

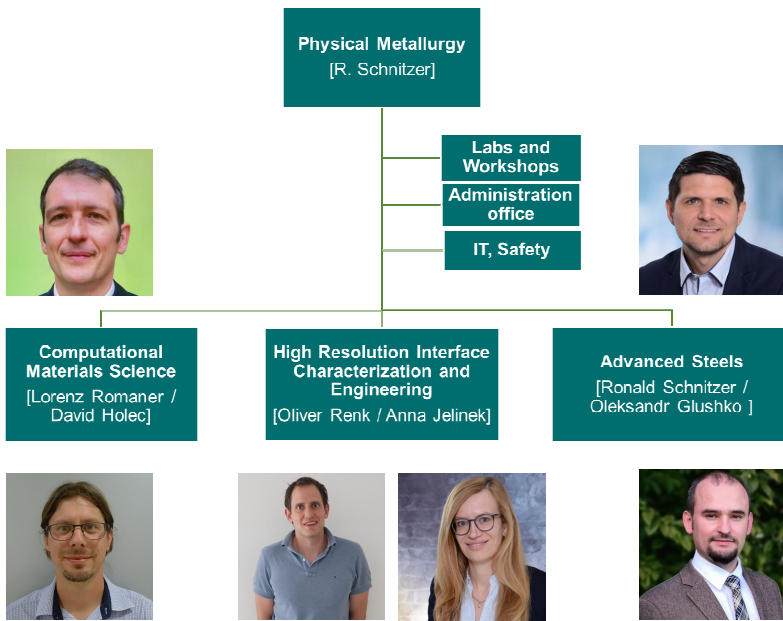
Table of contents

Nr.	Name	Title	Page
1	Schnitzer Ronald	Chair of physical metallurgy	2
2	Schnitzer Ronald	Christian Doppler Laboratory for knowledge-based design of advanced steels	3
3	Romaner Lorenz	Christian Doppler Laboratory for advanced computational design of crystal growth	4
4	Jelinek Anna	Atom probe tomograph	5
5	Glushko Oleksandr	Advanced steels	6
6	Schrittwieser Daniel	Structure-property relationship of high-strength weld metal	7
7	Holec David	Computational design of hydrogen technologies	8

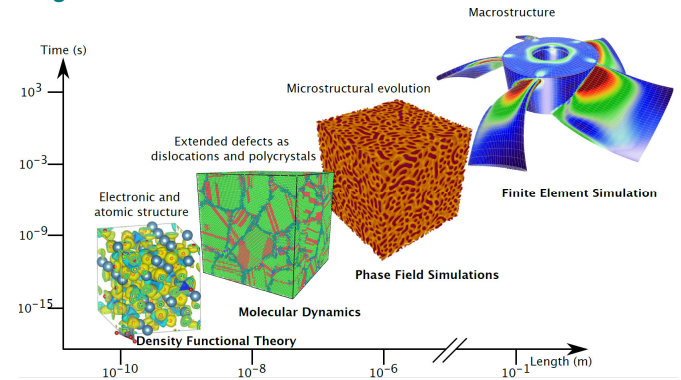
Chair of Physical Metallurgy

Lehrstuhl für Metallkunde

The mission of the chair is to carry out fundamental and applied research in the form of industry-related collaborations and scientific research projects.

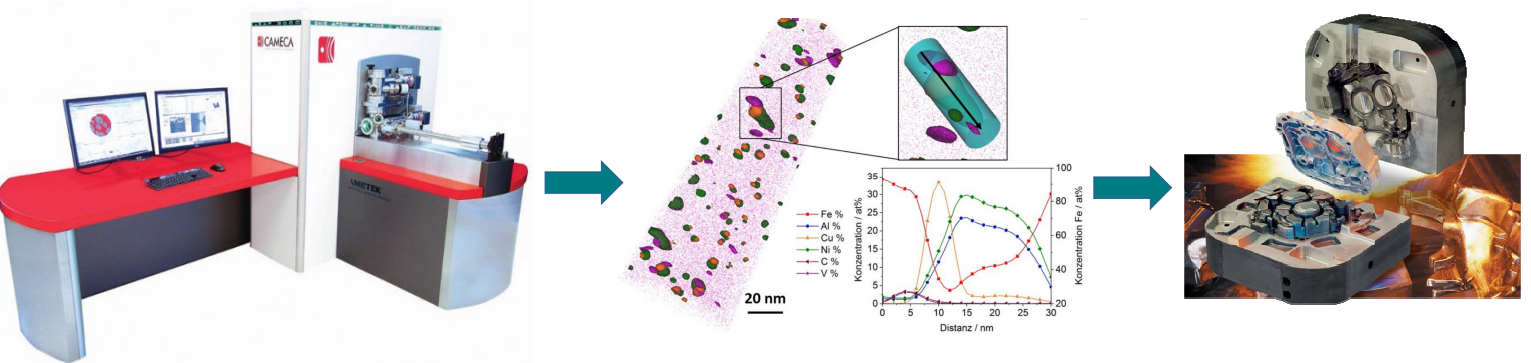


Computational Materials Science – Bridging all length scales



Computer-aided modelling has become an integral part of materials science. Methods range from the atomistic to the continuum level and are used to support and interpret experimental observations as well as to explore new research questions. Our activities target modeling of crystallographic phases or precipitates, modeling of nanostructures, modeling of crystallographic defects such as dislocations, grain boundaries or interfaces, and thermodynamic and kinetic simulations of phenomena on the mesoscale. In addition, approaches to combine physics-based simulations with data-driven modeling approaches are being explored.

Experimental Materials Science - High Resolution Characterization by Atom Probe Tomography



In atom probe tomography, a DC voltage of several kilovolts is applied to a tip with a radius of 20-50 nm. Atoms are removed from the surface one-by-one by field evaporation and accelerated onto a position-sensitive detector equipped with time-of-flight mass spectrometer. As a result, the position of each atom is reconstructed in 3D with **sub-nm resolution**.

Atom probe tomography of a dual hardening steel with a concentration profile of a selected cylinder volume. The purple-coloured areas correspond the V enriched carbides, the green areas to intermetallic NiAl precipitate and the orange areas to Cu particles.

The thermo-mechanical fatigue strength is connected with the nanostructure of this dual hardening steels, which are used as plastic mould steels.



Univ.-Prof. Dr.
Ronald Schnitzer
Chair of Physical Metallurgy
Department of Materials Science
materials@unileoben.ac.at

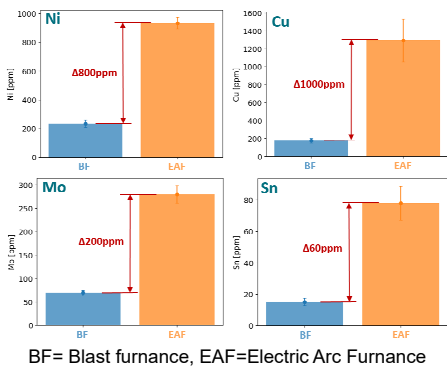


Christian Doppler Laboratory for Knowledge-based Design of Advanced Steels

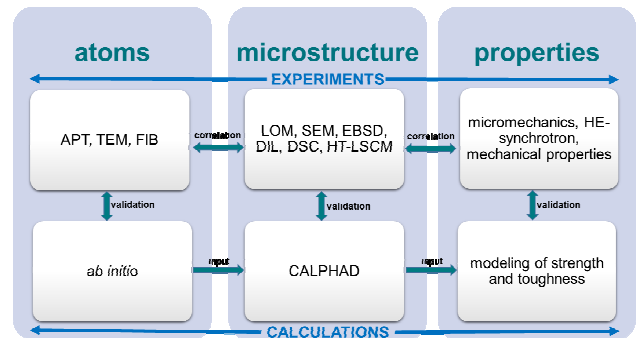
– from ab initio methods to components produced with low CO₂ emissions

The key development trends in the 21st century include sustainability, energy saving and recycling, which require a development of environmentally-friendly material processing technologies and knowledge-based design of structural materials such as steel. In order to reduce the amount of CO₂ emissions, the steel industry aims for increasing the amount of scrap in its production route by shifting the used technology from blast furnaces to electric arc furnaces. Thereby, the amount of unwanted tramp and trace elements will inevitably increase. To enable this technological milestone, knowledge about the influence of these elements on the properties of the steel products is a necessary requirement. The detailed analysis and chemical information of elements segregating on grain and phase boundaries or within different phases in steels is not known. However, revealing their influence on the nano- and microstructure, mechanical properties and processability is a prerequisite for the development of advanced steels, produced with low CO₂ emissions. This is the key research focus and main goal of this Christian Doppler Laboratory (CDL).

Higher element contents due to higher scrap rates



Concept and methodological approach of the CDL

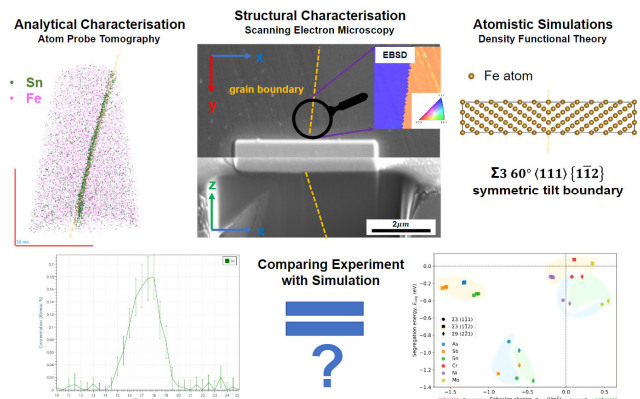


Structure and methods of the CDL

Head of the CDL: Ronald Schnitzer	
area A David Holec	<ul style="list-style-type: none"> Ab initio CALPHAD Machine learning / High-throughput calculations
area B Ronald Schnitzer	<ul style="list-style-type: none"> APT, TEM, FIB, TKD LIMI, REM, EBSD, DIL, DSC Modeling of mechanical properties
area C Jozef Keckes	<ul style="list-style-type: none"> HE-synchrotron radiation (in-situ methods) Micromechanics and macro-mechanical properties

One exemplary result of the CDL

Grain Boundary Segregation Analysis in Ferritic Steels



Univ.-Prof. Dr.
Ronald Schnitzer
Department of Materials Science
Chair of Physical Metallurgy
materials@unileoben.ac.at

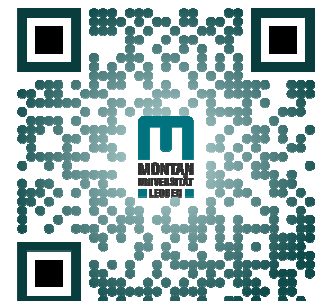
Research partner:



Funding:



Bundesministerium Arbeit und Wirtschaft



Christian Doppler Laboratory for Advanced Computational Design of Crystal Growth

Creating next generation materials for power electronics

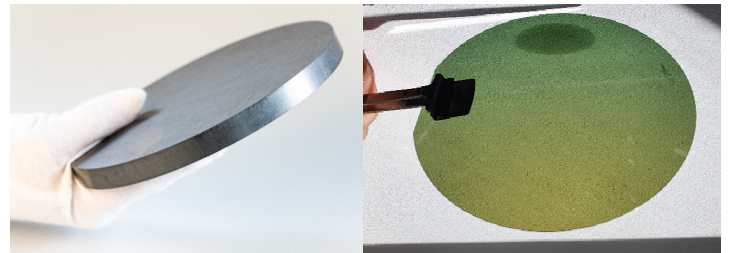
We develop novel modelling methods for the virtual description of crystal growth processes. Physics-based and data-driven modelling approaches are combined to achieve the most efficient and predictive approach possible.

Growth facilities for silicon carbide (SiC)



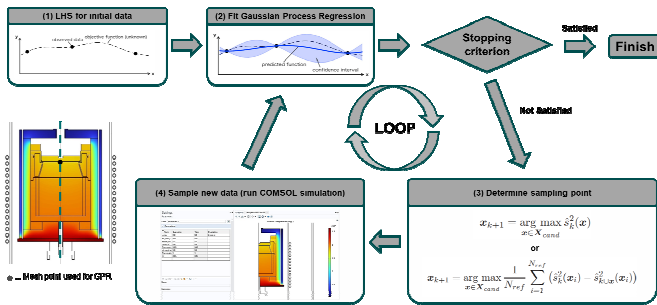
Single crystals of SiC are grown in furnaces (left) with the physical vapor transport method. Simulations (right) allow to virtually observe quantities such as magnetic field, temperature and mass transport which remain hidden experimentally.

High quality single crystal SiC



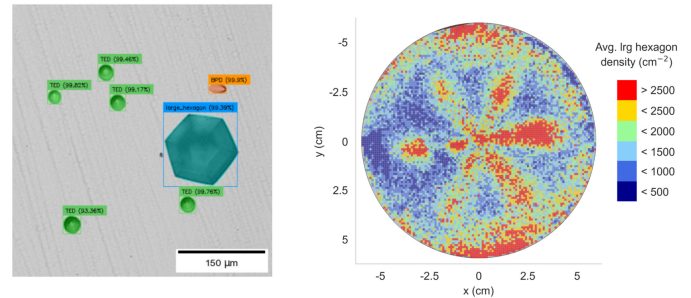
The company partner EEMCO grows the single crystals, shapes them into a puck (left) and cuts it into wafers (right) which are needed for producing devices for power electronics applications such as electric cars, trains or charging stations.

Active learning for creation of surrogate furnace model



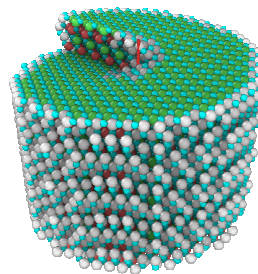
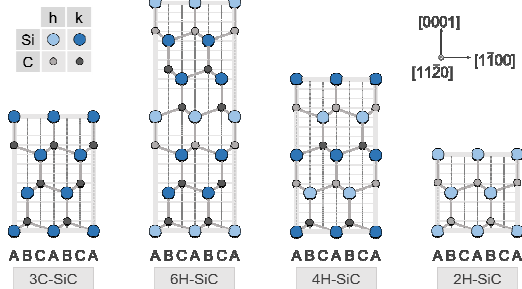
The multiphysics COMSOL simulations are accelerated via machine learning to enable optimization of the growth process in high-dimensional parameter spaces.

Automatic detection of dislocations with neural networks

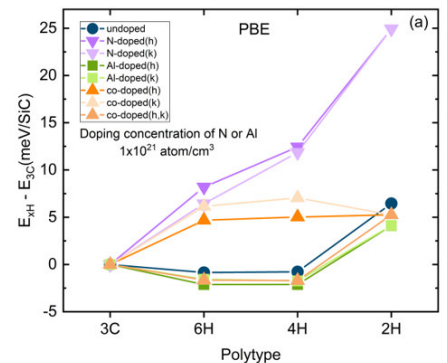


Neural networks allow to automatically detect different dislocations in etch images (left) and to create density maps for whole wafers (right) relevant for quality monitoring.

Atomistic simulations



Modeling of threading screw dislocations allows understanding their core structure and impact on growth phenomena.



Doping of SiC with N or Al can strongly alter the polytype energy differences. N has the strongest impact while Al and Al-N co-doping pairs show minor influences.



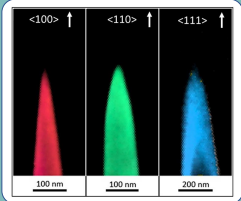
Univ.-Prof. Dr.
Lorenz Romaner
Chair of Physical Metallurgy
Department of Materials Science
materials@unileoben.ac.at



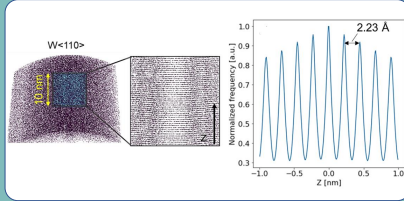
Atom Probe Tomography

Field-evaporating ions from a sharp tip provides 3-dimensional images with atomic resolution and quantitative chemical analysis of materials. To learn more about this fascinating microscopy technique, scan the QR code below!

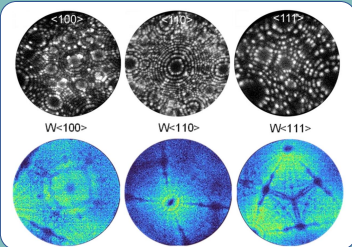
Atom Probe Crystallography



Transmission Kikuchi diffraction enables correlation with orientation of specimens



In the 3-dimensional reconstruction, lattice planes become visible and are measurable using spatial distribution maps



Field ion microscopy images and field desorption maps of tungsten

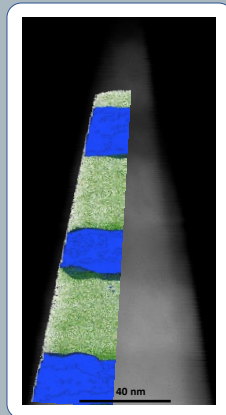
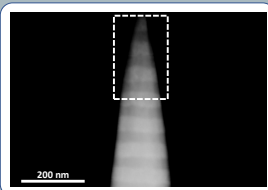
D. Rainer, Master Thesis, MUL (2023).



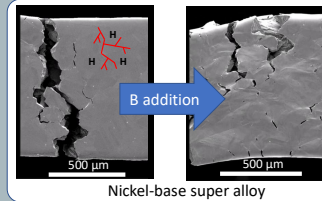
Correlative microscopy of multilayer coatings

The combined application of microscopy techniques to the same area of a single specimen is called correlative microscopy. APT is preferably combined with transmission electron microscopy (TEM) to ensure a reliable reconstruction, as in the example shown.

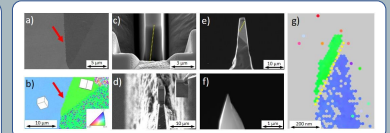
In the research and development of multilayer coatings, which are used e.g. as wear resistant coatings, but also in energy storage and harvesting applications, we use correlative microscopy to enhance their performance.



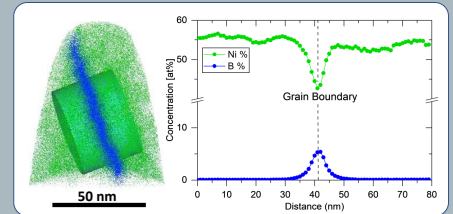
Grain Boundary Segregation Engineering against Hydrogen Embrittlement



Grain boundaries of high-strength materials (e.g. steels and nickel base alloys) can be prone to Hydrogen Embrittlement

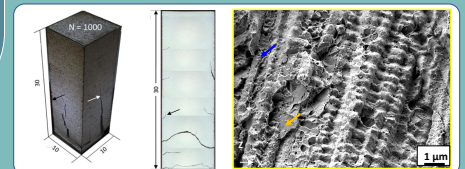


Site-specific preparation with a focused ion beam microscope allows preparation of a grain boundary inside the APT tip

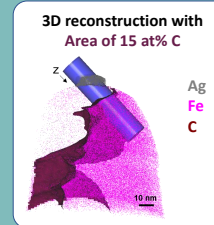


Amount of grain boundary segregation was successfully quantified with APT

Investigation of cracking mechanisms for Additive Manufacturing (AM)



Some AM materials are prone to cracking when used with inappropriate composition or process parameters.



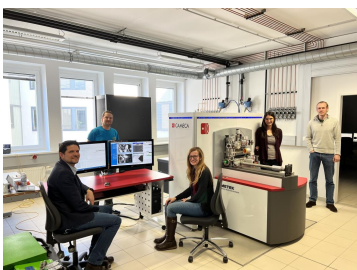
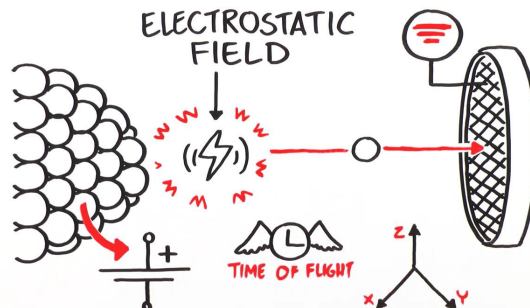
APT tip of crack surface with Ag and Pt protection coating

Stress-induced eutectic carbides, formed during solidification, could be identified with APT as predominant cracking mechanism.

J. Platl et al., Acta Mater. 225 (2022).

APT-Team

Dr. Anna Jelinek,
Dr. Michael Tkadletz
Department Material Science
apt@unileoben.ac.at

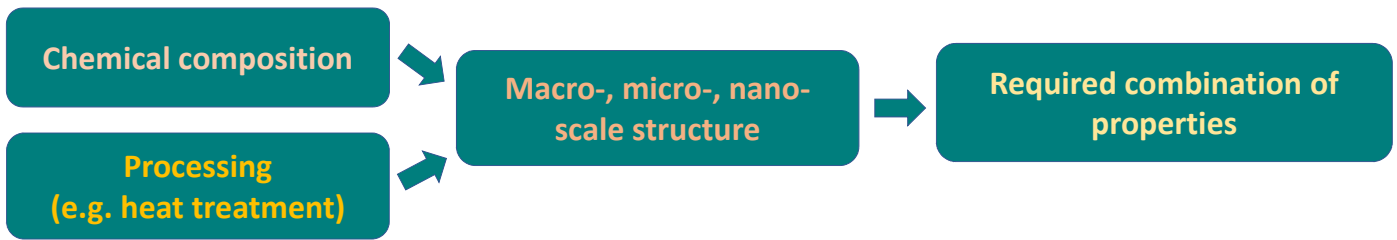


Advanced Steels

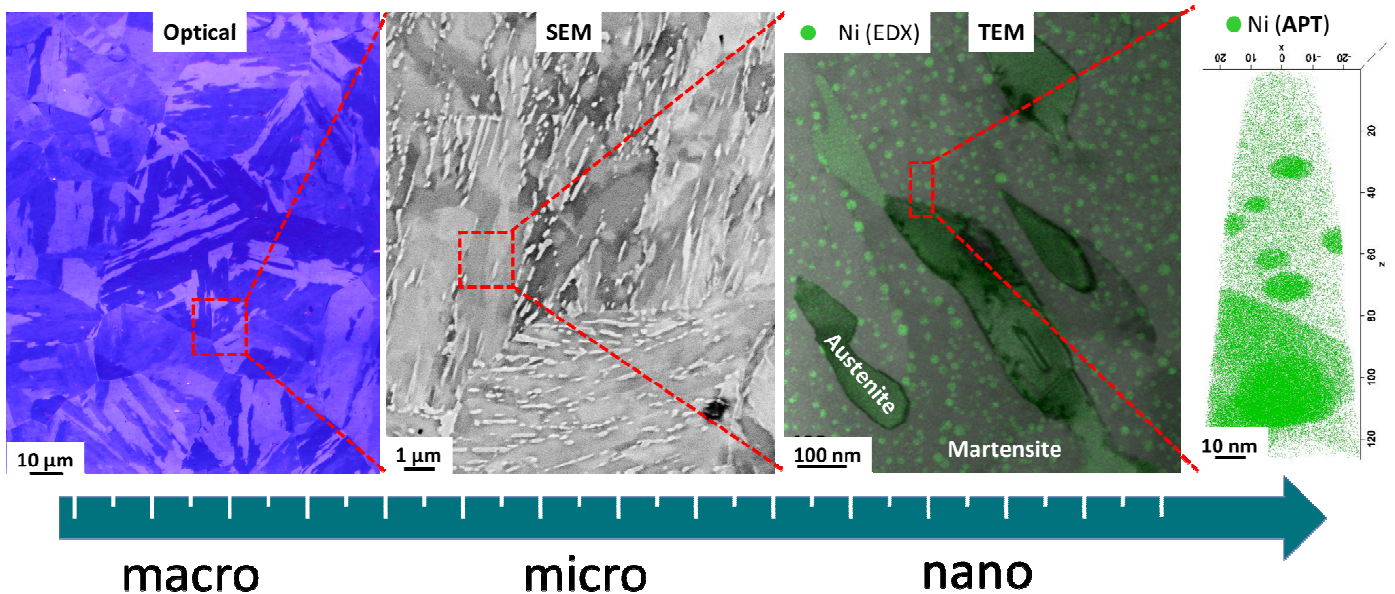
Designing stronger, tougher, lighter, more reliable, and more sustainable steels

Although steels are used by humankind for thousands of years, there is still a place for improvements of steel properties. Nowadays these improvements are achieved through targeted and specific design of steel structure on different length scales – from sub-nm to sub-mm. Such advanced steels are, in essence, complex hierarchical composite materials which can be produced in large scale by metallurgical means.

Advanced steels design concept



Example of multiscale hierarchical structure of PH13-8 Mo



Materials for aerospace applications must fulfil particularly high safety requirements. One such material is the maraging steel PH 13-8 Mo, which is used in the landing gear of long-haul aeroplanes. In order to achieve an excellent combination of strength and toughness, the structure of the material is precisely designed across length scales. Optical microscopy confirms macroscopic material quality and structural homogeneity. Scanning electron microscopy (SEM) shows martensitic structure with austenite islands on a micrometer scale. On sub-μm scale, transmission electron microscopy (TEM) demonstrates finely dispersed Ni-rich particles within the martensite matrix as well as higher Ni content of austenite. Finally, atom probe technology (APT) allows to resolve the distribution of Ni at a truly nanometer scale. Thanks to this correlative and high-resolution characterization, it is learned that the strength of PH 13-8 Mo is increased by fine NiAl precipitates, while the good toughness is ensured by sub-micrometer-sized austenite grains which are stabilized by Ni enrichment.



Dr.
Oleksandr Glushko
Chair of Physical Metallurgy
Department of Materials Science
oleksandr.glushko@unileoben.ac.at



Univ.-Prof. Dr.
Ronald Schnitzer
Chair of Physical Metallurgy
Department of Materials Science
materials@unileoben.ac.at



Structure-property relationship of high-strength weld metal



Materials Science
CHAMPIONS
LEAGUE

adapted from www.uefa.com (03.2024)



Materials Science
CHAMPIONS
LEAGUE

The Champions League of Physical Metallurgy

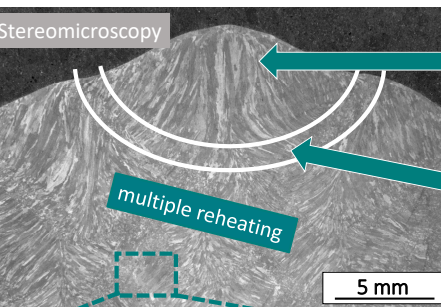
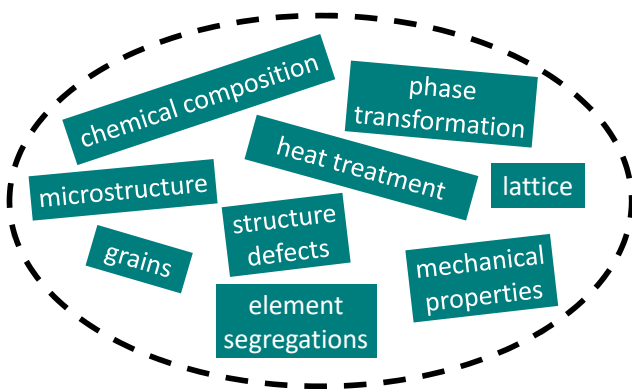
Due to an excellent combination of strength and toughness, high-strength steel enables constructions with an elevated load capacity by employing a diminished quantity of material. Consequently, a reduction in the production and transportation requirements is achieved, which leads to a decrease in the associated carbon footprint.

The bottleneck of building high-strength steel constructions is the joining process. Typically gas metal arc welding is employed by utilizing highly advanced welding consumables. Due to complex and locally varying temperature histories several difficulties occur:

- no controlled grain and dislocation hardening in the weld metal due to the primary solidification
- consequently, a higher content of alloying elements is required
- dilution of the high-strength steel (base metal) and the weld metal
- strong variation of the microstructure depending on the location
- local brittle phases occur
- **problem** → reaching sufficient **toughness**

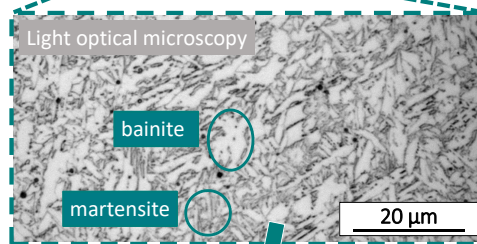


To accomplish a welded joint with an appropriate level of **toughness**, each facet of physical metallurgy must be considered.

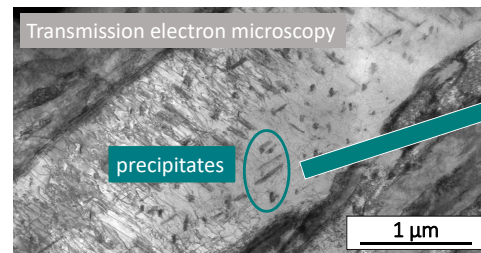
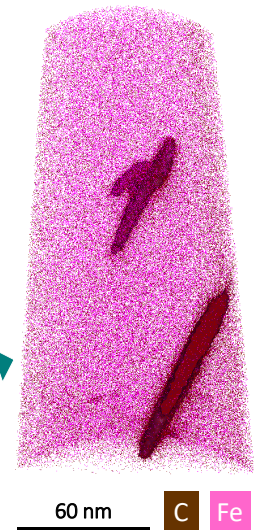


last bead → as-casted microstructure

weld metal heat treated by subsequent bead → heat-affected zone



Atom probe tomography



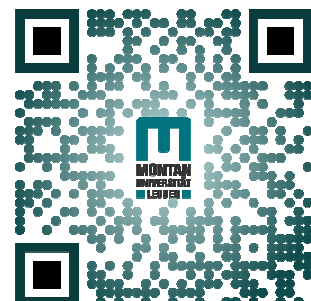
How to increase the toughness?

- *bainite and martensite fine and chaotic*
- *less precipitates*
- *reduced amount of local brittle phases*
- *small non-metallic inclusions*
- ...



Dipl.-Ing.
Daniel Schrittwieser
Chair of Physical Metallurgy
Department Materials Science
daniel.schrittwieser@unileoben.ac.at

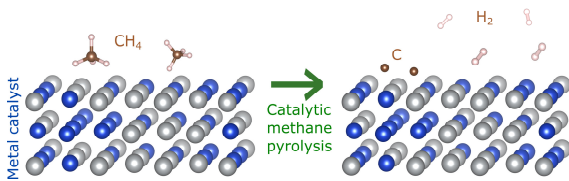
Research partner:



Computational Design of Hydrogen Technologies

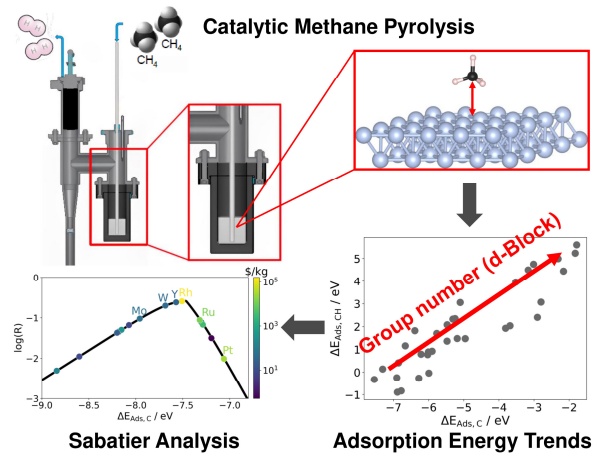
Using quantum mechanics and atomistic simulations to explore materials and processes for the hydrogen era

Hydrogen Production

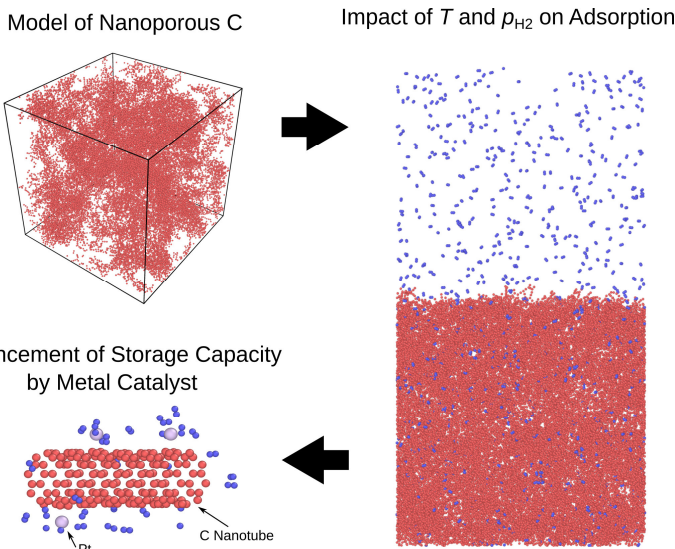


Methane pyrolysis is the heat decomposition of CH₄ into solid C and gas H₂ without causing CO₂ emissions. However, the operating temperatures are too high for large-scale hydrogen production by catalyst-free methane pyrolysis. Therefore, finding catalyst materials that lower the operating temperatures and thus make methane pyrolysis economically viable and environmentally bearable has become an important scientific goal.

We derived a model that allows a quantitative comparison of various catalyst materials. The model is based on a detailed description of the adsorption of C and H atoms and intermediate molecules in the methane pyrolysis reaction on the surface of the metal catalysts. The results obtained through screening 30 single-element catalysts, for example, show that the magnitude of adsorption energy increases with decreasing d-block group number of the catalyst element. Notably, various process conditions (operating temperature, CH₄/H₂ partial pressure) require various optimal catalysts. Hence, reaction parameters and catalyst choice have to be carefully matched. Therefore, our project establishes the foundation for future large-scale studies of catalyst surfaces, alloy compositions, or material classes.



Hydrogen Storage



Methane pyrolysis produces large amounts of *nanoporous carbon* (np-C). One of the possible applications has been suggested as a medium for H storage.

We employ atomistic simulations to construct realistic models of np-C based on inputs from small-angle X-ray scattering experiments. Next, we investigate its H storage capacity based on various external parameters such as temperature or pressure of H₂ gas. Our current activities are focused on quantifying the effect of metal decorations on the H₂ decomposition and adsorption in carbon nanostructures.



Priv.-Doz. PhD
David Holec
Chair of Physical Metallurgy
Department of Materials Science
david.holec@unileoben.ac.at

Research Team:



Martin Matas



Ulrich Pototschnig
(Univ. of Hamburg)



Thomas Leiner

Support:

SCoRe A+ H&C

