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Christian Doppler Laboratory for Knowledge-based Design of Advanced Steels

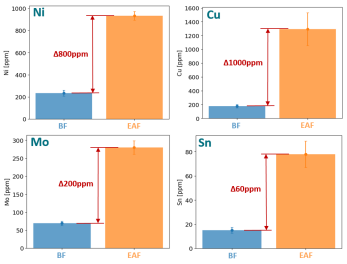
From ab initio methods to components produced with low CO2 emissions

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.

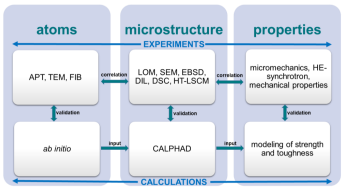
Motiviation

In order to reduce the amount of CO_2 emissions, the steel industry aims for increasing the amount of scrap in its production route by shifting the used technology from blast furnaces (BF) to electric arc furnaces (EAF). 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 amount 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 CO_2 emissions. This is the key research focus and main goal of this Christian Doppler Laboratory.

Influence of higher recycling rates

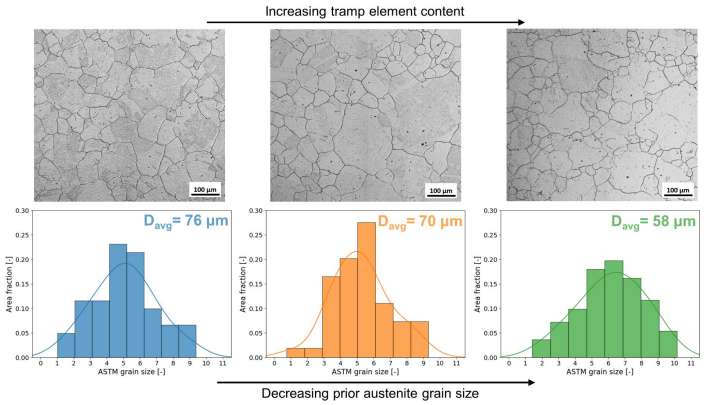


Concept and methods



Scale-bridging methods are used, starting from the atomic level. The research approach includes experimental methods paired with simulations and calculations.

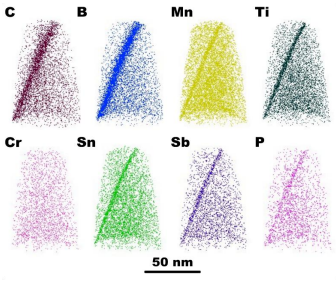
Influence of tramp elements on the grain size



The introduction of tramp elements is decreasing the prior austenite grain size, most likely due to a solute drag effect and the segregation of these elements to prior austenite grain boundaries.

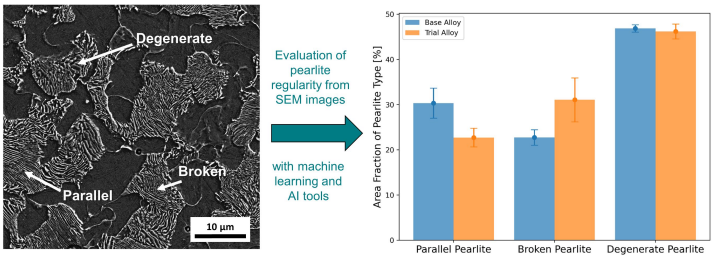
This can affect the subsequent phase transformations during cooling and the occurring phases in the final microstructure.

Segregation of elements to grain boundaries



The left image shows an atom probe tomography measurement of an alloy with increased contents of tramp elements. The segregation behavior of individual elements at a high-angle grain boundary can be clearly seen. Sn, Sb, and B, for example, show a strong tendency to segregate, whereas Cr is uniformly distributed in the matrix.

Microstructural evolution determined by using AI tools



Tramp elements affect the parallel growth of ferrite and cementite lamellae. Three pearlite types are determined with SEM: parallel, broken, and degenerate. The fractions of pearlite are analyzed with machine learning and AI tools. The presence of tramp elements increases broken pearlite at the expense of parallel pearlite.

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voestalpine ONE STEP AHEAD.

Christian Doppler Forschungsgesellschaft

References:
[1] L. Hatzenbichler et al., Praktische Metallographie, 2025, 62, 148-175
[2] L. Hatzenbichler, et al., steel research international, 2025, 2500172
[3] N. Kostwein, et al., Journal of Materials Research and Technology, 2025, 38, 4908–4916

Chair of Physical Metallurgy

The Chair conducts fundamental research in close cooperation with industry partners, driven by a strong commitment to sustainable and resource-efficient solutions. We combine scale-bridging experiments and modeling to explore process-structure-property relationships and design high-performance materials. We actively involve students in research to educate highly qualified experts who are ready to tackle the scientific, technical, and environmental challenges of today and the future.

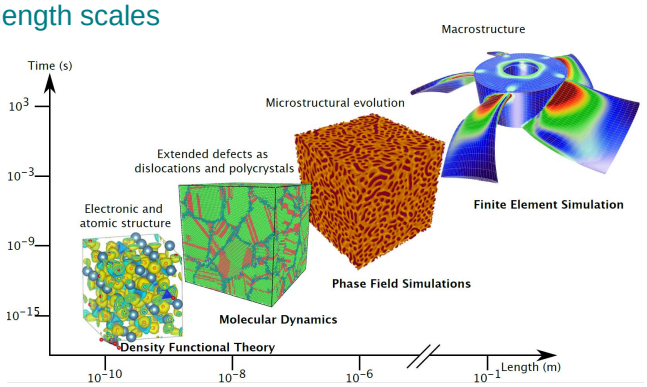
Physical Metallurgy
[R. Schnitzer]

- Labs and Workshops
- Administration office
- IT, Safety

Computational Materials Science	High Resolution Interface Charact-erization and Engineering	Advanced Steels	NeXt (Neutron and X-ray Team)
[Lorenz Romaner / David Holec]	[Oliver Renk / Ronald Schnitzer]	[Oleksandr Glushko / Ronald Schnitzer]	[Sabine Bodner / Ronald Schnitzer]

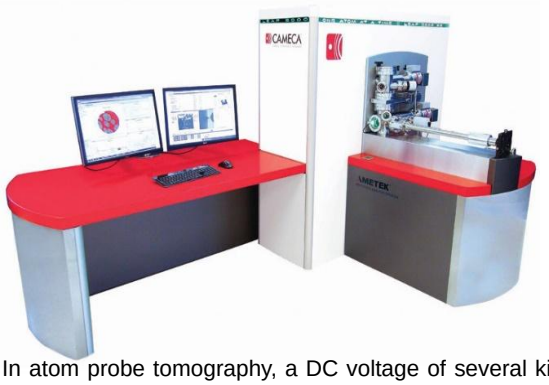


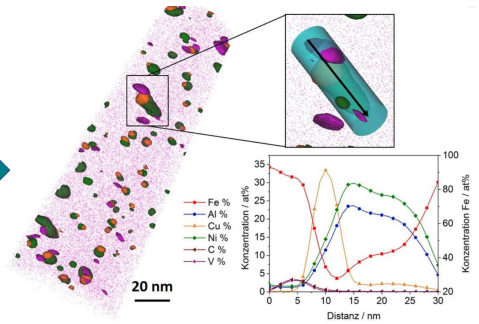

Computational Materials Science – Bridging all length scales



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.

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Harvesting and storing hydrogen: *in silico* approach

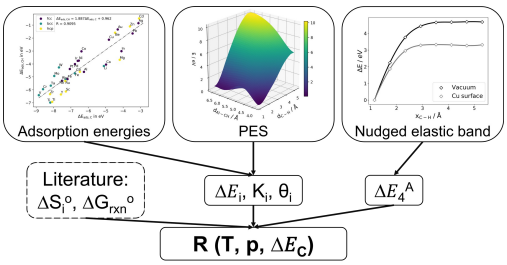
Atomistic modelling strategies for hydrogen era: Applications to methane pyrolysis and hydrogen storage

The growing demand for sustainable energy solutions requires advancements in hydrogen technology. This poster presents an overview of recent and current activities related to hydrogen harvesting rand storage performed by the Computational Materials Science Group at the Department of Materials Science.

Microkinetic modelling of catalytical activity for methane pyrolysis: static calculations

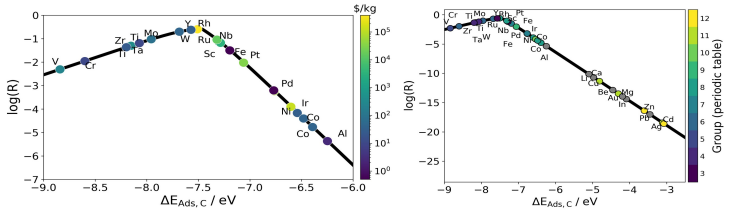
- Sabatier principle

U. Pototschnig, M. Matas, D. Scheiblehner, D. Neuschitzer, R. Obenaus-Emler, H. Antrekowitsch, D. Holec
Predictive Model for Catalytic Methane Pyrolysis
J. Phys. Chem. C 128 (2024) 9034–9040

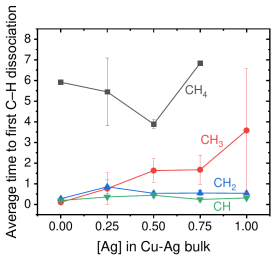


- Energetics from Density Functional Theory

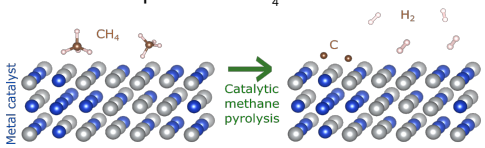
$$R(T,p,\Delta E_{\mathrm{Ads,C}}) = \frac{k_B T}{h} e^{-\frac{\Delta E_4^A}{k_B T}} \theta_{CH} \theta_* (1-\gamma)$$



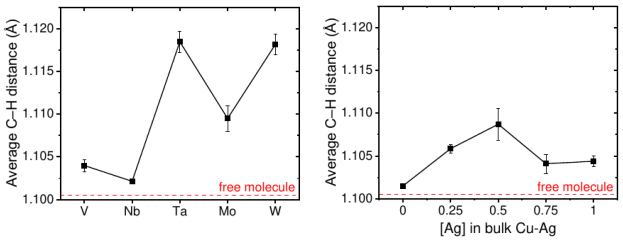
Dynamic simulations of pyrolysis using AIMD



- Bottleneck: decomposition of CH_4

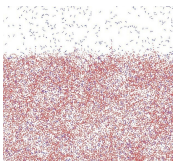


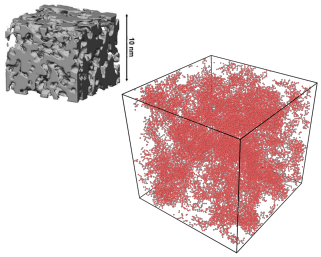
- BCC metals (CH_4 at 300 K)
- Cu-Ag alloys (CH_4 at 300 K)

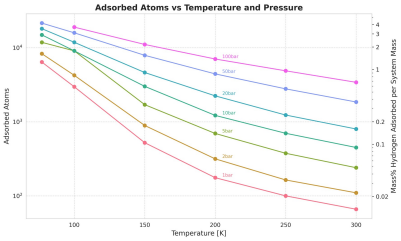


Experimentally-inspired atomistic model of nano-porous carbon for H storage

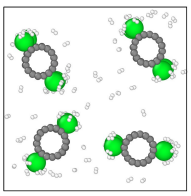
- From SAX scattering experiment via a continuum model obtained through Gaussian Random Fields to and atomistic model in molecular dynamics

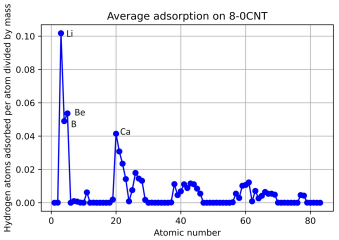


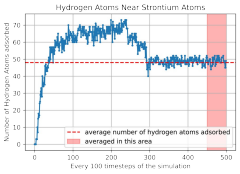




Enhancing hydrogen-storage capacity of carbon nanotubes by metallic decoration







T. Leiner, D. Holec
Revealing trends in catalytic activity of adatoms for hydrogen adsorption on carbon: A case study of graphene and carbon nanotube
Carbon Trends 20 (2025) 100535

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Ulrich Pototschnig


Martin Matas


Thomas Leiner

NEXT - From Structure to Performance

In-situ High-Energy X-ray Diffraction for Advanced Materials Development

Particle Accelerators for Studying Materials in Real time

Synchrotron-based characterization merthods enable non-destructive probing of bulk materials under realistic conditions. In-situ diffraction provides time-resolved access to phase transformations, lattice strain and texture evolution during thermal or mechanical loading. By linking experiments with simulations, we establish quantitative structure-property relationships and capture microstructure evolution during application relevant conditions. This approach enables a mechanistic understanding of materials behavior which provides a robust foundation to design and optimize advanced materials systems.

Fig. 1: Synchrotrons generate X-rays for high-energy materials science.

In-situ process investigation: PBF-LB/M at 250 Hz

Various metal systems (e.g., Al-, Fe-, Ni-, Co-, Cu-based) can be processed into complex components by laser beam powder bed fusion. However, industrial processing of more specific alloy systems, often characterized by outstanding mechanical properties such as high strength, remains challenging and requires specialized environments not available in commercial PBF-LB/M systems. The integration of a synchrotron-compatible module into an industrial machine at the high-energy materials science beamline P07 at DESY enables in-situ process investigation using hard X-rays at 250 Hz. In this way, residual stress build-up, phase transformations, texture formation, and microstructure evolution can be monitored, enabling development of optimized processing conditions and improved understanding of process failures such as cracking and severe warpage.

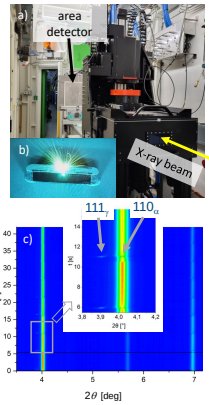
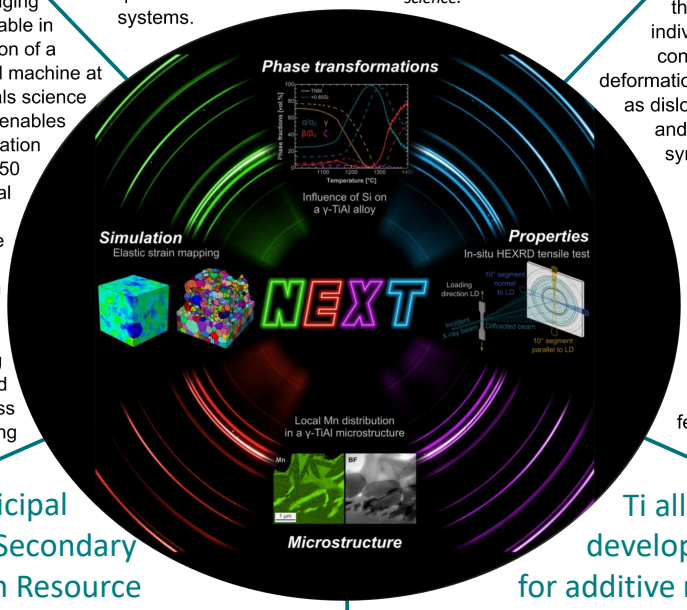


Fig. 2: PBF-LB/M device (a) with synchrotron module (b) and first results (c).



Efficient TiAl development aided by finite element simulations

Titanium aluminides (TiAl) exhibit complex multiphase microstructures that enable their mechanical response. Their properties arise from the interplay between individual phases, each contributing distinct deformation mechanisms such as dislocation slip, twinning, and creep.Using in-situ synchrotron diffraction, we resolve phase-specific lattice strain evolution and quantify load partitioning during deformation. This enables a direct link between local deformation mechanisms and microstructural features, providing insight into how phase interactions control the macroscopic mechanical behavior of these alloys.

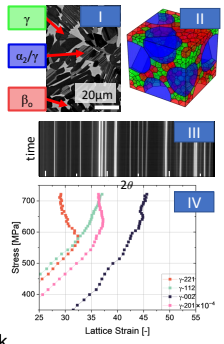


Fig. 3: Synchrotron results combined with simulations for efficient TiAl development.

B. Seligmann

Municipal Waste as Secondary Aluminium Resource

Aluminum's industrial and economic relevance is underscored by its ranking at the top of the European list of critical materials. Compared to primary Al production from ore, the use of secondary Al can reduce energy demand and CO_2 emissions by about 95%, highlighting the importance of recycling. Secondary Al in municipal waste originates from everyday products such as tubes, cans, coffee capsules, and foil. Approx. 1,000 t of secondary Al per year can be recovered from slag produced by waste incineration. Because secondary Al often contains higher levels of impurities (trace and tramp elements), synchrotron experiments are performed to understand their interactions with phase formation and microstructure evolution during processing, enabling reuse in wrought alloys, which are more sensitive to alloying elements than cast alloys.

F. Brandstetter

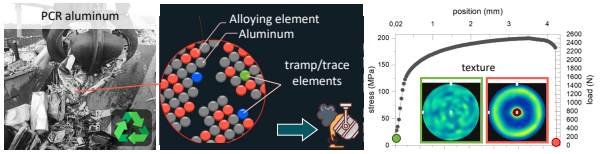


Fig. 4: Synchrotron experiments elucidate the influence of impurities on the microstructure and properties enabling optimized circular reuse of aluminum.

Ti alloys development for additive manufacturing

Additive manufacturing of titanium alloys is challenged by the formation of columnar grain structures, which limit isotropy and mechanical performance. Achieving a columnar-to-equiaxed transition (CET) remains a key objective and cannot be addressed by process optimization alone. Alloy design provides an additional pathway, where selected alloying elements (e.g. Cu) modify solidification behavior and promote equiaxed grain formation. These newly developed alloys require detailed investigation of phase transformations and precipitation kinetics. Using in-situ synchrotron diffraction across complementary experimental setups, we resolve microstructure evolution during processing, enabling a mechanistic understanding of how alloy composition influences solidification and resulting material properties.

D. Obersteiner

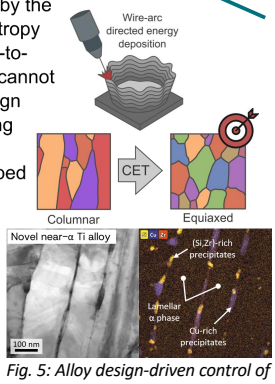


Fig. 5: Alloy design-driven control of solidification and microstructure evolution in Ti alloys.

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NEXT Neutrons and X-ray Team

FFG Forschung wirkt.

Materials Science

Helmholtz-Zentrum hereon

Further information:

Christian Doppler Laboratory for Advanced Computational Design of Crystal Growth

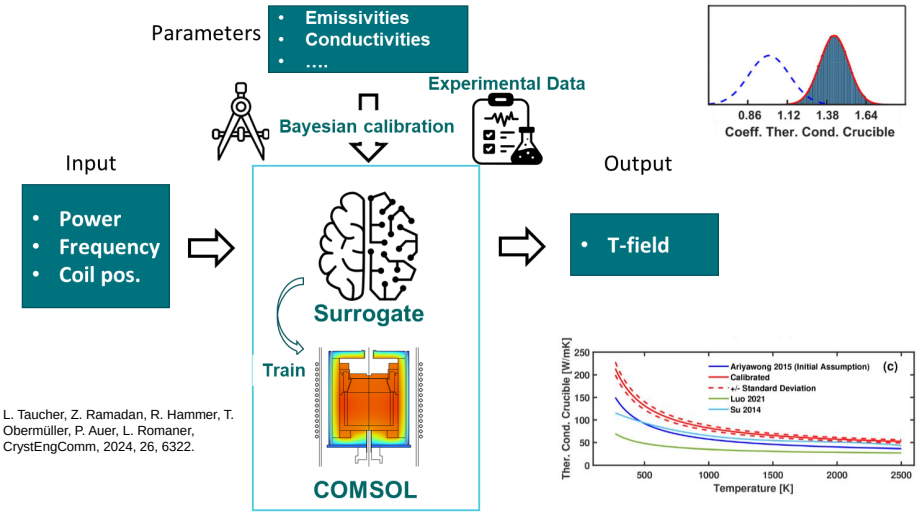
Physics-based and machine learning approaches for SiC crystal growth

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.

PVT furnaces for SiC crystal growth

Single crystals of SiC are grown in furnaces with the physical vapor transport (PVT) method. A schematic is shown in the window of the right furnace. An example of an obtained single crystal boule is shown on the bottom left.

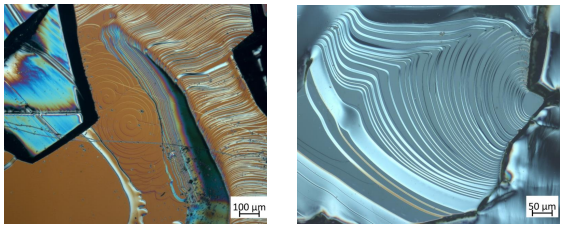
Calibration of multiphysics simulations via machine learning



L. Taucher, Z. Ramadan, R. Hammer, T. Obermüller, P. Auer, L. Romaner, CrystEngComm, 2024, 26, 6322.

Multiphysics simulations allow to calculate the temperature field as well as mass transport and the conditions of the single crystal boule. Bayesian calibration is used to obtain probabilistic models that speed-up the COMSOL FEM model, calibrate the FEM model to experimental data, measure the material data at service T and propose optimized sensor placements.

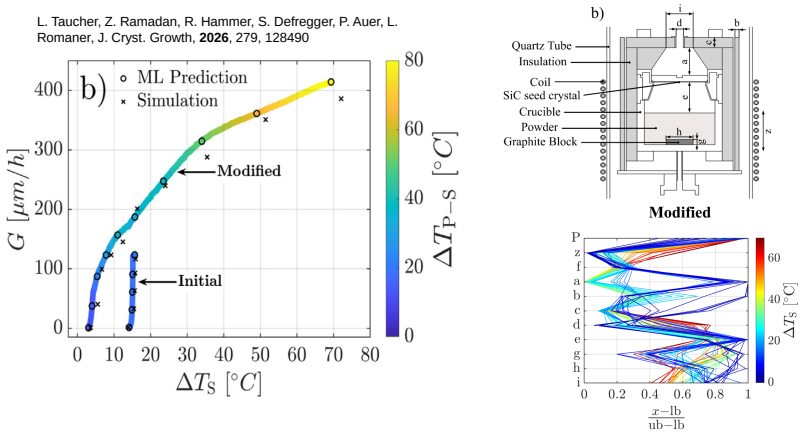
Exploration of growth phenomena



Crystal growth exhibits rich phenomena on the surface such as threading screw dislocations or step flow growth. A precise understanding of crystal defects is essential to control the crystal growth.

Furnace geometry optimization

L. Taucher, Z. Ramadan, R. Hammer, S. Defregger, P. Auer, L. Romaner, J. Cryst. Growth, **2026**, 279, 128490



Surrogate models allow to optimize the geometry of the furnace to achieve high growth rate *G* while keeping the temperature gradients small.

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EEMCO®
EBNER EUROPEAN MONO CRYSTAL OPERATIONS

CDC
ADVANCED COMPUTATIONAL DESIGN OF CRYSTAL GROWTH

Christian Doppler Forschungsgesellschaft