Materials Science

4th Materials Science Colloquium in Lech

(69. Metallkunde-Kolloquium)

07. – 10. April 2025

MONTAN UNIVERSITÄT LEOBEN

List of participants & Abstracts

Department Materials Science

Montanuniversität Leoben

4th Materials Science Colloquium

(69. Metallkunde-Kolloquium)

Lech am Arlberg

07. - 10. April 2025

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in alphabetical order

applications until 21. March 2025

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Unraveling the Structure-Property Relationship of innovative Materials using Advanced Electron Microscopy

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As materials scientists, we have the mission to contribute to a sustainable future by developing materials for green technologies. Using Transmission Electron Microscopy (TEM), we can analyze the interplay between microstructure and the functional properties of innovative materials at the atomic scale, which helps improve the performance of next-generation devices. In combination with advanced techniques, insights into application-relevant mechanisms can be obtained. Spectroscopy methods, such as Electron Energy Loss Spectroscopy (EELS), are used to characterize the local composition, while nanobeam diffraction (4DSTEM) enables the local resolution of microstructures. By employing *in situ* techniques, such as heating and mechanical straining, the changing microstructure under external stimuli can be observed. This provides insights into dynamic processes and allows for tuning the microstructure through a direct feedback loop.

In this talk, the (i) impact of short-range ordering (SRO) on electronic properties of semiconductors for green computing, (ii) the loading process within state-of the art battery materials, and the (iii) effect of microstructural changes within thin film on their ability to generate green hydrogen will be presented.

In-situ STEM investigation of primary phase formation of high Fe-content Al alloys

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Recycling of Al alloys is gaining evermore importance with the increasing use of Al alloys as structural alloys in the automotive industry, accelerated also by the rise of electric vehicles. Fe is one of the main contamination elements introduced by increased recycling rates, it is critical for ductility limiting primary phases and is therefore often strictly limited by alloy limits. Nowadays transmission electron microscopes are capable of a broad range of in-situ experiment capabilities also including possibilities for investigation of solidification. In our in-situ scanning transmission electron microscope experiments we utilize a simple but time-efficient sample preparation for specimens determined for melting and solidification on a MEMS-based chip heating system. In this presentation we demonstrate that slow-cooling experiments are possible, present results, analysis options of formed phase and the in-situ observation of primary phase formation in a high-Fe, Al-Fe-Si alloy. Furthermore, we will discuss challenges particularly present for slow-cooling experiments.

Making steels greener: challenges for structure and properties

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This talk will provide a physical metallurgy perspective on the challenges posed by the growing use of scrap in steelmaking. The focus of this brief review will be on tramp elements and their impact on phase transformation kinetics, microstructure evolution, and resulting material properties, in particular, addressing the following questions:

- Which elements are trapped in a scrap-based steel?
- What can go wrong in terms of structure and properties of a final product?
- Why even “good” elements such as Cr, Mo, Ni might cause problems?

Multiple effects of tramp elements are demonstrated through illustrative examples, including phase transition temperature shift, delayed phase transformations and recrystallization, grain refinement, grain boundary segregation, precipitation, strengthening, loss of ductility, as well as reduction of fracture toughness. Finally, potential strategies for effective management of tramp elements to ensure both sustainability and material performance are discussed.

The Future of Sustainable Materials in Energy Production

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One of the leading research efforts in materials science and engineering today is the simultaneous improvement of known and sustainable materials and the exploration of new alternative material options for sustainable applications in demanding environments for the energy sector. A unique combination of corrosion resistance, toughness, strength, machinability and wear resistance is required in materials used in energy sector applications. In the last 5 years, a new process called cryogenic processing (CP), a sustainable and green technology, has emerged as an additional step in the heat treatment of various ferrous and non-ferrous alloys to improve aforementioned properties. CP involves subjecting materials to temperatures below 0 °C. There are 3 known cryogenic processing types: conventional (-0 °C to -80 °C), shallow (-80 °C to -150 °C) and deep (below -150 °C). For cryogenic applications, liquid nitrogen is usually used. CP, through the main mechanisms of enhanced austenite transformation into martensite and increased carbide precipitation, fundamentally changes the material properties (hardness, toughness, strength, ductility, corrosion and wear resistance, etc.). CP advances microstructure by retransforming ART's reverted austenite into tertiary α-martensite, ε-martensite and carbides. This unique phenomenon is called the cryogenic austenite retransformation (CAR) effect, which provides an alternative transformation route that results in a new set of properties for the same alloy system. Within our comparative study we are discovering new ways to achieve the optimised microstructure, improved residual stress state, surface and corrosive resistance, magnetic properties of selected ferrous alloys (EUROFER97 and AISI 431) in combination with deep CP as a response to the increasing demand for material improvement in the energy sector (including fusion).

Deformation-Precipitation Interactions in Sustainable Aluminum Alloys

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Aluminum alloys are critical for reducing emissions in industries like aviation, owing to their low density and energy efficiency. However, challenges such as the energy-intensive production process and the reliance on primary materials highlight the need for sustainable innovations. Recent developments in crossover alloys, such as CrossAlloy.57 and CrossAlloy.68, have shown that combining elements from different alloy series can optimize mechanical properties and recyclability. CrossAlloy.68 demonstrates that primary phases, previously considered detrimental, can enhance strength and performance under specific conditions, suggesting new avenues for alloy design.

Despite these advances, managing tramp elements like iron remains a challenge due to their negative effects on processability and material properties. The presence of dispersoids also presents difficulties, often limiting formability and mechanical performance. A deeper understanding of how microstructural constituents, deformation and precipitation interact is essential for overcoming these obstacles and developing robust, composition-tolerant alloys.

The study of deformation-precipitation interactions aims to advance the fundamental understanding of how microstructural features influence alloy behavior using advanced material characterization techniques. This will support the development of aluminum alloys that not only meet the high performance and sustainability requirements for structural applications but also extend to broader material research, with a focus on sustainable design for next-generation materials, including anode materials for energy storage.

Current developments and process strategies for sustainable steelmaking

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A drastic reduction of CO_2 emissions in steelmaking requires new or adapted processing routes for primary and secondary raw materials. The precondition is maintaining the quality of the final steel product that is demanded. The paper overviews current research approaches and challenges related to sustainable steelmaking. Different process examples, including their technology readiness levels, will be discussed. Production routes based on iron ore as the primary raw material and the related role of hydrogen in the reduction step will be addressed. Fluidized bed technologies to produce Direct Reduced Iron (DRI) will be highlighted and the influence of varying iron ore quality on the further processing of DRI in different aggregates will be explained. Moreover, the concept of hydrogen plasma smelting reduction, comprising highly reactive excited hydrogen species with a substantially higher reduction potential than molecular hydrogen, offers significant potential for industrial decarbonization. The effects of varying hydrogen and feed material introduction points, alongside the use of oxidic alloying elements, will be discussed. Another important aspect is the increased scrap rate in terms of circularity. The resulting higher levels of trace elements are hardly removable from the liquid steel. They can negatively influence material properties and reactions in the steel-slag-refractory system in secondary metallurgy. Finally, the potential consequences of new production technologies on further processing and the usage of by-products will be shown.

Towards safer batteries – Characterization of Li-ion batteries for simulation purposes

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In recent years, the safety of lithium-ion batteries (LIBs) has become an increasingly important issue, not only due to their growing usage, but also because of their larger capacities, such as those used in electric vehicles (EVs). Addition

ally, the lifespan of LIBs in electric vehicles is still a relatively new topic, both in the used car market and among manufacturers aiming to improve cell longevity. A comprehensive understanding of how LIBs behave under thermo-mechanical stress is therefore crucial to predict catastrophic failure, such as thermal runaway, as well as the behaviour of aged cells.

Our project aims to develop an advanced model to predict the behaviour of LIBs under mechanical loads, such as those experienced during accidents. However, even the most advanced modelling tools are only as effective as the quality of their input parameters, making accurate and repeatable measurements of the mechanical properties of electrode materials essential. For conventional LIBs, the mechanical characterization of electrode materials is still in development, primarily due to the sensitivity of the materials used, such as foils, as well as the variety of used material combinations and cell chemistries.

Therefore, the first step involves the development of safe methods for opening single cells, followed by a gentle and repeatable process for cleaning and sample preparation. Once this foundation is established, the individual electrode elements will be characterized in regards of their composition, as well as their mechanical and thermal properties. These properties will then be used to aid the development of the mentioned simulation models.

Sustainable solid oxide cell air electrodes: complexity versus simplicity

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Electrochemical solid oxide cells (SOCs) are promising future technologies for sustainable and efficient energy conversion and storage. Solid oxide fuel cells convert the chemical energy of a fuel into electrical energy with high efficiency, while solid oxide electrolyser cells store electrical energy from fluctuating renewable sources in a chemical energy carrier such as H_2 or syngas. In line with the UN's Sustainable Development Goals, the most important challenges are improving the performance and long-term stability of the cells. State-of-the-art SOC air electrodes like (La,Sr)(Co,Fe)O_3 contain cobalt, which increases the electronic conductivity and enhances the oxygen exchange kinetics, as well as strontium and lanthanum, all of which are on the list of critical materials that should be avoided.

In our research, we follow two complementary strategies to develop sustainable air electrodes for the next generation of SOCs: (i) "complex" high-entropy perovskites containing 6 different cations, excluding Co, (ii) "simple" brownmillerite-type calcium ferrates containing 2-3 different cations, excluding Co, Sr and rare earth elements. The present talk provides a discussion of the difficulties associated with these two approaches and presents strategies to mitigate drawbacks such as limited electronic conductivity and insufficient current collection. Results obtained on the material level, as well as electrochemical tests on symmetrical and full cells are presented. Promising first results show that it is indeed possible – by careful studies of the fundamental mass and charge transport properties, as well as adaptations in the cell design – to develop air electrodes based on sustainable raw materials with high performance and good long-term stability.

Stabilizing Cu nanoparticle films via atomic layer deposition for CO_2 reduction: Enabling Sputtering-Based Synthesis of Novel Catalyst Materials

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Metallic nanoparticles (NPs) exhibit intriguing properties as a consequence of their spatial confinement and their high surface-to-volume ratio. A topic rising in importance is the utilization of NPs as catalysts for energy conversion and storage. To facilitate more advanced use of NPs, a thorough understanding of their synthesis-structure-property relations is crucial. In this study, porous 300 nm thick Cu nanoparticle films (particle diameter 10 nm) are fabricated via hollow cathode sputtering and subsequently coated with an amorphous Al_2O_3 layer (0-20nm) via atomic layer deposition (ALD). Top-view scanning electron and cross-sectional transmission electron microscopy analyses confirm conformal ALD coverage of the porous structures. Thermal annealing with in-situ X-ray diffraction is used to study particle mobility (RT-800°C) as a function of oxide thickness. Nanoparticle films without ALD undergo densification and dewetting, while particle mobility is significantly reduced with the protective ALD coating. These results are crucial for and in good agreement with their catalytic performance peaking at an oxide layer thickness of 2-5 nm, with a minimal tradeoff between stability and catalytic activity/selectivity of Cu. Our findings should facilitate the deposition of NP-based films with higher efficiency and tailored morphology, making this technique more attractive for e.g. the synthesis of thin film catalysts for various applications.

Rare-earth free magnetic material by combining severe plastic deformation and thermomagnetic processing

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Many magnetic materials rely on rare-earth (RE) or other critical elements. The global supply chain for these materials depends on a few countries, posing risks related to supply disruptions, geopolitical tensions, and price volatility. There are several strategies to reduce the dependency on REs: recycle materials containing REs, reduce the content of REs, seek for a novel ultra-high-performance material and broaden the diversity with new materials without REs bridging the magnetic properties' gap between the strong RE based magnets and the weaker hard ferrites. This talk will cover the last strategy using RE free MnBi magnets as an example. The α-MnBi phase possesses unique magnetic properties as function of temperature, which makes this material suitable for high-temperature environment applications. Direct fabrication of the α-MnBi phase with classical metallurgical methods is only possible to a limited extent. For processing, we combine severe plastic deformation with thermal treatment and a magnetic field increasing the final α-MnBi phase content up to 76 vol%. In-situ X-ray diffraction experiments with and without augmenting magnetic field were further performed to study the influence of the magnetic field on the evolution of the α-MnBi phase in detail.

This research was funded in part by the Austrian Science Fund (FWF) 10.55776/TAI4821824. We acknowledge DESY (Hamburg, Germany), a member of the Helmholtz Association HGF, for the provision of experimental facilities. Parts of this research were carried out at PETRA III and we would like to thank M. Blankenburg for assistance in using P21.2. Beamtime was allocated for proposal I-20220454 EC.

Transparent Ceramic Materials for Advanced and Multifunctional Optical and Photonic Applications

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Transparent ceramics are highly promising materials, offering properties that often surpass those of single-crystal and amorphous materials. These advantages make them ideal for a broad range of applications in optics and photonics, including lasers, scintillators, armor protection, and optoelectronic devices. To develop high-quality transparent ceramics for such applications, it is crucial to investigate the fundamental scientific aspects of their synthesis and processing. Achieving the desired transparency and microstructural characteristics requires a deep understanding of the mechanisms governing optical scattering and chemical defect behavior. The primary scientific objective is to minimize material defects that contribute to light absorption and scattering, thereby enhancing optical performance. Processing transparent optical materials with anisotropic crystal structures presents additional challenges due to the inherent optical anisotropy in polycrystalline materials. Research efforts focus on understanding how different processing techniques influence birefringence behavior in transparent photonic ceramics.

Sustainable metal production via hydrogen- and ammonia-based direct reduction of metal oxides

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Fossil-free metal production is critical for reducing the substantial CO_2 emissions from the metal industry, which accounts for approximately 10% of global emissions and is a major contributor to climate change. Hydrogen-based direct reduction of metal oxides, including the use of hydrogen carriers such as ammonia, represents one of the most promising strategies for mitigating these emissions. In this study, we investigate the reduction behavior of metal oxides (e.g., iron oxide and mixtures of iron and nickel oxides) using hydrogen [1-3] and ammonia [4,5], with a particular focus on the spatial and temporal evolution of the microstructure during the multistep solid-gas reaction. Advanced characterization techniques were employed to analyze phase transformations, porosity, and local chemistry throughout the reduction process. The fundamental reaction mechanisms are discussed, providing new insights into the sustainable production of metals and alloys via hydrogen- and ammonia-based direct reduction, ultimately enabling a pathway to metal production with minimal CO_2 footprint.

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Homogenization heat treatments of porous, intermetallic Ni_3Al fabricated by laser powder bed fusion and in-situ alloying

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Nickel is a common and well-researched catalyst material with a wide variety of industrial applications. Pure Ni, however, also comes with limitations such as catalyst poisoning and sintering at the elevated temperatures required for some catalytic processes such as H_2 production. Intermetallic Ni_3Al, by contrast, has been found to exhibit catalytic properties comparable to Ni, while being less prone to both poisoning and sintering. These circumstances motivated this work to investigate potential approaches to fabricating a porous Ni_3Al catalyst by additive manufacturing.

Additive manufacturing and in particular, laser powder bed fusion was used to obtain a large surface area as required to obtain good catalytic properties by utilizing the intrinsic possibilities of this method to produce complex, high-resolution structures, while the printing parameters were optimized for maximum bulk porosity. Furthermore, in order to keep the fabrication route economically competitive, so-called in-situ alloying was used to print the samples. In-situ alloying refers to the procedure of mixing two elemental powders mechanically and creating the alloy by laser-melting during the printing process.

In the case of a nominal chemical composition of 76 at.% Ni and 24 at.% Al, the printing parameters optimized for a porous structure were found to cause an inhomogeneous microstructure with pronounced local variations in the chemical composition. Although the powder particles were fully melted during the printing process, the melt solidified before complete mixing and equilibrium could not be reached. Using high-energy X-ray diffraction, the phases Ni(Al), Ni_3Al, NiAl, Al_3Ni_5, and Al_3Ni were detected in these as-printed samples. To homogenize the microstructure and increase the phase fraction of Ni_3Al, heat treatments have been conducted. The dissolution of the Al-rich phases with relatively low melting points has been investigated in the course of a step-wise heat treatment with isothermal segments at 600°C and 1000°C as well as a slow, but continuous heating experiment up to 1100°C. To obtain further information about the phase fractions and to trace the phase evolution in dependence on the printing parameters, in-situ heating experiments were conducted in a dilatometer setup at the Hereon-run beamline P07B at the Deutsches Elektronen-Synchrotron in Hamburg, Germany. The data collected through high-energy X-ray diffraction offer valuable insights into the effect of the various heat treatments on the as-printed samples and allow us to draw conclusions as to their final catalytic properties.

Insights from mechanical testing under electrochemical hydrogen charging to evaluate structural materials for future hydrogen applications

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Hydrogen is a key energy carrier in the transition to a sustainable future, making the structural integrity of materials in hydrogen infrastructure critical. Steel components must endure hydrogen-rich environments where hydrogen embrittlement poses a serious risk, necessitating advanced experimental methodologies to assess the complex interplay between mechanical loading and hydrogen-induced degradation. This presentation highlights the importance of mechanical testing—specifically tensile and fatigue tests—in evaluating steel performance under hydrogen exposure. The experiments were designed to validate the reliability of the testing setup and methodology. Ex-situ hydrogen-charged tensile tests on martensitic PH13-8Mo and austenitic AISI 303 steels confirmed significant reductions in ductility, and experiments were supplemented with scanning electron microscopy and thermal desorption spectroscopy investigations. Complementing these findings, fatigue tests using an integrated in-situ hydrogen charging setup further demonstrated hydrogen's detrimental effects under cyclic loading. Tests on the soft martensitic steel (X3CrNiMo13-4) showed that hydrogen pre-charged samples failed immediately, indicating direct hydrogen-induced failure, while in-situ charged samples exhibited reduced fatigue life. Fracture surface analysis revealed both, typical fatigue features and distinct hydrogen embrittlement characteristics, such as intergranular brittle fractures. In summary, mechanical testing under hydrogen exposure is crucial for developing safer and more resilient hydrogen infrastructure. Our department's advanced testing facilities enable systematic investigations into hydrogen-induced degradation, ensuring that materials used in hydrogen applications meet the rigorous demands of modern energy systems.

Turning The Tables – From microstructure-enhanced metal hydrides to metal hydrides for microstructure enhancement

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Severe plastic deformation (SPD) enables the preparation of advanced functional materials, particularly for emerging hydrogen-related applications. This includes hydrogen storage materials, such as FeTi or TiVZrNbHf, which promise superior storage capacities at low pressures and moderate temperatures.

By combining high-pressure torsion (HPT) with selective phase dissolution, we synthesized nanoporous FeTi from FeTi-Cu nanocomposites. Overcoming challenges in processing finally resulted in strategies to achieve uniform microstructures in mechanically demanding material pairings.[1,2] Subsequent selective removal of the Cu enabled the formation of well-defined mesoporous FeTi. However, this FeTi absorbed only low amounts of hydrogen, suggesting that an oxide layer confines the FeTi, thereby limiting the hydride formation associated with volume expansion.

It is well established that SPD can significantly impact the properties of metal hydrides. However, we reveal that the reverse is also true: *The presence or absence of hydrogen can drastically impact the microstructural evolution in the context of SPD*[3]. HPT was applied to the high-entropy alloy TiVZrNbHf and hydrogen pressure and heat treatment were subsequently applied during in-situ X-ray synchrotron diffraction. Interestingly substituting the HEA with its hydride suppressed grain growth during high temperature annealing and allowed for the formation of a nanocrystalline structure stable under cyclic hydrogen charging conditions.

In conclusion, by combining SPD with hydrogen loading we can harness hydrogen´s potential to tailor microstructural development, paving the way for advanced materials design that could leverage hydrogen-based metallurgy.

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Divorced eutectoid transformation (DET) in a low-alloy hypereutectoid steel and the influence of increased tramp and trace element contents on this transformation

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Current efforts to reduce CO_2 emissions in the iron and steel production through the increased use of scrap in electric arc furnaces can lead to higher contents of tramp and trace elements in steels. This can lead to a change in the steel properties, such as a delay of phase transitions to lower temperatures [1]. It can also have an influence on the divorced eutectoid transformation (DET), which is a non-cooperative eutectoid transformation in steel that can occur instead of or together with the pearlitic transformation. The resulting microstructure is composed of a ferritic matrix and spherical cementite particles (see left Figure below) [2].

In order to investigate the influence of various heat treatment parameters as well as of different tramp and trace element contents on DET, hardness measurements and AI-assisted image analysis [3] of high-resolution scanning electron micrographs (see right Figure below) were performed on a low-alloy hypereutectoid steel and variants thereof with increased tramp and trace element contents.

In the present study, it has been shown that a low undercooling or cooling rate after austenitization, as well as an austenitizing temperature closer to the A_1 temperature, favors DET. These investigations show that there are indications that an increased content of tramp and trace elements can have a favorable effect on DET.

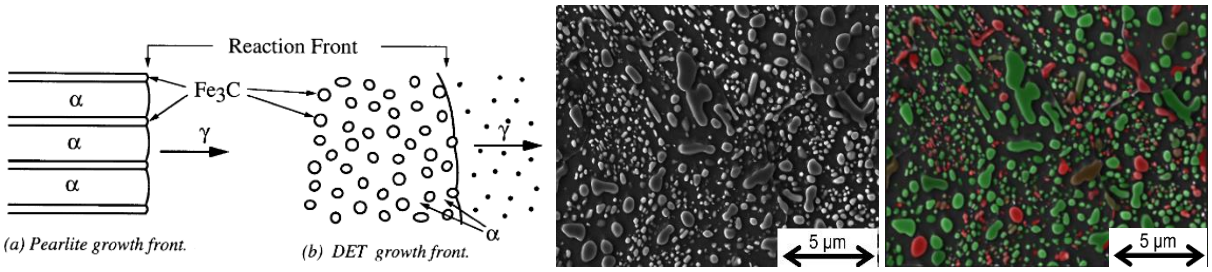

Figure: Left: Schematic representation of the different eutectoid transformation forms in steel [3]. **Center:** SEM image of a fully spheroidized microstructure after DET. **Right:** AI-assisted evaluation of particle size and aspect ratio distribution.

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Influence of atmosphere changes in reheating furnaces on scale formation and decarburization of low-alloyed steels

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One aspect of the recent transformation of the steel industry is the replacement of natural gas used in combustion furnaces by green energy sources. Hydrogen was found to be a candidate which can contribute to the decarbonization of steel production. Replacement of natural gas by hydrogen in reheating furnaces will lead to changes in the furnace atmosphere which could influence the high-temperature oxidation of the reheated products. Additionally, the use of higher amounts of scrap in steel mills will lead to increased contents of tramp elements which could form low-melting constituents on the steel surface during scale formation. Currently, investigations in cooperation with scientific partners are ongoing to identify changes in scale formation and/or decarburization depending on both described influences. Steel samples were heat treated in a directly heated laboratory-scale furnace to compare hydrogen combustion with natural gas combustion. The results of this study will be presented and put in perspective with regards to the current transformation pathway.

Microstructural-based mitigation strategies to improve the mechanical performance in the presence of hydrogen

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This work focusses on the development of better performing materials in contact with hydrogen from a microstructural viewpoint. Generic concepts of alloy design in terms of modifications in chemical composition, applied thermal treatments, processing strategy, nano-sized precipitate addition, grain boundary engineering and the use of pearlite or retained austenite are introduced with a particular focus on their hydrogen trapping ability and potential beneficial effect on the hydrogen embrittlement resistance. Thermal desorption spectroscopy, hydrogen permeation testing under simultaneous mechanical load, local hydrogen characterization and in-situ mechanical testing combined with post-mortem advanced microstructural characterization is done for this purpose. The different alloy design concepts are applied on several industrial case examples where the microstructural-based mitigation strategy demonstrated to improve the mechanical performance of steel alloys, based on their hydrogen trapping ability.

The use of recyclates in plastics pipes: Possibilities and Limits

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Engineering structures, such as operating plastic pipes, are often submitted to unexpected influences that may shorten their lifetime. An increasing understanding of processes that govern these sudden failures has been attained in the last decades. This has led to a remarkable improvement of pipe performances by enhancing the material's slow crack growth (SCG) resistance (e.g. from PE63 to PE100RC). Still, a great deal of uncertainty is associated with the use of non virgin grades. This is mainly, because of the unknown effects of impurities that are found in recycled materials. The effects on lifetime relevant properties concerning impurities can be divided into three categories:

i. polymeric contaminants of a different kind (e.g. PE in PP)

ii. polymeric contaminants of the same kind (e.g. PE LD in PE HD, PP-R in PP-H)

iii. non polymeric contaminants (e.g. inorganic particles)

In that context, the effects of polymeric as well as non polymeric impurities were studied by mixing virgin polypropylene (v PP) grades with actual polypropylene recyclates (r PP) into different compositions (v PP/r PP in %: 100/0, 90/10, 75/25, 50/50 and 0/100). Subsequently, these materials were tested via internal pressure pipe tests. A profound dependency of impurity content on final failure time (tf) could be demonstrated, thereby. Additionally, a deeper analysis of fractured pipe samples revealed a clear correlation between the maximum size of incorporated inorganic impurities and tf. This indicates, that two seemingly identical pipe samples, with regard to the content of recycled material, can still have vastly different resulting failure times, based on the size of the introduced critical contaminant. Results show, that it is not only necessary to understand the influence of the content and distribution of recyclates on the resulting lifetime of pipes, but more importantly the maximum introduced defect size as well. Consequentially, pipe manufacturers should choose recycled grades carefully, and only after knowing about the feedstock of origin, treatment- and mechanical sorting history.

Sustainable iron aluminide-based laser claddings

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Approximately 3% of the world's total energy consumption (~16 EJ) is used to remanufacture worn parts, highlighting a significant potential for emission reduction—a crucial factor in combating climate change. To achieve this, alternative wear-resistant materials must be developed that minimize environmental impact and eliminate critical raw materials like Co, Cr, and Ni, which are commonly used for high-temperature wear protection but have a high ecological footprint. This study explores sustainable iron aluminide-based alternatives that align with four key strategies for reducing a material's carbon footprint: (i) lightweight design, (ii) improved production efficiency, (iii) extended service life, and (iv) enhanced recyclability.

Iron aluminides offer a significantly lower CO_2 footprint (~8.4 t CO_2eq/t) compared to high-Cr cast steels (~13.8 t CO_2eq/t), Ni-based alloys (~20–22 t CO_2eq/t), and Co-based alloys (~31–39 t CO_2eq/t). Their low density supports weight reduction, while laser metal deposition enables localized surface functionalization. To enhance wear resistance, Fe_3Al matrices were strengthened using different strategies: (i) Si, C, and Ti+B additions provided stable hardness up to 600 °C, with a self-protective mechanically mixed layer forming at higher temperatures, resulting in low wear rates (0.01–0.05 mm^3/m at 700 °C); (ii) precipitation hardening with borides and carbides increased hardness to ~800 HV10, ensuring wear resistance up to 700 °C (0.03–0.05 mm^3/m wear rates); and (iii) reinforcement with up to 70 vol.% recycled hardmetal scrap and sustainable TiC cermets yielded 1100 HV10 hardness at RT, maintaining a stable plateau up to 700 °C with excellent wear rates (0.04–0.05 mm^3/m).

In summary, all developed Fe_3Al-based claddings match or surpass the performance of conventional high-temperature wear protection solutions while reducing environmental impact by over 60% (GWP100) compared to Co-based alternatives.

Development of Coating-Substrate Combinations for Sustainable Ceramic Data Storage Media

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Nowadays, data storage and its sustainability are topics of great importance, not only for cloud providers but also for other companies and even for people in their personal lives. Most of the data stored is referred to as cold data, meaning it is very rarely changed and accessed e.g., photos, research results. That cold data is currently stored by running server farms utilizing hard drive discs (HDD). These server farms need a lot of energy and provide limited capacity, making them very insufficient as the demand of storage capacity is increasing. To overcome the issue of the high amount of required energy and limited capacity, a new form of storage media is in the focus of our research. By utilizing a certain coating-substrate combination, it is possible to literally write data into ceramic layers by a femtosecond laser. Using this method, it is possible to write a large amount of data onto a relatively small area. Within our research we analyzed different coating-substrate combinations regarding their mechanical properties and laser ablation characteristics. The coatings investigated were synthesized by magnetron sputtering using different composite targets e.g., Cr, CrB_2, AlCr on various substrates including sapphire, silicon, glass, and austenitic steel. All the coatings were investigated by XRD showing a single-phase structures and hardness values ranging from 21 to 33 GPa. Additionally, laser ablation tests were conducted to determine the laser-ablation threshold and to find suitable coating-substrate combinations. Furthermore, after writing data into the samples, the samples were tested regarding their thermal stability, oxidation and corrosion resistance. These studies prove the exceptional stability and durability of such ceramic data storage media. Once written, storing the data does require almost no energy and allows to save up to 99 % of the currently used energy for data storage.

Computational design of hydrogen embrittlement resistant alloys

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The global transition towards extensive use of renewable energy sources, such as hydrogen and hydrogen-bearing fuels, introduces new safety requirements and calls for innovative material solutions for both emerging and existing energy sectors. A possible way towards these solutions is offered by modern multiscale computational methods and approaches that allow one to significantly accelerate material development and to mitigate potential material-related safety risks already at an early stage of a material development cycle.

In this overview, we present computational approaches that have been successfully applied in the past to propose various mitigation strategies for hydrogen embrittlement in high-strength steels and Ni-base alloys. Additionally, we introduce new methods developed at our center, applied to investigate this phenomenon under various conditions. Our approach spans multiple length and time scales, from quantum mechanical density functional theory calculations at the atomic scale to continuum meso and macro scales represented by phenomenological thermodynamic and kinetic models, as well as by the finite element method. These methods enable us to study and predict the evolution of hydrogen-material interactions as a function of material composition, microstructure, time, temperature, and mechanical load.

Green steel from red mud: Turning industrial waste into sustainable metal with hydrogen plasma-based smelting reduction

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Aluminum is the forefront metal for lightweight design of transport vehicles and civil engineering structures. For its primary production, bauxite ore needs to be refined through the Bayer process to produce alumina, during which waste, called bauxite residue or red mud, is formed. Due to the large scale of alumina production, red mud production is massive, amounting to about 180 million tons per year that is mostly disposed into large ponds. It has amassed to one of the largest environmentally hazardous waste (due to high alkalinity and presence of heavy metals) on the planet (cumulatively 4 billion tons). However, red mud can be rich in iron oxide, even up to 60 wt.%, making red mud a potential source for production of iron and other materials, if properly processed and neutralized. Here we demonstrate how red mud can be processed with hydrogen plasma-based smelting reduction (HPSR) to produce sustainable iron in a fossil-free manner. The process enables simultaneously reducing the amount of red mud deposited on the planet and on the other it mitigates part of the steel-related CO_2 emissions. HPSR proceeds through rapid liquid-state reduction that simultaneously allows reduction of the iron oxides and chemical partitioning of the oxide melt into individual inert oxides and formation of high-grade iron in a form of macroscopic spheres. Additionally, the HPSR processing of red mud also neutralizes the pH of the residual portion of the unreduced red mud, enabling direct utilization of the residual oxide material for construction purposes. A techno-economical and life-cycle assessment is also performed with which the feasibility and long-time impact of the process on the environment is explored in relation to the different iron content within red mud.

Contact damage of silicon nitride bearing balls - how to characterise the material?

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Ceramic bearing balls are essential components for electro-mechanical systems that require electrical insulation, like bearings in modern wind turbines. Silicon nitride is favored for this application due to its high hardness, stiffness, and strength combined with low density. However, premature failure of ceramic bearing balls may occur due to crack initiation and propagation under contact stresses. Therefore, assessment of relevant mechanical strength properties is essential.

Generally, the tensile strength of ceramics can be understood within the framework of linear elastic fracture mechanics. The scatter of strength arises from a size distribution of fracture origins and is conventionally described by Weibull statistics. This encompasses a size effect on strength. A standardised tensile strength test for balls is the “notched ball test”.

Hertzian contact tests are well-suited for assessing the loads required to initiate contact cracks – typically ring cracks. These tests involve pressing two ceramic balls together with increasing load until cracks are formed. The critical load corresponds to a contact stress field, where the maximum tensile stress amplitude defines the contact stress, occurring immediately outside of the compression zone. An attempt was made to predict the contact strength distribution on the basis of notched ball test results using Weibullian size extrapolation, but this attempt was unsuccessful. Experiments showed that predictions significantly underestimate empirical strength data, which exhibit greater strength and much lower scatter than anticipated. The reasons for this discrepancy remain unclear, but possible explanations will be discussed.

Characterization of dislocations in SiC single crystals

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Silicon carbide (SiC) is a wide band-gap semiconductor that has gained popularity in various industries due to its unique properties, including higher voltage handling capacity and lower switching losses compared to Silicon. This makes SiC an ideal candidate for use in high-performance power devices, which could play a significant role in energy efficiency, reduced power consumption, and lower carbon emissions [1, 2]. A key to utilize this high performance is a low density of dislocations and micropipes (MP) in manufactured single crystals. MPs are a special hollow form of threading screw dislocations and are considered to be “killer defects” in SiC devices [2].

In this talk, we present molecular static simulations of dislocations and MPs as well as defect densities obtained from KOH etching. The atomistic simulations calculate explicitly the strain energy of the dislocation that, when exceeding a critical value, makes it energetically more favorable to remove the dislocation core according to the effect predicted by Frank [3]. We obtain smaller radii than experimentally observed, showing that this effect cannot be explained by an energy balance alone. A common way to visualize dislocations on the surface of SiC single crystals for subsequent characterization is defect-selective etching using molten KOH [4, 5]. To detect and characterize these etch pits, we employed a Mask R-CNN, a region-based convolutional neural network, which produces superior results compared to previously used threshold-based methods. This way, etch pit density maps on a whole-wafer scale can be produced. Further, we used the generated segmentation masks of the BPD-type etch pits to characterize the extent of prismatic slip on the investigated substrate.

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Machine learning of multi-physics simulations of SiC single crystal growth

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Silicon carbide (SiC) is a wide-bandgap semiconductor with exceptional chemical and physical properties that surpass silicon (Si) in several key characteristics for electronic applications. Its high thermal conductivity, high break-down electrical field strength and high electron saturation velocity enable its use in applications involving high temperatures, high voltages and fast switching speeds, all while maintaining minimal energy losses. These attributes position SiC as a highly promising material for the next generation of high-power electronic devices, playing a key role in advancing large-scale, sustainable energy generation in the future.

Nowadays, machine learning (ML) algorithms have shown to be highly practical and effective in many research fields, including the statistical analysis of expensive computer simulations. They have proven to be able to serve as low-fidelity surrogates, approximating the simulation with satisfactory accuracy while being orders of magnitude faster and computationally inexpensive.

We demonstrate the effectiveness of ML surrogates on the basis of multi-physics finite element method (FEM)-based physical vapor transport (PVT) simulation for SiC single crystal growth. Our approach focuses on the computational and time efficient creation of a ML model and its application for several downstream tasks. These tasks include sensitivity and uncertainty analysis as well as the calibration of the simulation to experimental data and the search for optimized growth conditions. The benefits and forthcoming opportunities of such approaches for materials development and facilities will be discussed.

Tracing Techniques to Determine the Origin of Non-Metallic Inclusions in Steel: An Overview

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The presence and characteristics of microscopic particles, known as non-metallic inclusions (NMIs), significantly influence the properties and quality of steel. Hence, it is critical for optimizing production processes and enhancing steel cleanness by understanding the origin, formation and modification of NMIs during steelmaking. The application of tracing techniques allows for tracking specific NMIs throughout the process and identifying their sources. Tracing methods can be divided into active and passive approaches, depending on whether an external tracer is required. The state-of-the-art method is an active tracing technique, where rare-earth elements (REEs) are directly added to the steel melt and mark NMIs by partial reduction. Due to the addition of REEs, the properties of the investigated NMIs are modified, leading to the necessity of the implementation of novel tracing approaches. Furthermore, two innovative techniques will be presented. The first one, the isotopic spiking, is also an active tracing approach, where one potential source for NMI formation is modified by enriched stable isotopes. This method allows a more detailed investigation of interactions in the steel/slag/refractory system. The second technique, that will be introduced is the REE-Fingerprint. By applying this passive approach, no additional tracer is required for the determination of the source of NMIs. Within this study, benefits, application fields and challenges of these three tracing methods will be discussed.

Designing materials for the hydrogen age: the need for nanoscale insights

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Decarbonation of society is necessitated by growing concerns about climate change, and motivates the search for clean and sustainable industrial processes and fuels. Hydrogen is a strong candidate to be a carbon-neutral energy vector for the future. Yet, from a materials standpoint, hydrogen is synonymous with challenges: first for material durability and sustainability in hydrogen-rich environments, and second for the green production of hydrogen. For both aspects there is a need for developing new materials, and to guide their design requires insights, on the finest scale, into how hydrogen distributes within the material or how the electrochemical reactions used for generating clean hydrogen modify the microstructure. Quantitative imaging of hydrogen at the nanoscale is not yet routinely achievable.

My research focuses first on developing the methodologies to probe hydrogen at the ultimate scale, based on the latest developments of cryogenic atom probe tomography in correlation with electron microscopy. I then apply these frontier techniques to model materials relevant to the hydrogen economy in the broader context. I aim to unveil mechanisms that limit their performance or operational lifetime to establish the feedback loop necessary to design new materials. In this overview presentation, I will draw examples from both high-strength steels, in which even trace amounts of hydrogen can cause severe and catastrophic degradation of the mechanical properties, and catalytically-active thin films to advance the understanding of the influence of microstructural defects and how to exploit them to boost the catalysts' performance and optimize their design.

By combining nanoscale characterization with microstructural control, my work provides insights into designing more efficient catalysts and hydrogen-resistant materials, contributing to the development of a sustainable hydrogen economy.

Impact of tramp elements on steel properties: Insights through microstructural and high-resolution characterization

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To reduce CO_2 emissions, the steel industry shifts its production route from classical blast furnaces towards recycling increasing amounts of steel scrap within the electric arc furnace. However, this practice introduces higher levels of tramp elements such as Ni, Cr, Mo, Cu, Sn, and Sb into the steel. Some of these, unless already present as alloying elements, can significantly alter the microstructure and mechanical properties. Sn and Sb are especially detrimental among these elements, as they tend to segregate to grain boundaries leading to intergranular embrittlement.

This work investigates the effects of tramp elements on a 51CrV4 quenched and tempered steel and a Titanium interstitial free steel subjected to various heat treatments. Small-scale laboratory alloys were produced with controlled additions of Sn, Sb, Cu, Cr, Mo, and Ni to simulate increased levels that may occur due to recycling in the future. Heat treatments consisting of annealing at 400 °C to 700 °C and slow cooling to room temperature were used to determine the embrittlement potential of the different tramp elements. The mechanical properties of the alloys were evaluated using tensile and Charpy V-notch impact tests. At the same time, multiple microstructural characterization methods were employed to identify the cause of the embrittlement.

The investigations revealed only minor changes in the tensile strength and microstructure of the materials. However, the impact toughness of the 51CrV4 quenched and tempered steel decreased drastically with increasing amounts of Sn, Sb, and Cu. Advanced site-specific sample preparation methods using femtosecond laser ablation and focused ion beam techniques enabled higher throughput atom probe tomography measurements to identify grain boundary segregation or precipitation that may be responsible for the embrittlement. Atom probe tomography revealed nm-sized Cu clusters and precipitates along grain boundaries and significant segregation of Sn and Sb to high-angle grain boundaries after tempering at 650 °C. This suggests that segregation is the primary factor driving the embrittlement of such alloys instead of bulk microstructural changes.

This work highlights the critical role of tramp elements, particularly Cu, Sn, and Sb, in the embrittlement of multiple steel grades under specific heat treatment conditions. It shows that different steel grades with widely different microstructures can suffer from the same mechanical degradation due to increased tramp elements, therefore underlining the need for a fundamental understanding of the segregation behavior of tramp elements in ferritic steels.

Segregation of P in polycrystalline Fe: Bringing atomistic predictions towards reality

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Solute segregation at grain boundaries (GBs) significantly affects material behaviour, with most studies focusing on substitutional solute segregation while neglecting interstitial segregation due to its increased complexity. The site preference, interstitial or substitutional, for P segregation in α-Fe is still under debate. This work investigates both substitutional and interstitial GB segregation in a polycrystalline model using classical interatomic potentials and machine learning. The method is validated with H and Ni, whose segregation behaviour is well understood. For P, we find segregation to both GB site types, with a preference for substitutional sites based on the mean segregation energy. However, the abundance of interstitial sites means that interstitial segregation also contributes significantly to GB enrichment with P. This highlights the importance of considering interstitial P segregation alongside substitutional segregation. In addition, obtaining a representative spectrum of segregation energies is crucial for accurate, experimentally based predictions.

Influence of scrap introduced tramp elements on phase transformations and deformation behavior of non-metallic inclusions in steels

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The Green Deal of the European Union requires a change of steel production routes including increased scrap recycling rates. While high quality scraps are already remelted at a high percentage, lower-quality scraps containing copper or tin are mostly downcycled to concrete steels since these elements lead to various issues during processing such as hot-shortness or an altered phase transformation behavior resulting in restrictive limits in many steels. Furthermore, physical and chemical properties of steel melts are influenced as most tramp elements decrease the surface tension which is connected to a higher nucleation rate of non-metallic inclusions (NMIs). With an increased NMI density, a harder microstructure, and possible accumulation of tramp elements around NMIs, the deformation behavior of NMIs during forming processes can be affected. While hard NMIs such as spinel types deform in steels with and without tramp elements in a similar manner, softer NMIs show altered deformation behavior in steels with tramp elements. This property is assessed using quenching and deformation dilatometry combined with scanning electron microscopy to measure the aspect ratio of NMIs before and after deformation. This work connects the change in microstructure with deformation behavior of NMIs of medium carbon steels due to elevated tramp element levels.

Insights into weld metal hot cracking of austenitic stainless steels: Atomistic characterization of crack surfaces

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Austenitic stainless steels (ASS) are prone to weld metal hot-cracking as a result of detrimental segregation of elements such as S, P, Nb and Ti. Nevertheless, accurate quantification of these segregating elements is central to comprehend the underlying mechanisms involved in hot-cracking phenomenon. Till now there were no attempts to characterize the hot-crack surfaces at atomistic scale as this partly involves complex crack opening protocols.

In the current scenario, using novel crack-opening methods, we successfully opened weld metal cracks (WMCs) in single and multi-pass ASS welds. The single-pass WMC is a ~ 20 mm long center line weld crack, and multi-pass WMC is a ~ 3 mm long crack located near the abutting weld-pass interfaces. Upon fractographic examination, these opened WMC surfaces were protected with ~ 500 nm Ag deposition prior to FIB-based sample preparation for TEM and APT investigations.

The SEM fractographic investigations implied ‘dendritic’ nature of the single-pass WMC surface, confirming its nature to be a ‘solidification’ hot-crack type. On the other hand, multi-pass WMCs showed ‘flat’ morphology. This, together with the location of multi-pass WMCs confirm them to be ‘liquation’ hot-cracks. The TEM and APT investigations indicated 25-33 at. % S segregation at both single and multi-pass WMC surfaces. The multi-pass WMCs were additionally enriched with ~ 14 at. % C, 0.4 at. % Nb and 0.4 at. % Ti. It was concluded that the segregation of these detrimental elements caused hot-cracking phenomenon. However, these WMCs occurred without phase formation, as possible stoichiometric phases such as M_2S and M_3S are thermodynamically unstable under weld pool conditions. There was no P detected and thus herein P did not contribute to WMCs formation.