### Karner, Matthias

Variation of the solution annealing temperature and strength modeling of Fe-12Ni maraging steels

#### Kutlesa, Kevin

Microstructural characterization and mechanical properties of nanocomposite AlCrSiN thin films

#### Marin-Morales, David

CCT diagrams of high-strength weld metal

#### Melcher, Verena

Characterization of electrically conductive ceramics for spark plug electrodes

#### Munz, Maximilian Luca

Comparison of technological and scientific methods for fracture toughness determination of silicon nitride

#### Nistelberger, Daniel

Microstructure variation of a secondary hardening tool steel through heat treatments

#### Pasterk, Michael Franz

Examination of contact damage in silicon nitride ball bearings

#### Paulik, Anna Margarethe

Ab initio discovery of novel hydride phases in NiTi shape memory alloys

#### Pototschnig, Ulrich Josef

Deriving a model for catalytic methane pyrolysis: A DFT study

#### Priet, Thomas Ernst

Strength testing of thin glass substrates

#### **Prötsch, Tobias Maria** Tape casting of Cr2AIC MAX phase for multi-material designs

**Rainer, Daniel** Towards atom probe crystallography of thin films

## **Materials** Science

# Final Theses

**Ribul, Elija** Mechanical characterization of zinc oxide produced by an optimized cold sintering process

**Rovira Ferrer, David** Synchrotron-based characterization of bulk metallic glasses

Ruderes, Katharina Reliability of copper-fiber reinforced laminates

**Strauss, Robert** Additive manufacturing of Fe-Si soft magnets

Stücklberger, Fabian Anton Mechanical response of textured alumina-based ceramics after Hertzian contact damage

Tabelander, Michael Timo Synthesis and characterization of high entropy alloy nitrides

#### **Taucher, Lorenz Johannes**

Microstructural characterization and investigation of the high-temperature forming behavior of an  $(\alpha+\beta)$  titanium alloy modified with boron

**Teusl, Sebastian** Intercritical annealing of PH 13-8 Mo maraging-steel

**Vukušić, Antonio** Influence of vacancies on the N K-edge ELNES response of fcc tantalum nitrides — Ab initio study

Wegscheider, Stefan Adhesive bonding of catalysts

#### Weissenböck, Thomas

Evaluation of high-temperature methods for the characterisation of recovery and recrystallisation processes in cold finished rolled molybdenum sheets from different sinter formats

#### Widowitsch, Nadine

Prediction of fracture toughness and DBTT of a 15-5 PH steel

#### Wurmitzer, Michael Martin

Computational analysis of chemical vapor deposition for nitride-based hard coatings

#### Zernatto, Gerald Nikolaus

In-situ thermo-mechanical fatigue of copper metallizations

#### Zetterberg, Keegan

The effects of grain size on the elastic response of FeCrMnNiCo high entropy alloy: a molecular dynamics study

# Final Theses

## **Doctoral theses**

In 2023, 19 doctoral students were awarded doctorates in montanistic sciences.

#### Biermair, Florian

Evaluation of microstructure and mechanical properties of a precipitation strengthened compositionally complex alloy

#### **Bodner, Sabine Carmen**

Cross-sectional characterization of functionally graded materials

#### Gehringer, Dominik Franz Josef

Atomistic approaches for investigating planar defects in compositionally complex alloys

#### Graf, Gloria Verena

Exploration of phase transformations in lightweight structural materials by means of in situ highenergy X-ray methods

#### Gruber, Georg Christoph

Refractory high entropy alloy thin films as diffusion barriers for microelectronic applications

#### Hofer, Anna-Katharina

Processing of ceramic materials with tailored microstructures deploying tape casting and stereolithographic 3D-printing

#### Jaszfi, Vince

Influence of temperature and microstructure on the magnetic properties of induction heat treated steels

#### Karner, Stefan

Strain engineering in trench power MOSFETs - characterization and optimization of mechanical and electrical transistor properties

#### Konstantiniuk, Fabian

Mechanical properties of Al<sub>2</sub>O<sub>3</sub> coatings for cutting tools deposited by chemical vapor deposition

#### Lintner, Arthur Rudolf

Impact behaviour and damage tolerance of selected g-TiAl alloys

#### Mayer, Florian

Structure-property relationships in substituted BaTiO3: A theoretical study

#### Moritz, Yvonne

Effect of Si alloying on Ti(Al)N hard coatings

#### Nayak, Ganesh Kumar

A multi-method atomistic study of protective nitride coatings: from crystalline to amorphous materials

#### Rezvan, Amir

Structural and mechanical property investigation of metallic glasses

## **Materials** Science

#### Staudacher, Maximilian

Strength testing of ceramics: Reassessment of methods and application to additive manufacturing

#### Trost, Claus Othmar Wolfgang

Advancing mechanical property characterisation for metallic foils using experiments, simulations, and machine learning

#### Weissitsch, Lukas Emanuel

Microstructure and magnetic properties of high-pressure torsion synthesized hard magnetic materials

#### Yuan, Xudong

Improving the mechanical properties of metallic glasses through structure and stress engineering: A molecular dynamics simulations study

#### Zeisl, Stefan

Process-structure-property relationships of β-NiAl and η-Ni3Ti strengthened Co-free maraging steels



# Conferences/Events

## **CONFERENCES AND EVENTS**

## **Organization of conferences**

Members of the Department were engaged in the organization of scientific conferences and other scientific events, as shown in the next pages.

## **Opening Christian Doppler Laboratorys** (17 Janury and 06 March 2023, Leoben)

In the year 2023 two new CD labs were started at the Department of Materials Science. The first, entitled "Knowledge-based Design of Advanced Steels", was opened on the 17<sup>th</sup> of January. The CDL is headed by Ronald Schnitzer and focuses on the effects of increased scrap use and the resulting increased amounts of undesirable tramp and trace elements on material properties. The research approach includes simulations and experimental methods, using cross-scale methods that start at the atomic structure. In addition to the presentation of the content and objectives of the CDL, the numerous participants had the opportunity to listen to presentations by scientific cooperation partners and to round off the event with a pleasant networking event.

The second CDL entitled "Advanced Computational Design of Crystal Growth" is headed by Lorenz Romaner and was opened on 6<sup>th</sup> of March. The research team will explore new modeling methods for the virtual description of crystal growth processes in the semiconductor industry combining physics-based and data-driven methods. Activities are centered around silicon carbide, one of the most promising semiconductors for high-power electronics. The inauguration was opened by representatives from CDG, the industry partner, and the rector of the MUL. After a concise overview of main activities planned in the CDL two high-level scientific talks were given on the subject of crystal growth and thin-film deposition. The event closed at the buffet with lively discussions and new acquaintances.



Foto Freisinger

### Berkeley Workshop "Manufacturing of Materials for Industry Applications" (27 - 29 March 2023, Berkeley)

After two successful previous workshops in 2017 and 2020, a third repetition took place following the annual TMS Conference in San Diego, fostering collaboration between the University of California, Berkeley, and the Montanuniversität Leoben in the faculty club of UCB in Berkeley. In 2023, the theme centered around "Manufacturing of Materials for Industry Applications", with Prof. Peter Hosemann and Verena Maier-Kiener assuming key roles. From March 27 - 29, a diverse group of 40 participants from the realms of science, research, and industry gathered to showcase their advancements in materials science, particularly in the fields of additive manufacturing and metallurgy for extreme material properties and harsh environments.

This workshop, complemented by the extensive TMS conference, provided an exceptional platform for in-depth discussions and the enhancement of research initiatives within a more intimate setting. Notably, Verena Maier-Kiener received the prestigious Family Care Grant from TMS for the third consecutive time. This grant not only acknowledges her contributions to the society, but also facilitates her participation by accommodating her family, exemplifying TMS's commitment to supporting individuals in building international networks while navigating familial responsibilities.



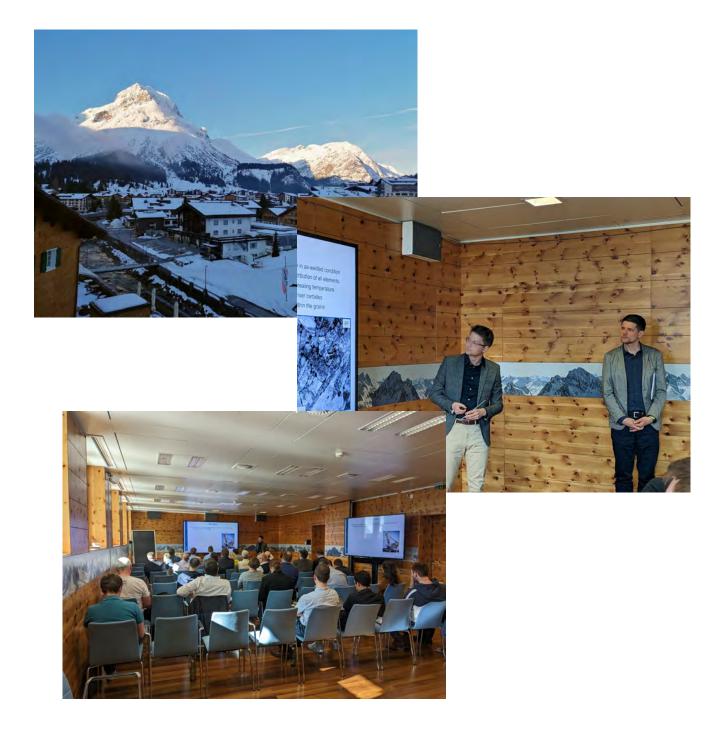
### 11<sup>th</sup> Annual Meeting of the Austrian Ceramic Society (13 April 2023, Leoben)

With 39 participants, the annual meeting of the Austrian Ceramic Society (AuCerS) on April 13, 2023 in Leoben set a new record. In addition to the members of AuCerS, we were able to welcome as guest of honour Prof. Clive Randall, the director of the Material Research Institute at the Pennsylvania State University, who visited the Montanuniversität Leoben due to a scientific cooperation. The focus of this annual conference was the student presentation competition with eleven applicants. All of them presented their research results with passion and honest effort.



### 2<sup>nd</sup> Materials Science Colloquium (67. Metallkunde-Kolloquium) (17 - 20 April 2023, Lech am Arlberg)

From April 17 - 20, the 2<sup>nd</sup> Materials Science Colloquium (67<sup>th</sup> Physical Metallurgy Colloquium) took place in Lech am Arlberg. The colloquium, organized by the entire Department of Materials Science, this year included the focus topic "Computational Materials Science". We saw 33 exciting presentations, especially from international invited speakers from Germany and USA, and lively scientific discussions in a relaxed winter atmosphere that left us wanting more.



## 49<sup>th</sup> International Conference on Metallurgical Coatings & Thin Films (ICMCTF) (21 - 26 May 2023, San Diego)

Barbara Putz and Michael Tkadletz were co-organizers of sessions within Symposium H: Advanced Characterization Techniques for Coatings, Thin Films, and Small Volumes at the renowned International Conference on Metallurgical Coatings and Thin Films (ICMCTF). Michael Tkadletz chaired the session "H1. Spatially-resolved and In-Situ Characterization of Thin Films and Engineered Surfaces," focusing on detailed and real-time analysis of thin films and engineered surfaces. Barbara Putz, was in charge of "H3. Characterization of Coatings and Small Volumes in Extreme and Cyclic Conditions," which concentrated on the study of coatings and small volumes under severe and varying conditions. These sessions highlighted their expertise in the field of materials science and engineering, emphasizing the importance of advanced characterization techniques in understanding and developing thin films, coatings, and engineered surfaces under various conditions.



## Joint International Symposium on Metastalble and Amorphous Meterials and Conference on Rapidly Quenched Materials (20 - 25 August 2023, Warsaw)

After 3 years of COVID-19 break the joint ISMANAM 27 (27<sup>th</sup> International Symposium on Metastable and Amorphous Materials) and the RQ 17 (17<sup>th</sup> Conference on Rapidly Quenched Materials) was held in Warsaw at the Technical University from August 20 - 25. The joint meeting was devoted to the celebration on behalf of 60 years of the discovery of metallic glasses in 1960. The quality of the presented research was outstanding. A strong delegation of the Chair of Materials Physics and the ESI gave presentations during the conference including a historical view on the community from a western European point of view given by Jürgen Eckert. During the conference dinner held at the Royal Castle in Warsaw the poster presented by Sepide Hadibeik was awarded with the "Best Poster Award".

After so many years the meeting was a great occasion to meet the colleagues and friends from the field and to foster the international collaboration, so important for scientific progress.



### 7<sup>th</sup> "young Ceramists Additive Manufacturing" Forum (30 August - 01 September 2023, Leoben)

During the 7<sup>th</sup> "young Ceramists Additive Manufacturing" (yCAM) Forum from August 30<sup>th</sup> to September 1<sup>st</sup>, the focus was on young scientists in additive manufacturing of ceramics. 84 participants from 15 countries joined the event, including 4 invited talks and 3 keynote talks from industrial partners.



# Conferences/Events

## 7<sup>th</sup> International Conference Fracture of Advanced Ceramics and Glasses (03. - 05. September 2023, Leoben)

The 7<sup>th</sup> International Conference "Fracture of Advanced Ceramics and Glasses - Fractography, Facture Mechanics and Fracture Testing" followed from September 3 - 5. The program committee, Tanja Lube (Montanuniversität Leoben) and Prof. Dr. Jan Dusza (Slovak Academy of Sciences, Kosice) welcomed participants from academic institutions in Europe and ceramic industry. The lectures about fracture analysis, materials testing and material characterization showed the current scientific developments and their applications in the industrial environment.



### 57<sup>th</sup> Metallography Conference (13 - 15 September 2023, Leoben)

From September 13 - 15, 2023, the 57<sup>th</sup> Metallography conference in the German-speaking area took place at the Montanuniversität Leoben, which is also the 16<sup>th</sup> International Metallography Conference and has been held in Leoben since 1963. Ronald Schnitzer from the Chair of Physical Metallurgy acted as scientific chair of the conference for the first time.

In seven plenary lectures and more than 60 technical presentations, the latest metallographic findings and achievements were presented and discussed in detail. The more than 260 participants were additionally provided with an impressive equipment demonstration by 20 exhibitors. The social program with a mayor's reception in the Gösserbräu and a conference dinner in the Live Congress provided a comfortable get-together and a good atmosphere during the conference.

Numerous prizes were awarded, such as the prestigious Roland Mitsche Prize to Prof. Ehrenfried Zschech from Dresden. The first place in the Struers Best Presentation Award, which was determined by the participants from all presentations by voting via app or ballot paper, was awarded to Daniel Schrittwieser from the Chair of Physical Metallurgy for his presentation in the field of high-strength weld metal.



## 93<sup>rd</sup> IUVSTA Workshop (15 - 19 September 2023, Leibnitz)

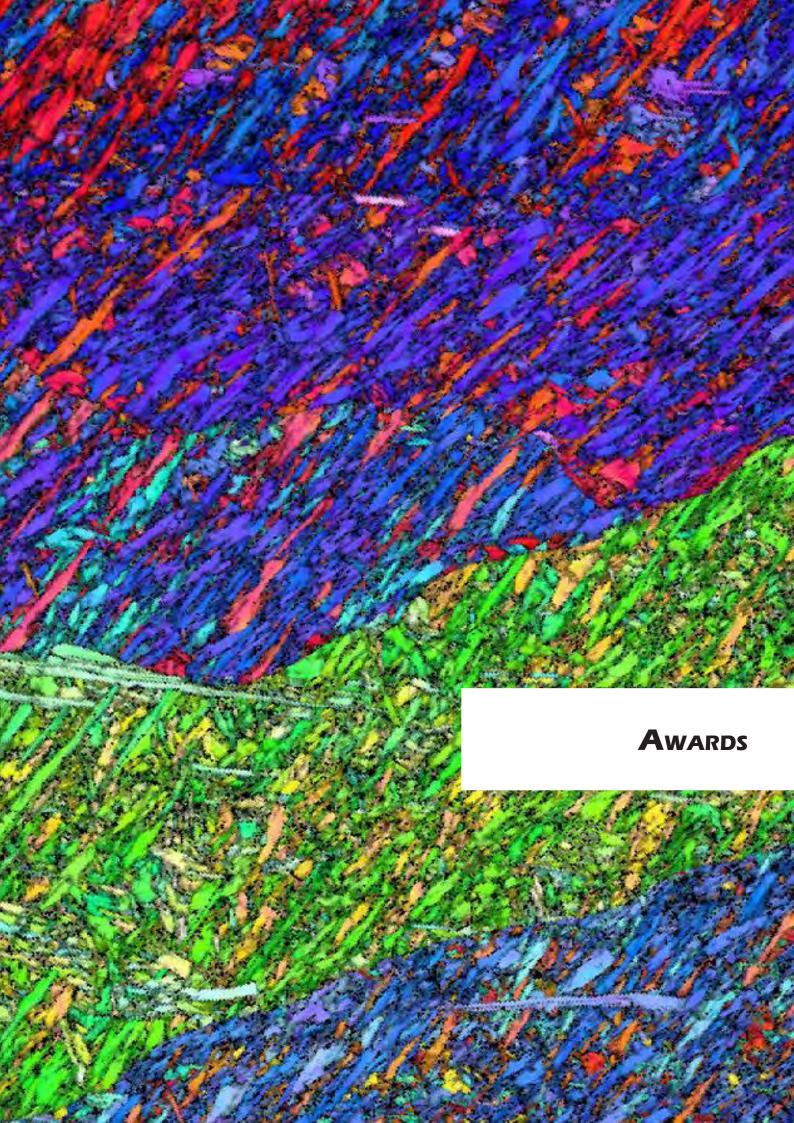
The 93<sup>rd</sup> IUVSTA Workshop, which was initially planned to take place in 2021 and was postponed due to the COVID-19 pandemic, was finally held at Schloss Seggau, Austria, from October 15 - 19, 2023. The organizing committee, consisting of Jozef Keckes, Nina Schalk, Michael Tkadletz (all Montanuniversität Leoben) and Prof. Ivan Petrov (University of Illionis, Linköping University), arranged an attractive scientific program with 15 invited talks from well recognized experts, 12 contributed talks and 15 posters, covering microstructural, chemical and residual stress characterization, nano-/micromechanics and in-situ/in-operando studies, as well as thermal properties, which was well-received by the participants. In addition to the excellent scientific program, the beautiful setting at Schloss Seggau and the social program including a castle tour and a wine tasting, which also left sufficient time for discussions contributed to the success of the workshop. The progress in the last years and the current state of research shown in advanced characterization of surfaces and thin films are impressive.



### MS&T23: Materials Science & Technology (01 - 04 October 2023, Columbus, Ohio)

The 2023 Materials Science & Technology Technical Meeting and Exhibition (MS&T2023) organized by TMS, AIST and The American Ceramic Society took place in Columbus, USA during October 1-4, 2023. Together with K.G. Prashanth (Tallinn University of Technology), Z. Wang (South China University of Technology, Guangzhou), J. Eckert organized a symposium on 'Additive Manufacturing of Metals: Microstructure, Properties and Alloy Development'. The symposium extended over four days and included invited presentation, 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. The scientific exchange and networking during the sessions was very lively and contributed to the success of the symposium.





# Awards

## **P**RIZES 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 in particular numerous younger employees 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.

# *"Wissenschaftspreise für Montanistinnen 2023" awarded to three female materials scientists*

Since 2019, the Montanuniversität Leoben has been awarding the "Wissenschaftspreis für Montanistinnen" every year on International Women's Day on March 8, in order to promote and focus on the work of young female researchers and thus strengthen women in the STEM subjects. The prize is awarded in three categories. This year, materials scientist from Leoben were honored in all three categories for their outstanding scientific achievements; Johanna Byloff from the Chair of Structural and Functional Ceramics was awarded in the Junior Scientist category, Gloria Graf from the Chair of Physical Metallurgy in the PreDoc category and Nina Schalk from the Chair of Functional Materials and Materials Systems in the PostDoc category.



### Awards to Jürgen Eckert

Jürgen Eckert was awarded the Distinguished Award at THERMEC 2023 (International Conference on Processing & Manufacturing of Advanced Materials) for his "seminal contributions to the understanding of phase formation and structure-property relationships of metastable materials". The award was presented during the THERMEC Meeting in Vienna (July 2-7, 2023)

Furthermore, Jürgen Eckert has been appointed Honorary Researcher by the Henan Academy of Sciences, Zhengzhou, China.

And additionally Jürgen Eckert has been elected a Foreign Fellow of the National Academy of Sciences, India (NASI), the oldest science academy in India.





#### Honor for Christian Fleißner-Rieger

Christian Fleißner-Rieger, former doctoral student at the Chair of Physical Metallurgy, received an award from the Fahrzeugverband Jubiläumsstiftung für his doctoral thesis, entitled "Titanium base alloys for laser powder bed fusion". Funded and supported by Pankl Racing Systems and voestalpine in Kapfenberg, his doctoral thesis dealt with the additive manufacturing of conventional, as well as self-developed titanium alloys for racing applications. Mr. Fleißner-Rieger has found process parameters that lead to the formation of a special phase that is able to reduce internal stresses caused during additive manufacturing. At the same time, the components have excellent mechanical properties. The award ceremony took place on July 11, 2023 in the auditorium of Graz University of Technology.



#### Franz Leitner Prize 2023 awarded to Hannah Fleißner-Rieger

Hannah Fleißner-Rieger was awarded the Franz Leitner Prize 2023 for her research achievements in the field of welding technology. This prize is donated by the board of the technical-scientific association ASMET and the management of voestalpine Böhler Welding Austria GmbH and is awarded every two years following the decision of a jury. During her doctoral thesis at the Chair of Physical Metallurgy, Ms. Fleißner-Rieger dealt with the structure-property relationships of heat-resistant weld metal and contributed significantly to their microstructural understanding and further development. Hannah Fleißner-Rieger focused on material characterization using atom probe tomography and in-situ synchrotron radiation. The award ceremony took place during the ASMET Forum on May 25, 2023.



## Awards

### Poster prize to Gloria Graf

Gloria Graf from the Chair of Physical Metallurgy received one of the two poster prizes awarded at the 7<sup>th</sup> International Workshop on Titanium Aluminides (IWTA 2023) for her research work on the solidification processes during additive manufacturing of intermetallic titanium aluminides. This conference provides a platform for intensive exchange between science and industry. Intermetallic titanium aluminides are mainly used in environmentally friendly aircraft engines. The workshop took place from June 11 - 16, 2023 in Toulouse, France.



### Graduate Student Award for Georg Gruber

Georg Gruber, PhD student at the Chair of Functional Materials and Materials Systems, was awarded the "Graduate Student Award in Silver" at the International Conference on Metallurgical Coatings and Thin Films in San Diego, USA, for his research work "Refractory high entropy alloy thin films as diffusion barriers for microelectronic applications". In his work, Georg Gruber investigated the influence of Ti, V, Cr, Mn, Zr and Hf in MoNbTaW-based high-entropy films on their microstructure, mechanical properties and thermal stability. In addition to the detailed characterization of the high entropy layers, their suitability as a diffusion barrier for applications in microelectronics and power electronics was examined. Mr. Gruber was able to show that the barrier effect can be shifted to higher temperatures by up to 300°C compared to conventional barrier layers.





# *"Best Poster Award" at the Metal Additive Manufacturing Conference (MAMC2023-Vienna) for Sepide Hadibeik*

Sepide Hadibeik, PhD-student at the Chair of Materials Physics, under the supervision of Jürgen Eckert and Florian Spieckermann, attended the MAMC-2023 in Vienna. In her poster, she presented her preliminary results regarding 3D-printing of Zr-based Bulk Metallic Glasses. One focus of the presented work is to optimize the crystallinity and relaxation of Zr-based amorphous alloys during laser powder bed fusion. In recognition of her research, she was awarded the "Best Poster Award" by Omar Al-Rawi, Member of the Vienna City Council and Conference Chairman and Gerhard Hackl from Austrian Society for Metallurgy and Materials (ASMET).



### 1<sup>st</sup> place in the student speech competition of the Austrian Ceramic Scciety (AuCerS)

Abdullah Jabr obtained the first place at the student speech competition held during the 11<sup>th</sup> Meeting of the Austrian Ceramic Society (AuCerS) on April 14, 2023, in Leoben. With his presentation titled "Structural integrity of cold sintered ceramics: effect of liquid phase chemistry and processing conditions," he secured the top position among the 11 participants. Mr. Jabr is working on his doctoral thesis at the Chair of Structural and Functional Ceramics. He is engaged in exploring new, alternative sintering methods with the aim of reducing the sintering temperature of ceramics (typically above 1000°C) to below 350°C. This significant reduction in temperature not only diminishes energy consumption in the manufacturing process but also facilitates the combination of different materials.



## **Materials** Science

# 1<sup>st</sup> place in the student speech competition of the European Ceramic Society

Abdullah Jabr, doctoral researcher at the Chair of Structural and Functional Ceramics (ISFK), won the student speech competition of the European Ceramic Society (ECerS), which was held as part of the "15<sup>th</sup> ECerS Conference for Young Scientists in Ceramics" from July 2 - 6, 2023 in Lyon, France. With his presentation "Understanding the cold sintering process of ceramics", he was able

to outperform 22 other candidates. He qualified to take part in this competition by winning the national student speech competition of the Austrian Ceramic Society (AuCerS) on April 13, 2023. This is the second victory in a row, that was achieved by an Austrian candidate and ISFK doctoral student. Mr. Jabr's research focuses on new, alternative sintering processes with the aim of lowering the sintering temperature of ceramics (typically above 1000°C) to below 350°C. This will significantly reduce the energy consumption in manufacturing and allows the combination of different materials.



### "Outstanding Reviewer Award" for Anna Sophie Jelinek

Anna Sophie Jelinek has been awarded with the "Outstanding Reviewer Award 2022" for her excellent reviewing activities for the journals ACTA MATERIALIA and SCRIPTA MATERIALIA. Both journals rank among the most prestigious journals for Materials Science with impact factors of 6.302 (Scripta) and 9.209 (Acta), status as of February 2023. The journals cover research topics on all aspects of the structure and properties of materials.







#### International Award for Tanja Lube

Tanja Lube, assistant professor at the Chair of Structural and Functional Ceramics, was awarded the "Fellowship" of the European Ceramic Society during the XVIII Conference and Exhibition of the European Ceramic Society. This biennial international event took place in Lyon (France) from July 2 - 6, 2023. The elevation to the grade of Fellow is a result of her exceptional contributions to the field of ceramic sciences. Her accomplishments include significant scholarly work in ceramic science and technology, remarkable achievements together with the ceramic industry, and outstanding service to the Society.

Tanja Lube has been actively engaged in ceramic research and teaching since the establishment of the Institut für Struktur- und Funktionskeramik at Montanuniversität Leoben in 1991. Furthermore, she holds a position as a board member of the Austrian Ceramic Society (AuCerS).





#### Presentation of the Award of Excellence 2023

On December 7, 2023, the Award of Excellence 2023 was presented to Michael Musi in the

Aula der Wissenschaften in Vienna by the Federal Minister of Education, Science, and Research, Martin Polaschek. This prestigious national award, funded through study support resources, has been acknowledging the top 40 dissertations of the past academic year since 2008. Nominations are submitted by individual universities and cover a broad range of topics. Under the guidance of Helmut Clemens, Michael Musi's dissertation focused on phase transformations in intermetallic titanium aluminide alloys for aviation.



# Participation at the Nanomat Conference in Warschau and Poster prize to Daniela Neumüller

Today, the focus on climate and responsible research is emerging as an ultimate global goal that will shape the future of our civilisation. The role of nanomaterials in the production of new, greener energy, including the long-term potential hazards of their use, was addressed by renowned researchers at the International Conference on Functional Nanomaterials and Nanodevices-Nanomat, held in Warsaw, Poland, from August 27 - 30, 2023. In such a setting, the understanding and pioneering role of the Montanuniversität Leoben through the Strategic Core Research Area, SCoRe A+ Hydrogen and Carbon, in meeting these global challenges gained international visibility and attention. Under the supervision of Jürgen Eckert, Chair of Materials Physics and ESI, and the active support of Lidija Rafailovic and Christoph Gammer, our young PhD students played an active role in the Nanomat conference. Adam Elbataioui, MSc, gave a talk on the importance of fundamental aspects for the preparation of free-standing electrodes for electrochemical  $CO_2$  reduction. Daniela Neumüller presented novel and exciting results on correlative characterisation methods to identify changes in the electrocatalyst during hydrogen evolution and was awarded 2<sup>nd</sup> prize by the jury.



### Josef Krainer Würdigungspreis 2023 for Nina Schalk

In memory of the work of former Styrian Governor Josef Krainer, the Steirische Gedenkwerk annually awards the Josef Krainer Würdigungspreis (appreciation prize) in recognition of outstanding achievements by young scientist, which are assessed by independent domestic and foreign experts. At this year's awards ceremony, on 20 March 2023 in the auditorium of the Old University in Graz, Nina Schalk was awarded the prize for her habilitation thesis in the field of materials science.



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#### Nina Schalk elected to the Executive Committee of the Advanced Surface Engineering Division of the American Vacuum Society

Nina Schalk has been elected to serve on the Executive Committee of the Advanced Surface Engineering Division (ASED) of the American Vacuum Society (AVS). The ASED provides a continuing forum for fostering the understanding of advanced surface engineering technologies. ASED brings together scientists and technologists from academia and industry, thereby merging research with application and promoting coating integration in materials design and engineering. ASED organizes and supports conferences, symposia and workshops, to promote discussion of basic aspects of surface's science, technology and engineering. Nina Schalk's election to the Executive Committee is a testament to her dedication and expertise in advanced surface science and engineering.



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#### Nina Schalk wins CDG Award 2023

The CDG Award for Research and Innovation is awarded to scientist who have been particularly successful in implementing the funding model of the Christian Doppler Gesellschaft in their CD Laboratories. Based on their outstanding findings in application-oriented fundamental research, award winners must have contributed to strengthening the innovative power and competitiveness of their company partners. Nina Schalk, head of the Christian Doppler Laboratory for Advanced Coated Cutting Tools, together with the company partner CERATIZIT Austria GmbH, succeeded in convincing the reviewers and was awarded the prestigious trophy. The award ceremony took place on 20 September 2023 at the Parkhotel Schönbrunn in Vienna.



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**Materials** Science



# 1<sup>st</sup> place in the poster competition at the Annual Conference of the German Ceramic Society (DKG)

Maximilian Staudacher from the Chair of Structural and Functional Ceramics achieved the 1<sup>st</sup> prize in the poster competition at the 98<sup>th</sup> Annual Conference of the German Ceramic Society, held from March 27 - 30, 2023, in Jena. On his poster titled "The B3B Strength Test," he presented new results on an important strength testing method for ceramic samples so effectively that the expert jury awarded his contribution the 1<sup>st</sup> prize out of 36 submissions. Mr. Staudacher is working on his dissertation as part of the "CharAM" project funded by the FFG. In this context, he explores strength testing methods for additively manufactured ceramic samples or those with exceptional geometries.



#### WKO Research Scholarship awarded to Sebastian Teusl from the Chair of Physical Metallurgy

The WKO Styria Research Scholarships have been awarded since the academic year 2013/14. In 2023, 22 works were selected for the scholarship from over 100 submissions. Among them is the master thesis of Sebastian Teusl, which deals with the influence of different heat treatments on the microstructure and mechanical properties of a PH 13-8 Mo maraging steel. The work was carried out at the Chair of Physical Metallurgy of the Department of Materials Science in cooperation with the company voestalpine Böhler Edelstahl. The scholarships were awarded on July 11 during a ceremony hosted by the WKO Styria in Graz.





#### Scholarship from the Hans List Fund

Helene Waldl was awarded a scholarship from the Hans List Fund for her dissertation entitled "Development of TiAlN based hard coatings by applying advanced characterization methods". The dissertation was written within the framework of the Christian Doppler Laboratory for Advanced Coated Cutting Tools at the Chair of Functional Materials and Materials Systems under the supervision of Nina Schalk. In her thesis, Helene WaldI focused on the synthesis, characterization and optimization of protective hard coatings for metal cutting applications. Advanced and high resolution characterization methods, such as micromechanical bending tests or atom probe tomography were used to gain a fundamental understanding of the structure-property relationship of the coatings. The award ceremony took place on October 16, 2023 at the AVL List GmbH in Graz.





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## 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	52	3	39
Chair of Physical Metallurgy	60	11	33
Chair of Materials Physics	42,8	9	50
Chair of Structural and Functional Ceramics	49	6	0

## Exams

Chair	Number of exams
Chair of Functional Materials and Materials Systems	595
Chair of Physical Metallurgy	629
Chair of Materials Physics	387
Chair of Structural and Functional Ceramics	310



# Cooperations



# Cooperations



# Forecast

## OUTLOOK

On a global scale, the past year has once again been characterized by worrisome and challenging developments, to say the least. While the conflict in Ukraine was at the forefront of our concerns, another deadly conflict erupted in Israel and Palestine. Additionally, record-breaking temperatures were reported at the poles, and 2023 has earned the unfortunate distinction of being the hottest year on record. The question remains: Is there still hope, or are we approaching a dystopian future? During the UN World Climate Conference COP 28, there was, at the very least, a global consensus to undertake efforts to reduce fossil fuels and cap global warming at well below 2°. The ambitious goal is to achieve a carbon dioxide-neutral planet by 2050. This commitment has been made, and now it is our task to develop the necessary technical solutions to ensure its success.

The Department Materials Science finds itself in a unique position to contribute a significant impact on these pressing global challenges. But to be successful in this attempt, we must attract the best minds and brightest students from around the world. Our new rectorate has been in place only since last October, but jointly we are committed to intensifying our efforts to increase student enrollment. In terms of educational opportunities, we eagerly look forward designing the Master phase of the new Materials Science and Technology study and providing our students with unique offerings from the European University EURECA-PRO. We anticipate welcoming even more international students through the innovative European School of Materials.

In our diverse spectrum of research activities, we will persist in developing responsible materials and processes that contribute to a carbon dioxide-neutral and energy-efficient future. Addressing significant challenges requires critical mass, and global impact necessitates collaborative efforts. To this end, we are excited about the upcoming launch of the Hydrogen and Carbon Center, as well as the establishment of a new Center of Excellence: Materials in the coming year. Pioneering research at an international level demands both, brilliant minds and state-of-the-art equipment and infrastructure, respectively. Whether in experiments, modeling, simulation, or data science, we eagerly await the completion of the Digital Science Center and the full operation of the high-performance computing cluster. Furthermore, we are thrilled regarding the arrival of advanced instrumentation, including for example a cryo-SIMS-FIB-TEM system for hydrogen and battery research, an advanced X-ray diffractometer, and new universal testing machines, among other significant investments.

As we have emphasized in previous years, we firmly believe that navigating the demanding and uncertain global landscape requires collaborative efforts. We are committed to contributing by providing diverse higher education in materials science, instilling a global perspective in our students, and offering high-level multidisciplinary research competences to our industry partners. This positions us at the international forefront to deliver substantial contributions to the societal needs of our times and future generations.

We eagerly anticipate a successful collaboration in the year 2024!

### Imprint

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