Helmholtz–Information
Programm „Materials Systems Engineering"
Topic "Scale-Bridging Designed Materials: From Fundamentals to Systems"

MSE-day
November 5th, 2024

Prof. Dr. Regine Willumeit-Römer / Prof. Dr.-Ing. Thomas Klassen
Spokes Person P3T4
Jülich, 05.11.2024

Karlsruher Institut für Technologie

Helmholtz-Zentrum hereon

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

KIT Karlsruher Institut für Technologie

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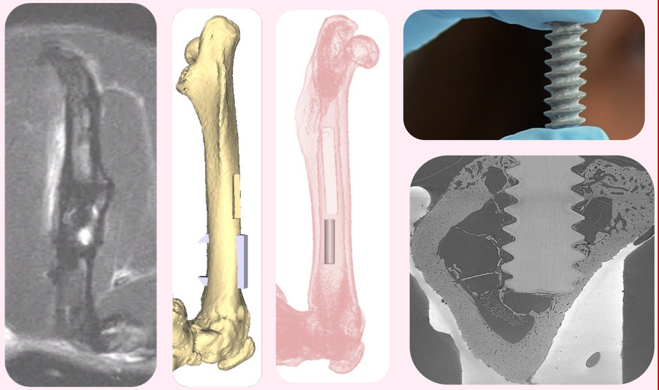
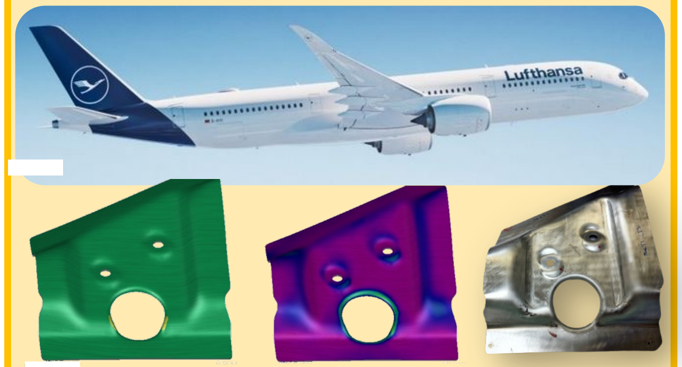
- from materials to components using in operando experiments & digital twins

Bio-Materials



biocompatible and resorbable implants

Light Weight Structures

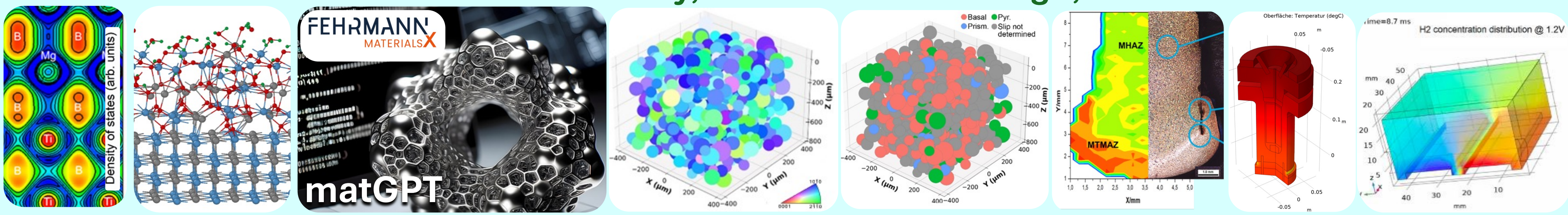


resource-efficient materials

Energy and Mobility

climate-friendly technologies

Information-Based Materials Discovery, Microstructure Design, Performance Prediction



from atomistic modelling to finite element simulation and property predictions

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

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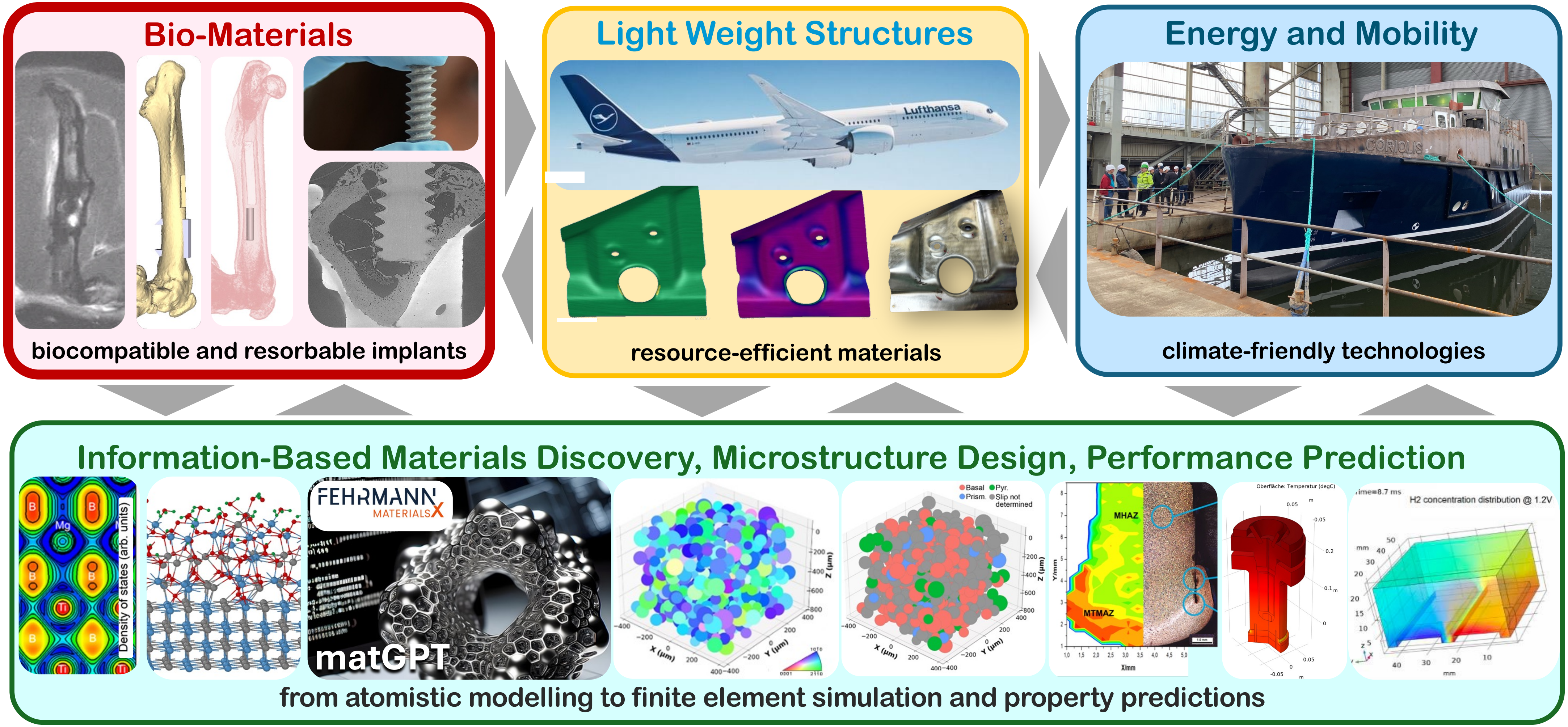


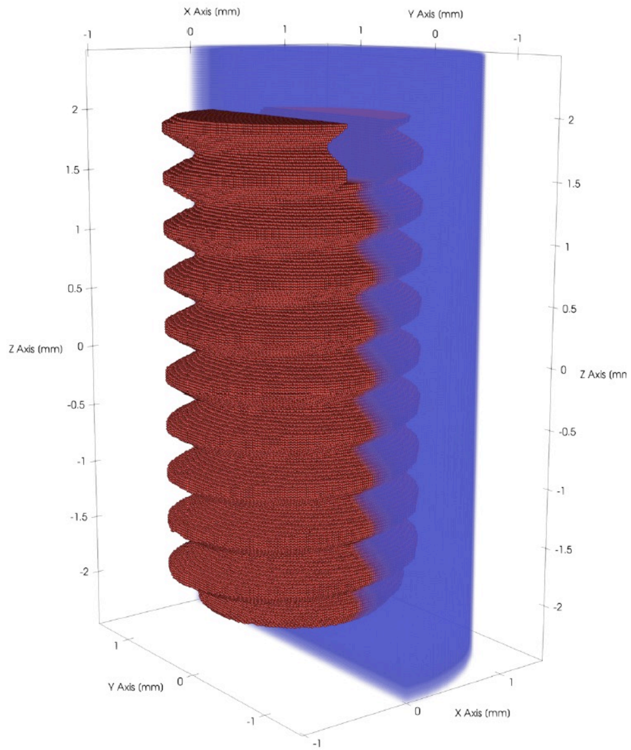
T4 Scale Bridging Designed Materials: From Fundamentals to Systems

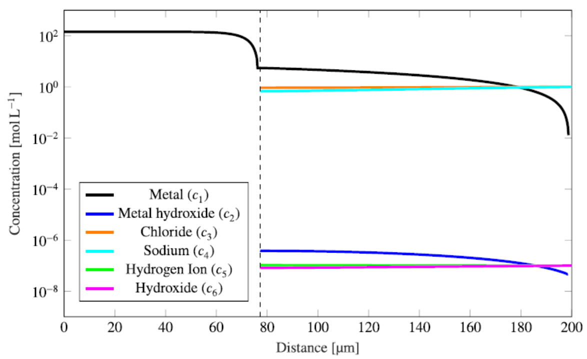
Implant degradation: peridynamics simulation of implant degradation in vitro

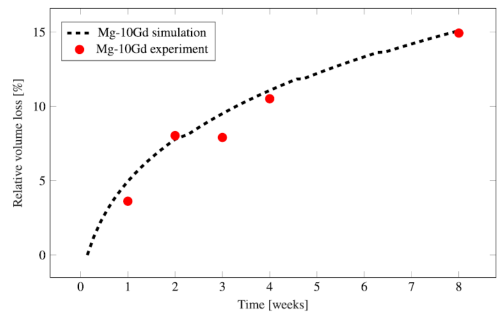
In vitro set up

- Biodegradation of new implant materials first assessed by experiments in vitro
- Computational model of in vitro degradation aims at thorough understanding of this process and allows for prediction of unknown materials
- Peridynamics model can capture in vitro corrosion including concentration of different chemical species involved

Cyron & Höche







A. Hermann et al. (2024) Journal of Peridynamics and Nonlocal Modeling

https://doi.org/10.1007/s42102-024-00125-z

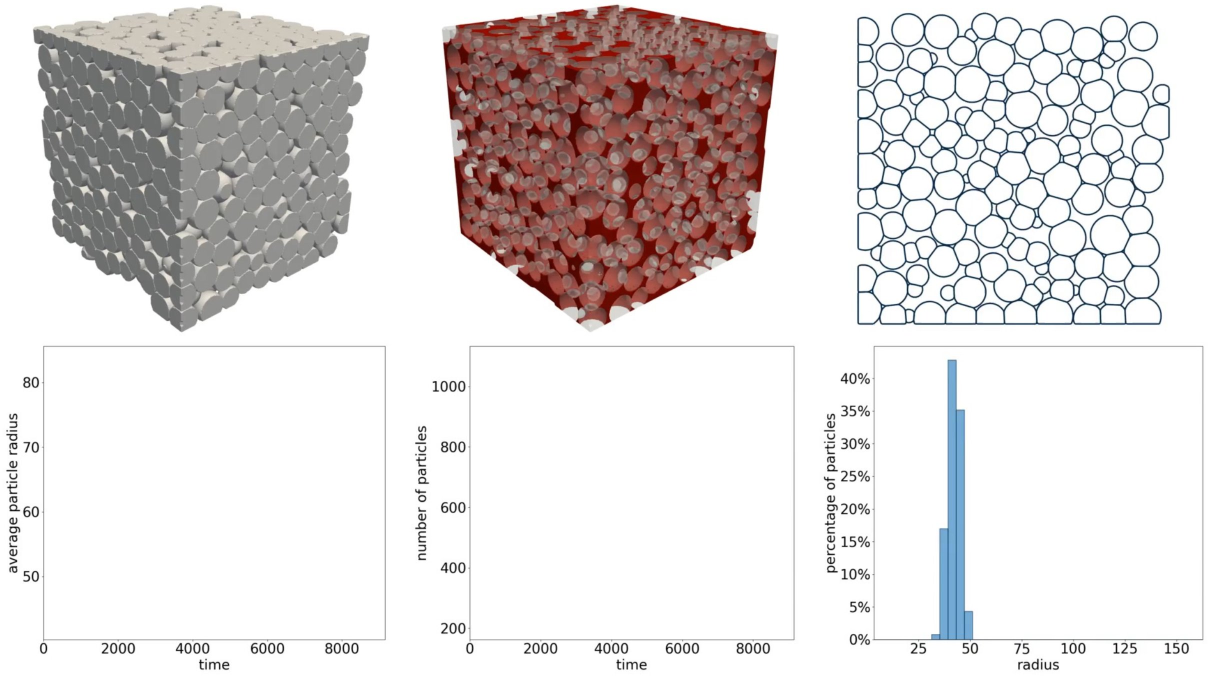
T4 Scale Bridging Designed Materials: From Fundamentals to Systems

Implant fabrication: HPC simulation of sintering

In vitro set up

- Fabrication of biodegradable implants often by sintering
- Development of new alloys requires time-consuming adjustment of manufacturing parameters
- We develop a computational model of implant sintering to accelerate this process by virtual process design
- Phase-field finite element model for massively parallel high performance computing (HPC) with billions of degrees of freedom

Cyron & Willumeit-Römer

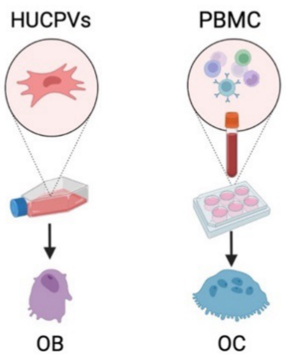


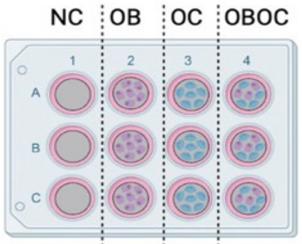
V. Ivannikov et al. (2024) Computational Materials Science
https://doi.org/10.1016/j.commatsci.2023.112589

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

Implant development: Impact of bone cell coculture on Mg degradation

In vitro set up

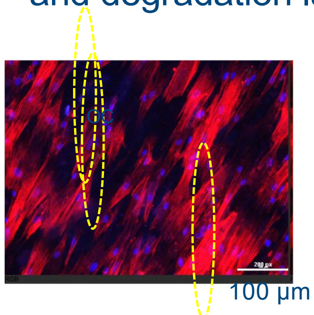




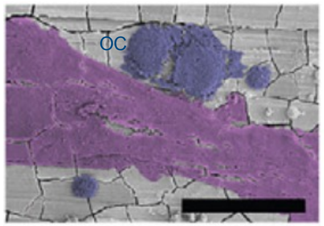
NC no cell control

The balance of bone forming cells (Osteoblasts OB) and bone resorbing cells (Osteoclasts OC) is essential for a functional bone remodelling

- OB were pre-differentiated from mesenchymal stem cells and OC from peripheral blood mononuclear cells
- Direct coculture at Mg surface for 14 days
- Correlation of cell layer density and degradation layer composition

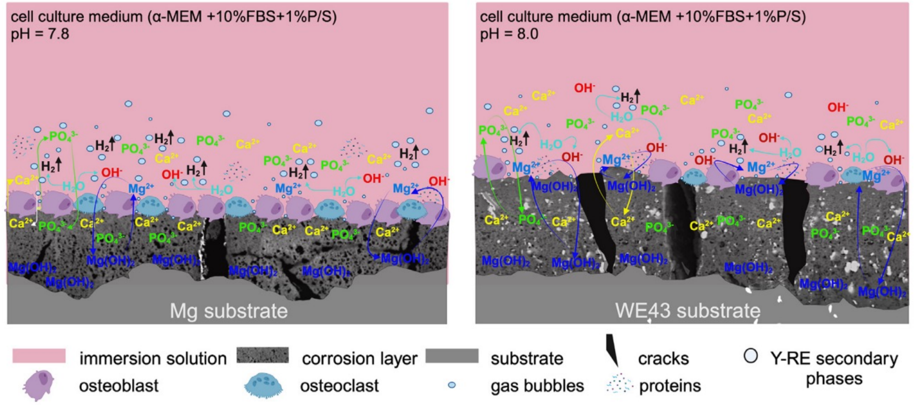


100 µm



50 µm

Degradation layer composition



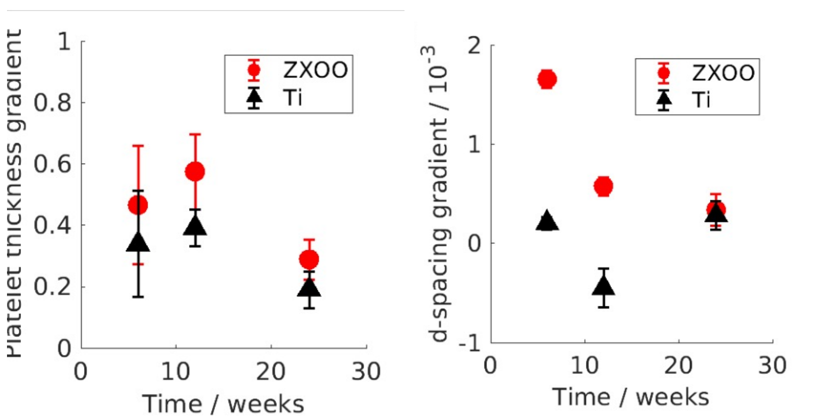
- the well-spread OB and OC on the pure Mg surface form a physical barrier
- Ca and P ions precipitate on the pure Mg surface in the uppermost corrosion layer
- No impact on degradation layer thickness

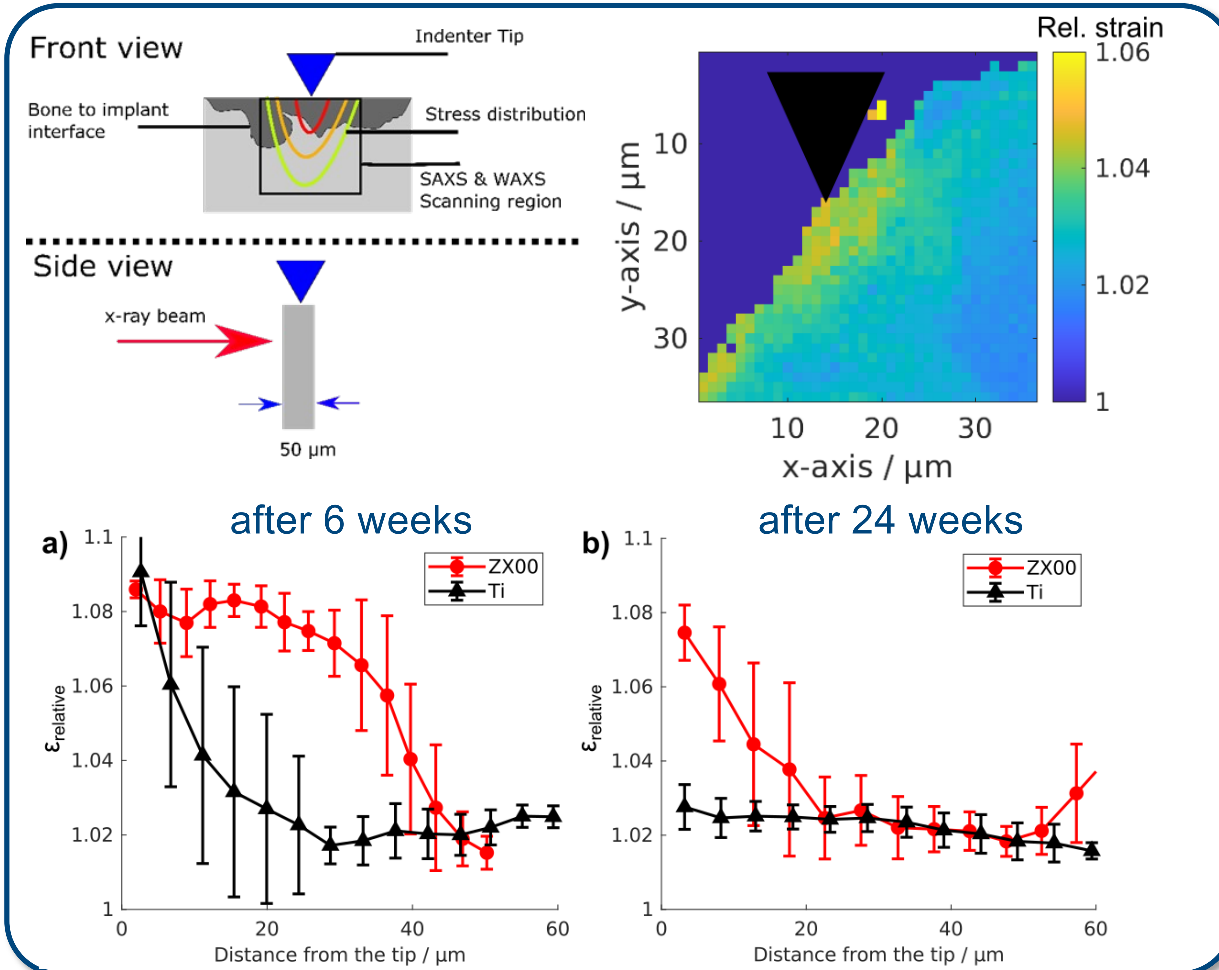
D. Martinez et al. (2024) Acta Biomaterialia
https://doi.org/10.1016/j.actbio.2024.08.015

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

Sheep Bone Ultrastructure Analyses Reveal Differences in Bone Maturation around Mg-Based and Ti Implants

- In situ nano-indentation x-ray scatterings experiments to investigate the ultrastructure and local mechanical properties at the bone-to-implant interface
- The data allows to conclude that the bone maturation and, thus, bone remodeling is delayed at Mg-implants as compared to Ti





P3T4

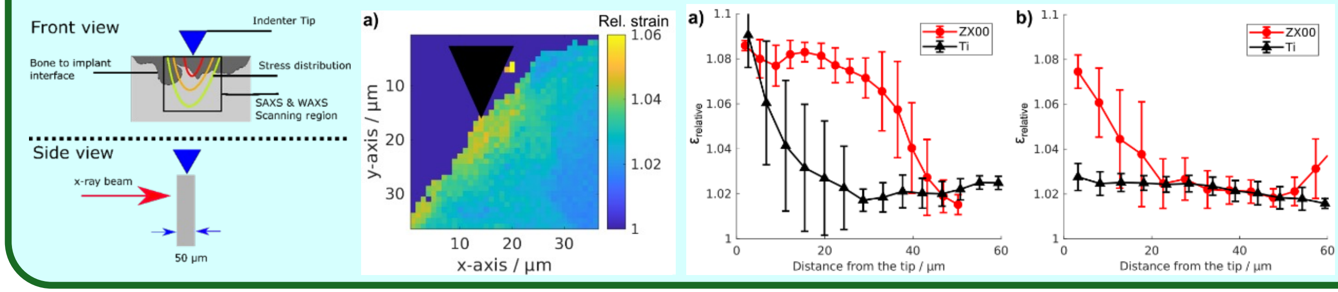
Ishkakova et al. J. Funct. Biomater. 2024, 15(7), 192

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

- from materials to components and assessment of environmental impact using in operando experiments & digital twins

Systems

Sheep Bone Ultrastructure Analyses Reveal Differences in Bone Maturation around Mg-Based and Ti Implants



- In situ nano-indentation x-ray scatterings experiments
- Bone maturation is delayed at Mg-implants as compared to Ti
- Still functionality is not altered

materials discovery

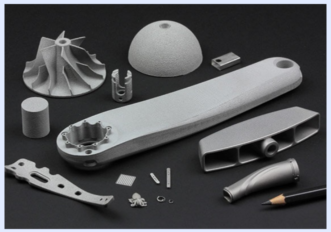
MatGPT: Using AI for materials development

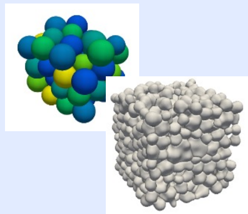
© Fehrmann Materials

FEHRMANN MATERIALS X

processing

Practical application of sintering modelling



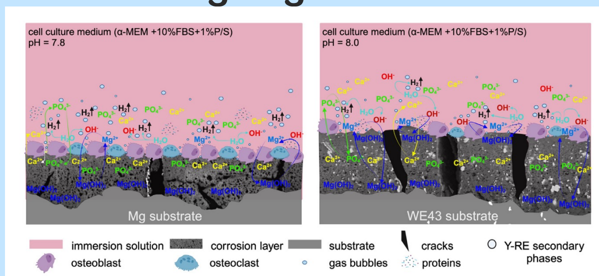


www.element22.com

ELEMENT 22

characterisation

Impact of bone cell coculture on Mg degradation

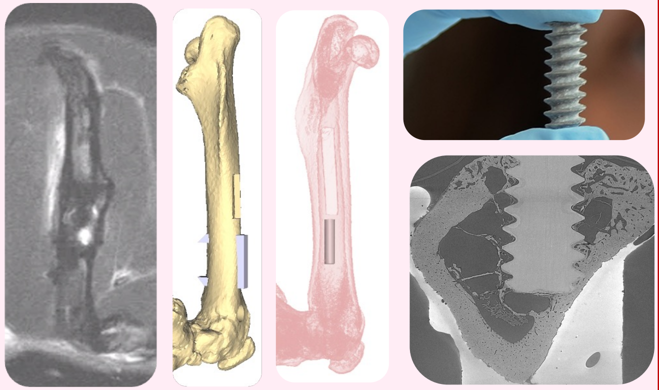


DMartinez et al. (2024) https://doi.org/10.1016/j.actbio.2024.08.015

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

- from materials to components using in operando experiments & digital twins

Bio-Materials



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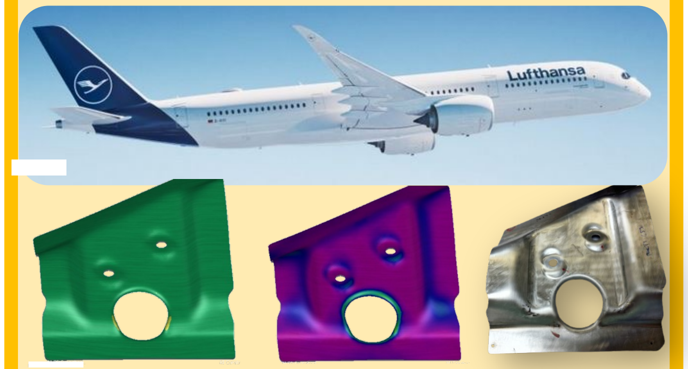

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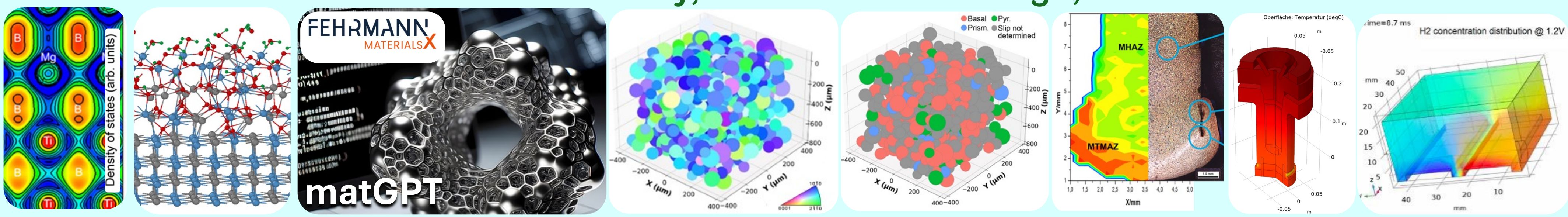


from atomistic modelling to finite element simulation and property predictions

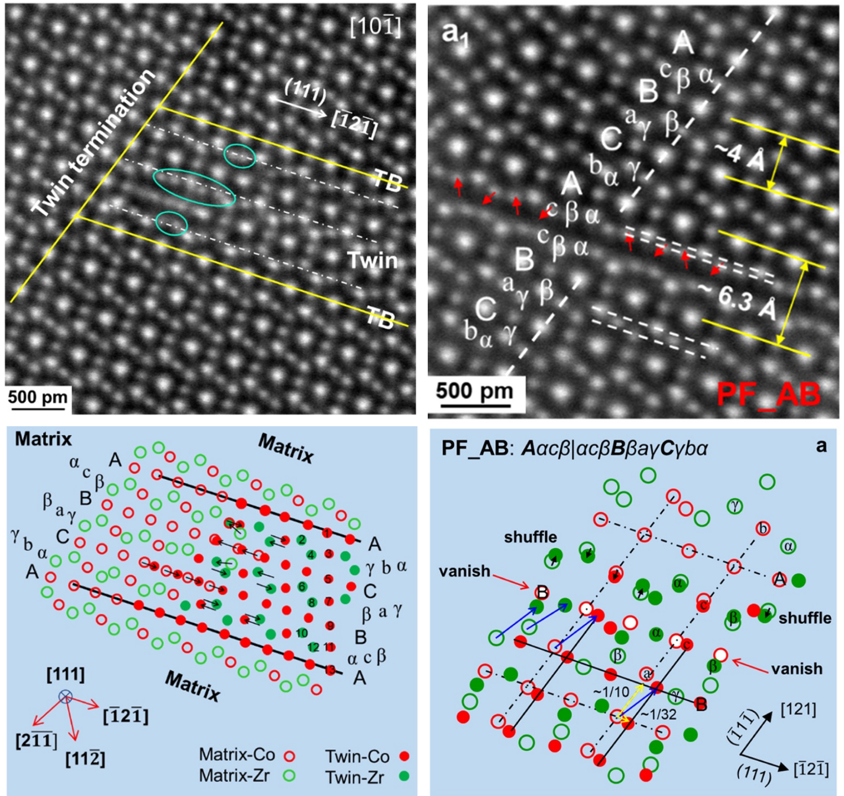
T4 Scale Bridging Designed Materials: From Fundamentals to Systems

Advanced Laves-Phase materials: novel deformation structures revealed by characterisation and modelling

Material characterisation

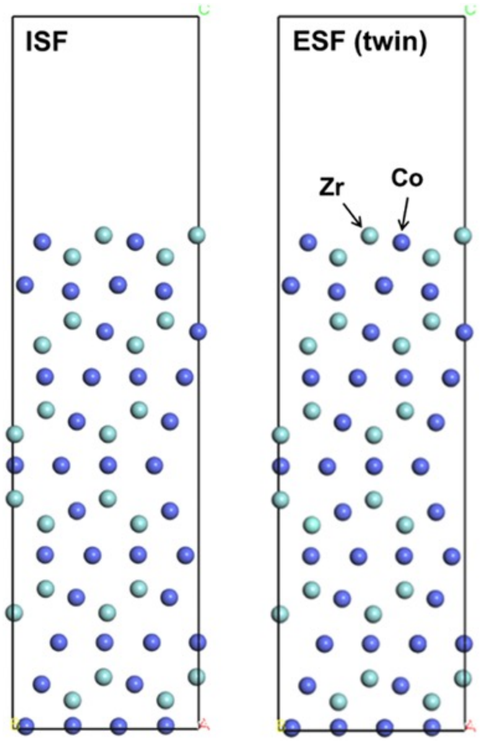
Synchro shear + atomic shuffling

Vacancy diffusion + atomic shuffling

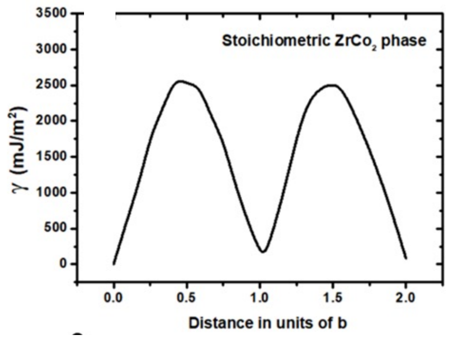


Accompanying Modelling

DFT supercell



Energy barriers



Defect energies

$ZrCo_2$	Energy (mJ/m²)
γ_{us}	2605
γ_{isf}	122
γ_{ut}	2548
$\gamma_{esf/tf}$	81
γ_{isf}/γ_{us}	0.047
γ_{us}/γ_{ut}	1.02
τ	1.14

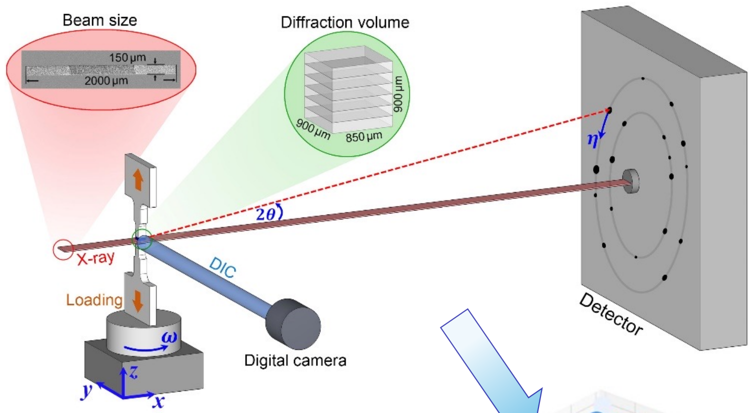
P3T4

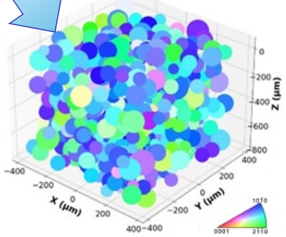
https://doi.org/10.1016/j.actamat.2023.119568

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

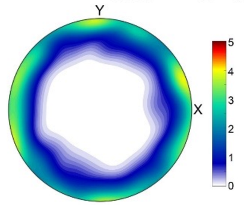
Grain-level insights into the deformation mechanisms of Mg alloys using in-situ 3DXRD

In-situ 3DXRD method

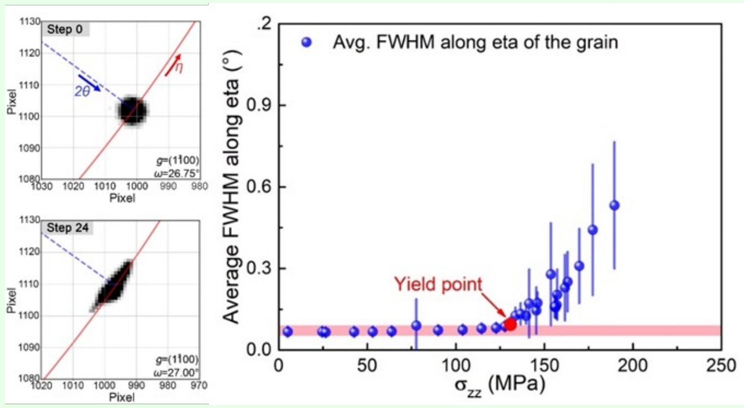




- Mg-3Al extruded alloy with a grain size of 100 µm
- In-situ experiments at DESY, Hamburg
- Grain reconstruction for grains at the 10^3 scale
- Combination with tension, compression, heating, etc.



{0001} Pole figure

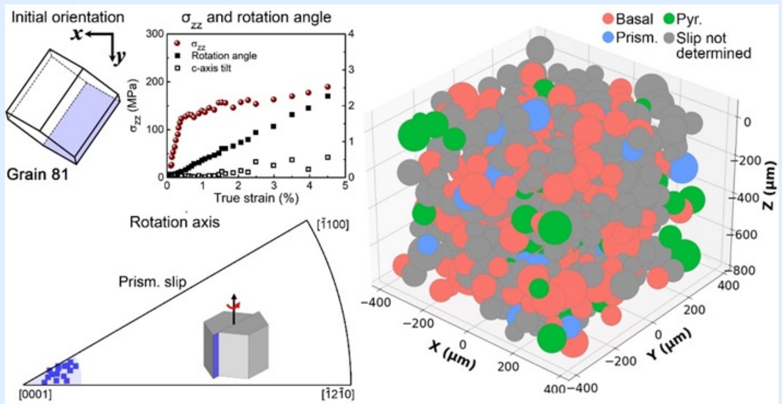


Grain-level yielding

- Diffraction spot tracking during loading
- Yield point of individual grains via spot broadening
- Grain-level stress tensor evolution via spot shift

Slip system identification

- Grain tracking during loading
- Slip system identification via rotation angle and rotation axis
- CRSS calculation for individual grains



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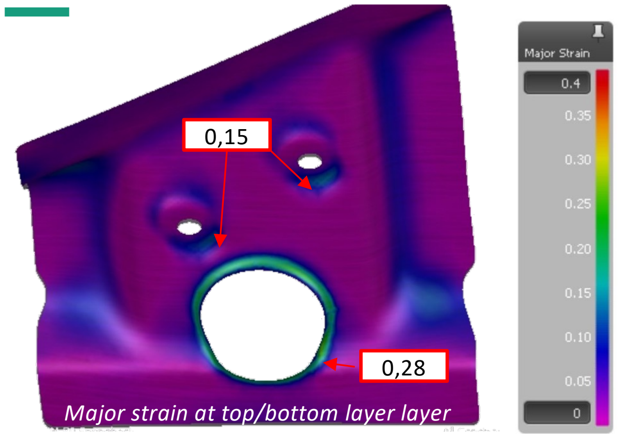
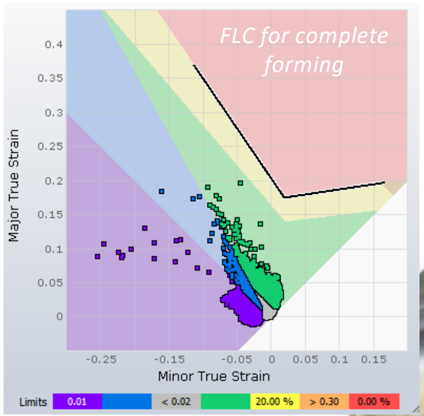
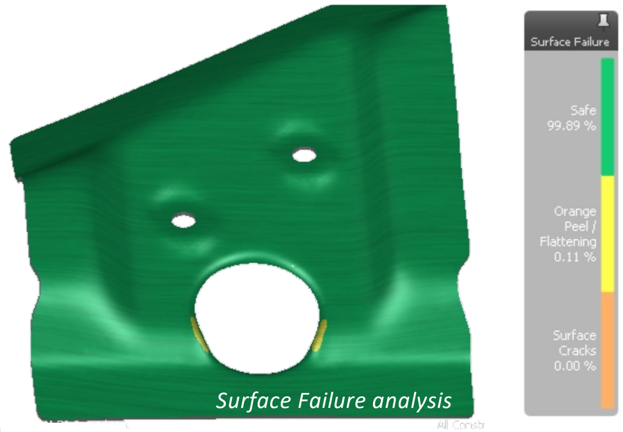
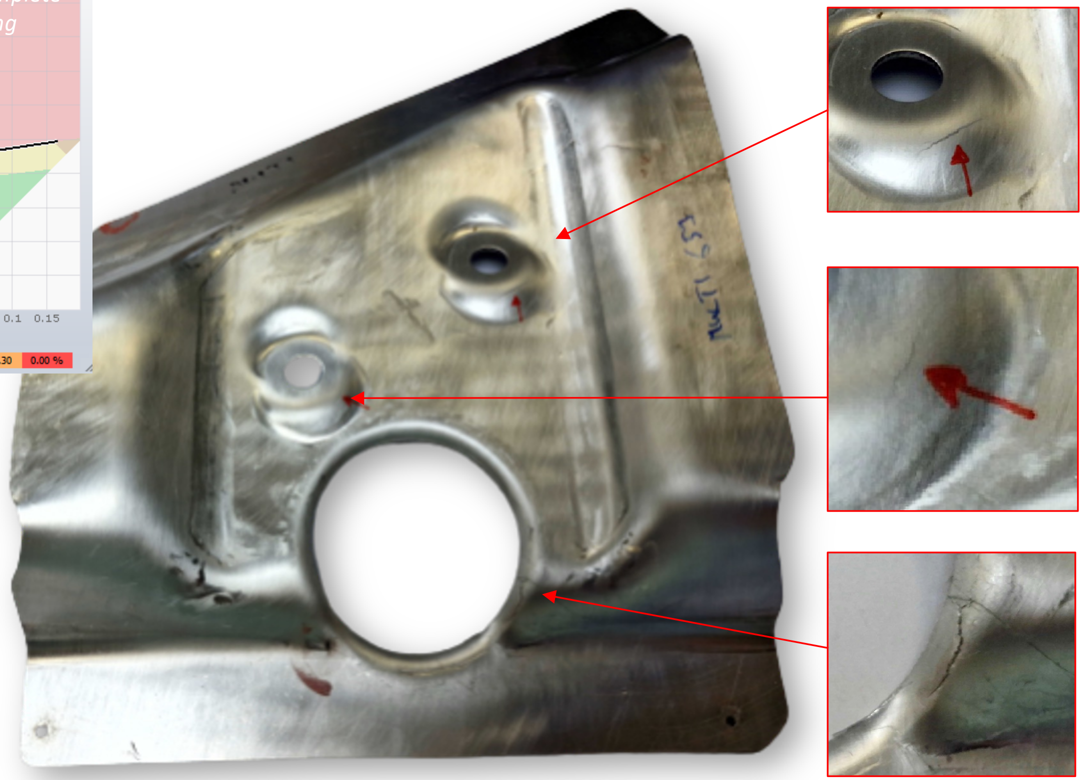
Demonstrator: FE-Simulation* results Mg-Zn-Gd*-Y (ZEW1) vs. Experiment (ZEWK)







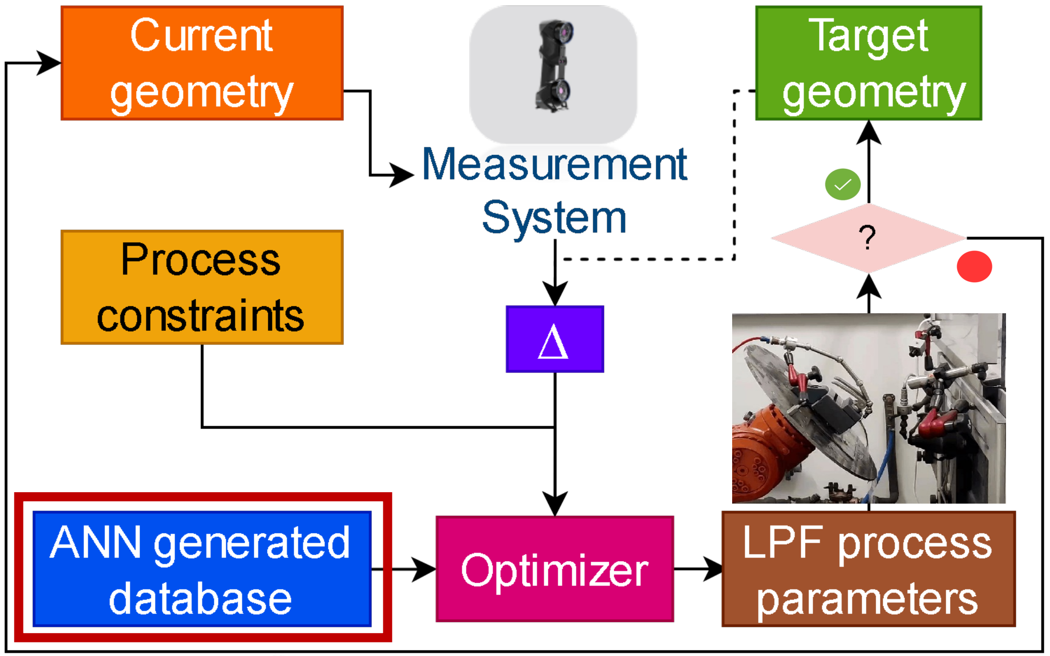


Public information

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

Data-driven approach to deform and modify thin titanium sheets by laser peen forming (LPF)

LPF process planning approach



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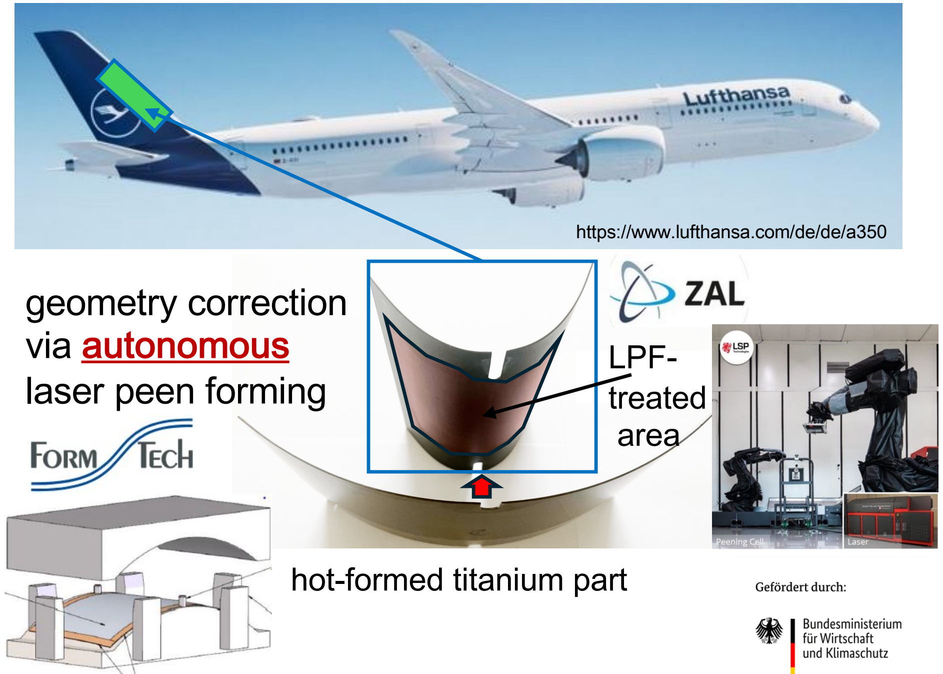
Demonstrator manufacturing and technology validation



Peencor

Gefördert durch:
Bundesministerium für Wirtschaft und Klimaschutz
aufgrund eines Beschlusses des Deutschen Bundestages

Sala, S.T., Bock, F.E., Pöltl, D., Klusemann, B., Huber, N., Kashaev, N.:
Journal of Intelligent Manufacturing (**2023**), https://doi.org/10.1007/s10845-023-02240-y

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

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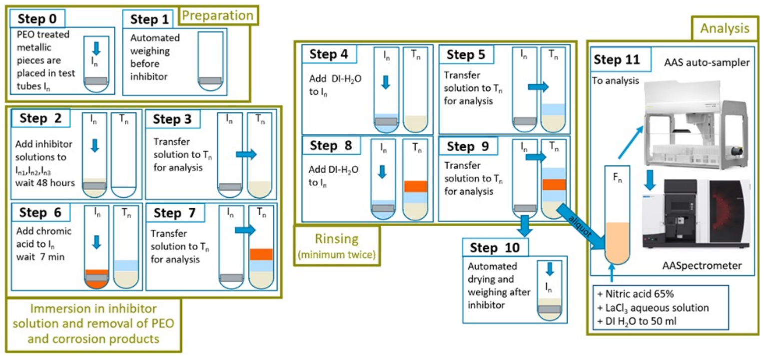
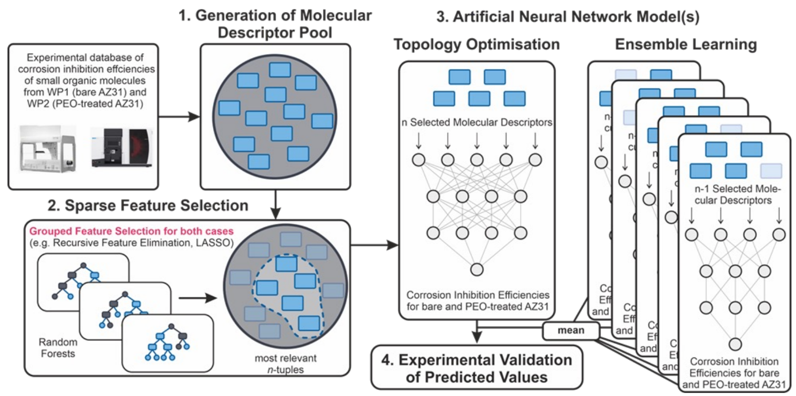
TUHH Technische Universität Hamburg

OPTIMA – Identification of optimal corrosion inhibitors for bare and PEO coated magnesium alloys by combining machine learning and robotic testing





The approach pursued in this project introduces a paradigm shift towards a highly automated and accelerated development of corrosion inhibitors on the example of magnesium alloys. Suitable chemical compounds will be identified through machine learning that relies on a large experimental database.

The project will show how machine learning combined with robotic experiments can help to identify optimal chemical compounds for corrosion protection for magnesium alloys with and without inorganic coating.

DFG Deutsche Forschungsgemeinschaft

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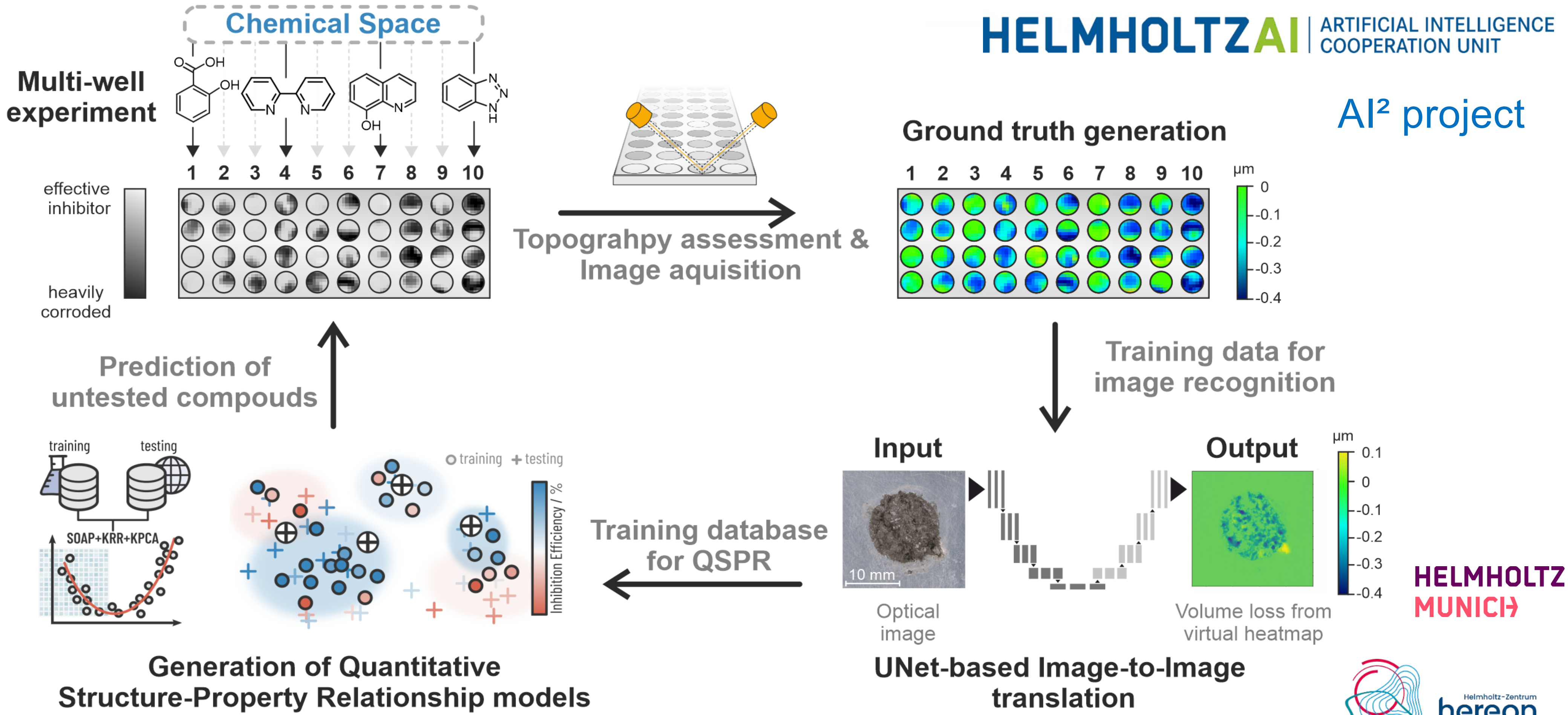
in-silico corrosion inhibitor discovery: coupling QSPR approaches with AI-based corrosion quantification



A. Lisitsyna, C. Song, T. Würger, B. Vaghefinazari, M. L. Zheludkevich, S. Albarqouni, S. V. Lamaka, C. Feiler, manuscript in preparation.

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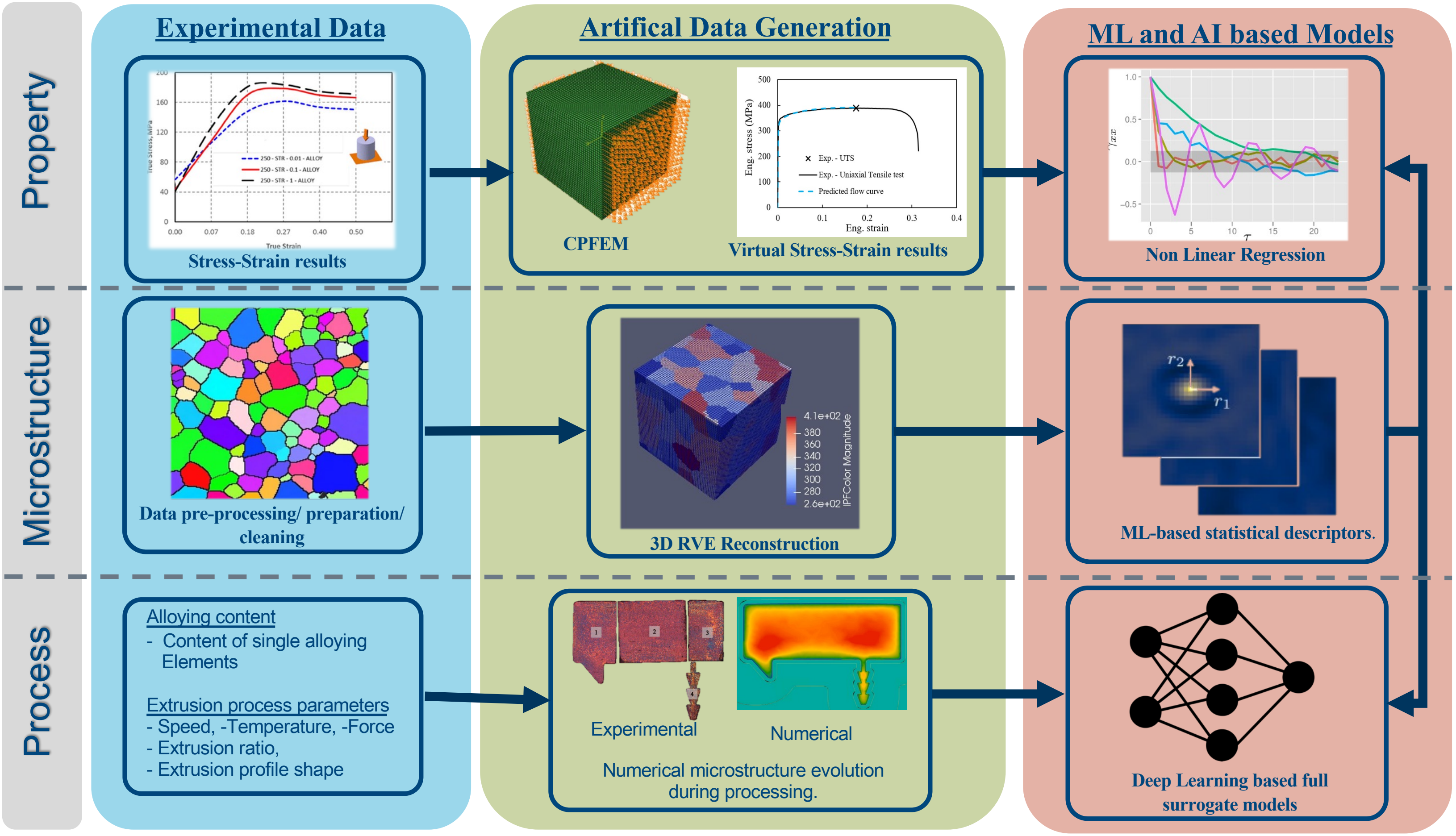
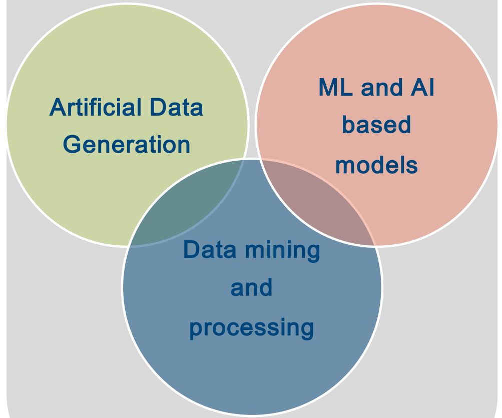
AI-enhanced Material Design Exploration



- Hybrid experimental and simulation-based Process-Structure-Property relation.
- Data collection, organization and generation.
- AI enhanced exploration for material and process design space.



“Process-Structure-Property” of extruded Mg alloys for tailored property profiles

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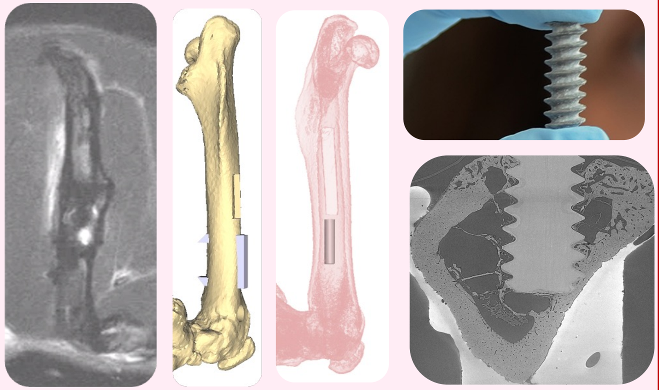

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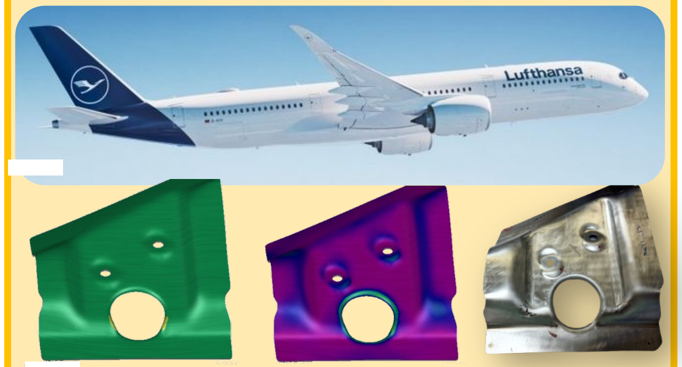

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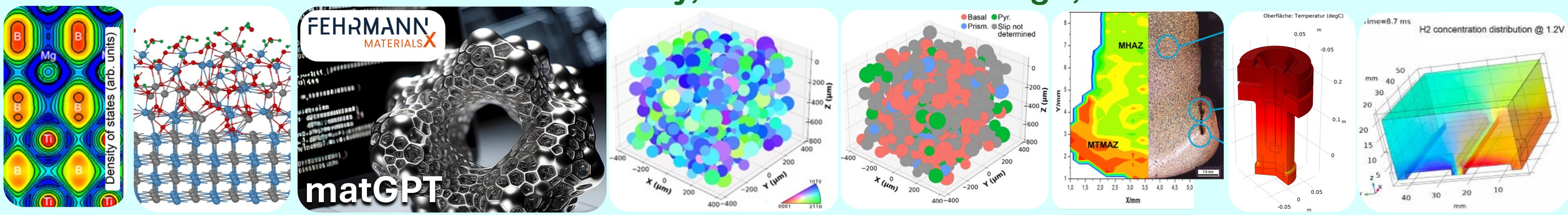
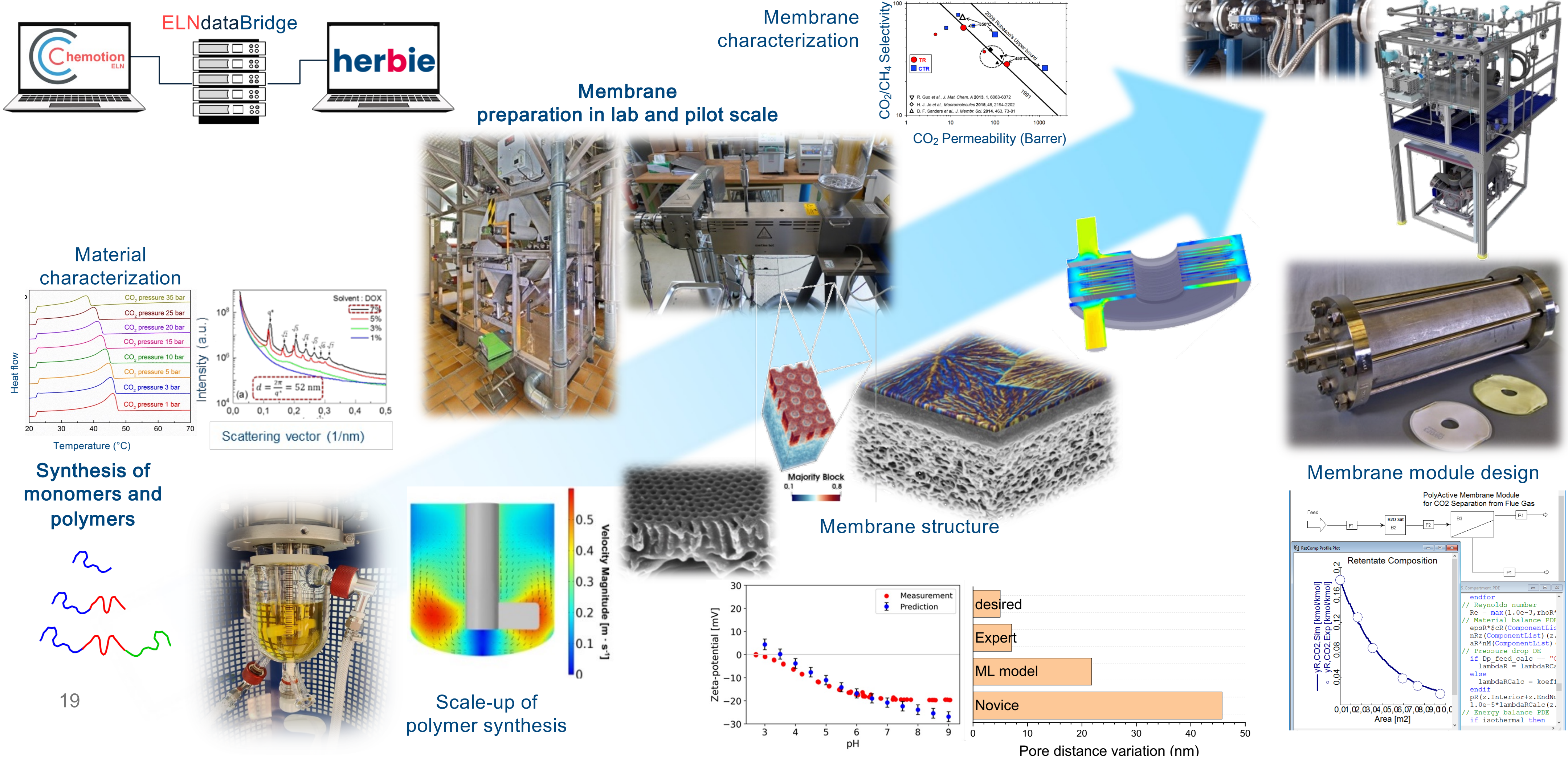


from atomistic modelling to finite element simulation and property predictions

Polymer Membranes for Efficient Separation

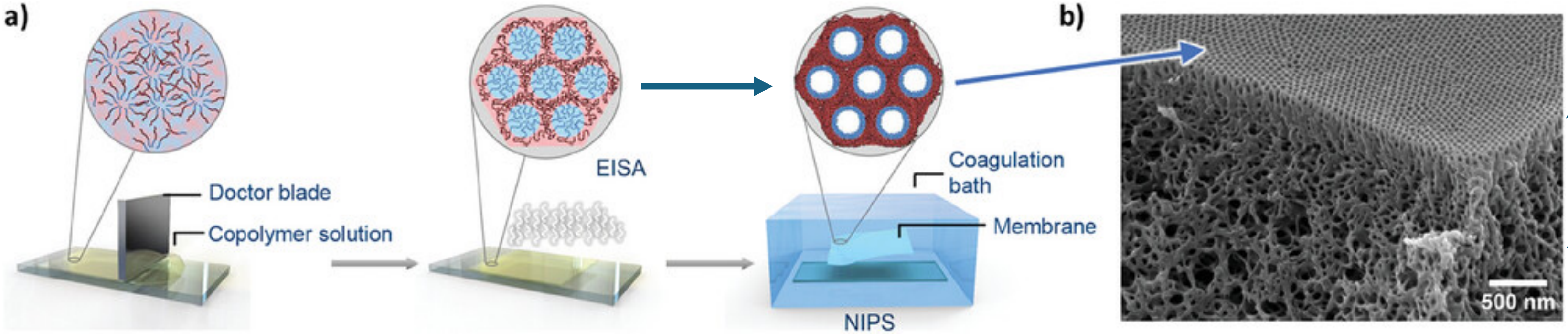
T4 Scale Bridging Designed Materials: From Fundamentals to Systems

From Polymer Synthesis to Membrane Technology



T4 Scale Bridging Designed Materials: From Fundamentals to Systems

Complete digital twin for predicting formation of integral-asymmetric isoporous diblock copolymer membranes



Isoporous top layer
EISA
➔ selectivity

Macroporous bottom structure
NIPS
➔ mechanical support

EISA
evaporation induced self-assembly
+
NIPS
nonsolvent-induced phase separation
=
SNIPS-process for membrane preparation

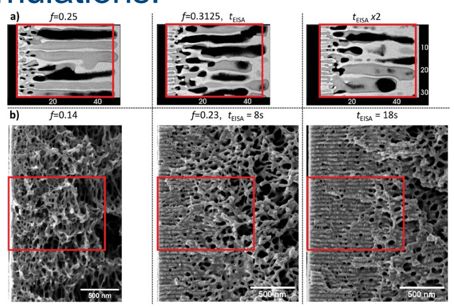
In collaboration with Georg-August University Göttingen: N. Blagojevic et al., Advanced Materials 2024, DOI: 10.1002/adma.202404560, supported by (BMBF) within the project 16ME0658K MExMeMo and European Union

Simulation of the entire SNIPS process via large-scale particle simulations:

Simulation of EISA
O. Dreyer et al., Macromolecules 2023,
DOI 10.1021/acs.macromol.3c01220
O. Dreyer et al., Macromolecules 2022,
DOI 10.1021/acs.macromol.2c00612

Simulation of entire SNIPS-Process
This work

CONFIRMATION VIA EXPERIMENT



polystyrene (PS)-block-poly(4-vinylpyridine) (P4VP)

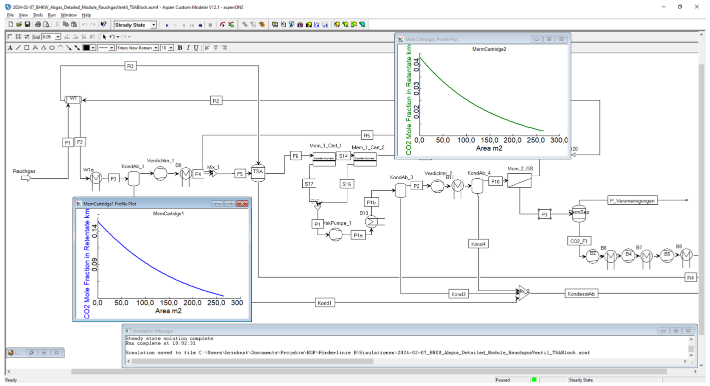
P3T4

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

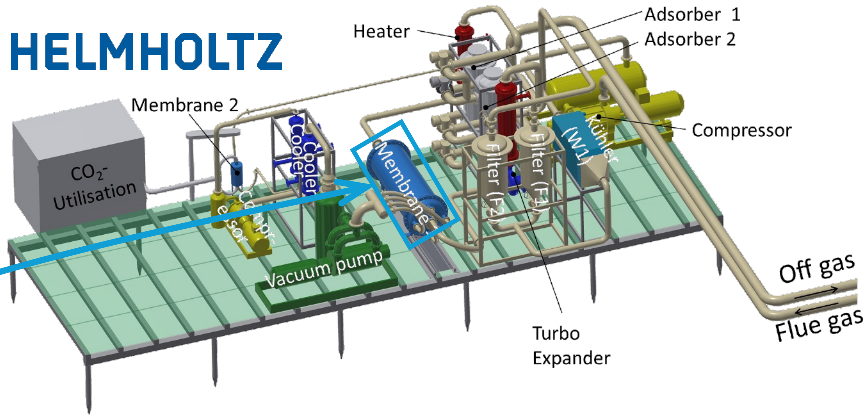
From Polymer Synthesis to Membrane Technology

Chem. Ing. Tech. 2019, 91, No. 1–2, 30–37
US 10,010,832,B2
EP 3 227 004 B1
EP Pat Application 4461400

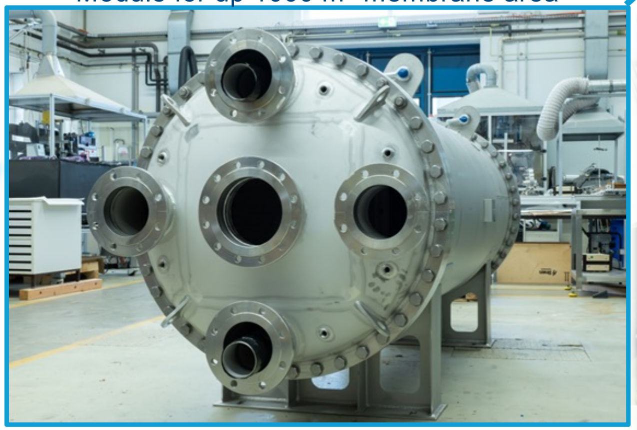
Membrane based CO_2 separation from flue gas: process simulation



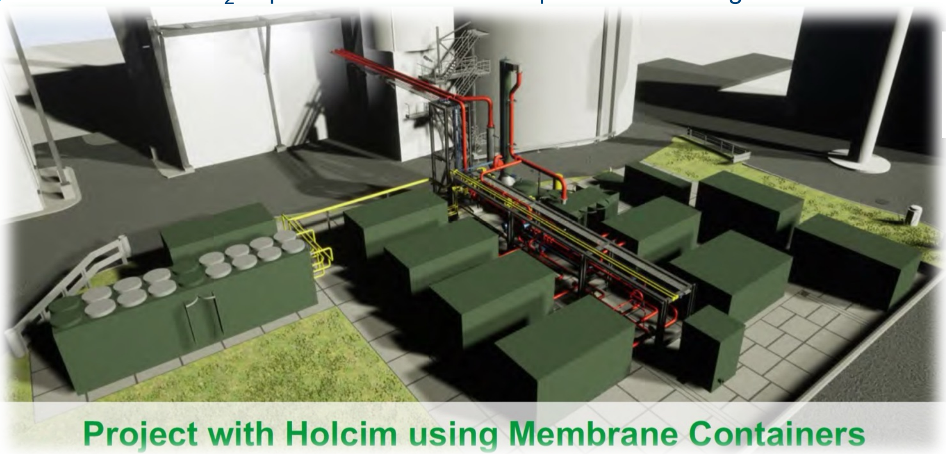
Membrane process for CO_2 separation at Hereon combined heat and power plant



Module for up 1000 m² membrane area



CO_2 separation from cement production flue gas



Cool Planet Technologies

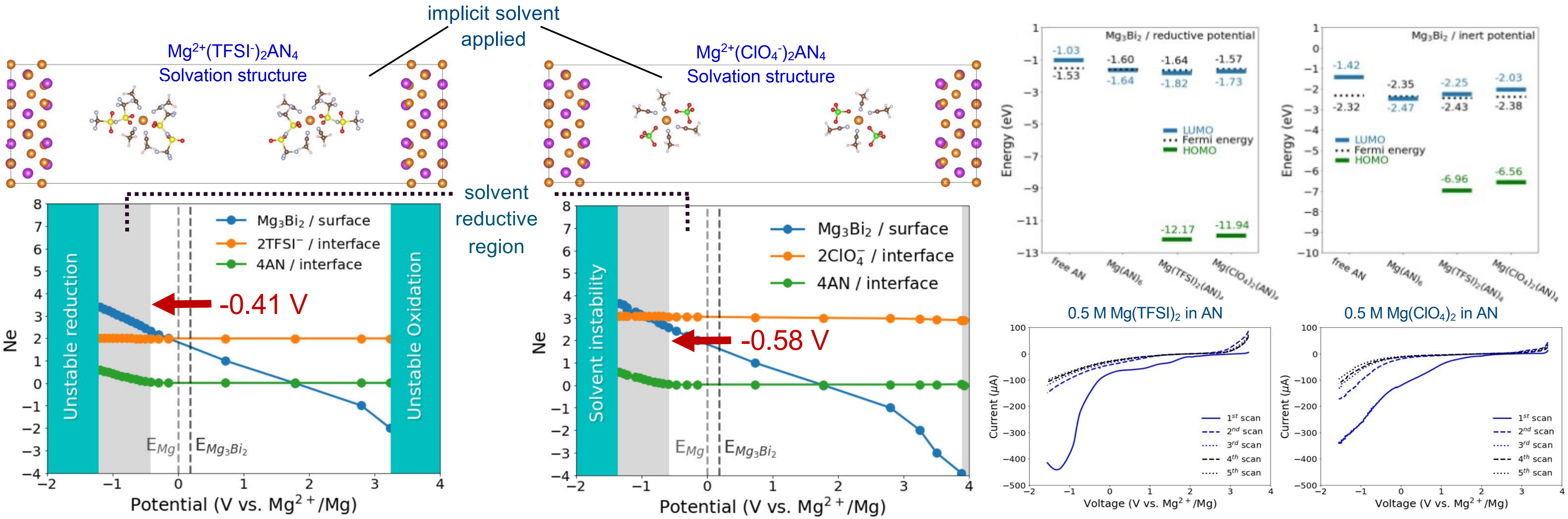
HOLCIM

Efficient Mg-Ion Batteries

T4 Scale Bridging Designed Materials

From potential-dependent DFT study to improved stability of electrolyte for Mg battery

- Accurate atomic / molecular scale methodology to define electrolyte stability required, accelerate Mg anodes interface study, overcome limits of translation of existing Li battery knowledge.
- Expanded methodology reveals different electrolyte's degradation behaviour, including anion effect in solvation structures, suggesting broader applicability in multi-component electrolyte solutions research.



P3T4 H. Kim, M. Deng, A. Fortuin, T. Würger, P. Georgopanos, D. Kramer, M. Zheludkevich, D. Höche, Advanced Energy Materials (2024)

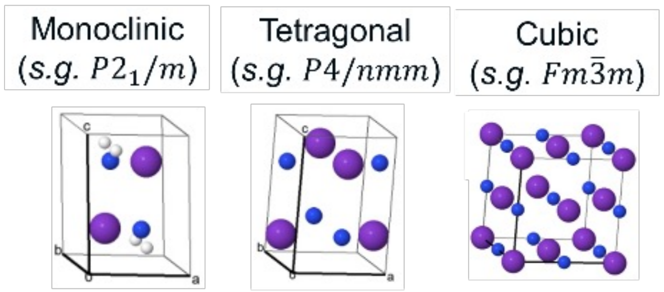
Efficient Hydrogen Storage

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

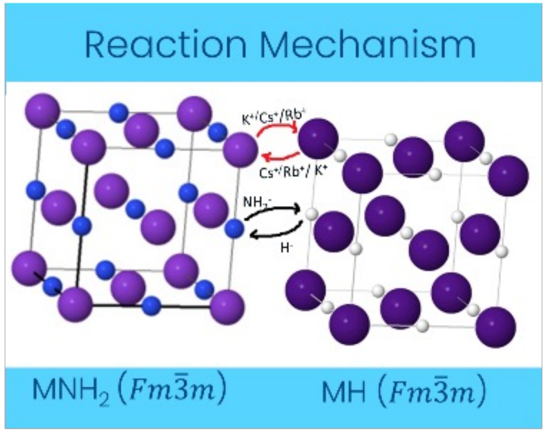
First-principles study on interfacial property in MgB_2-based reactive hydride composites

➔ generating a metal hydrides database for machine learning

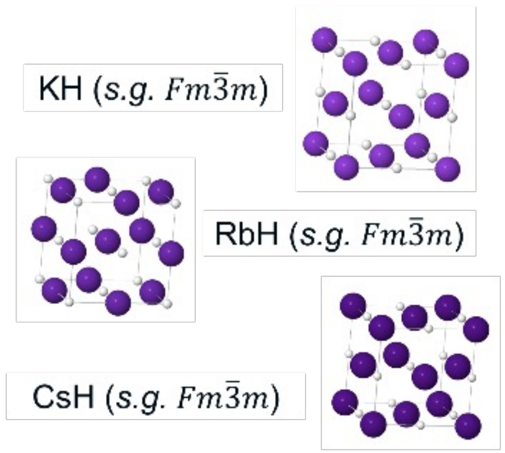
STRUCTURE OF AMIDES MNH_2



	Monoclinic (s.g. $P2_1/m$)	Tetragonal (s.g. $P4/nmm$)	Cubic (s.g. $Fm\bar{3}m$)
KNH_2	RT	~ 50 °C	~ 75 °C
$RbNH_2$	RT	-	~ 65 °C
$CsNH_2$	-	RT	~ 55 °C



STRUCTURE OF HYDRIDES MH



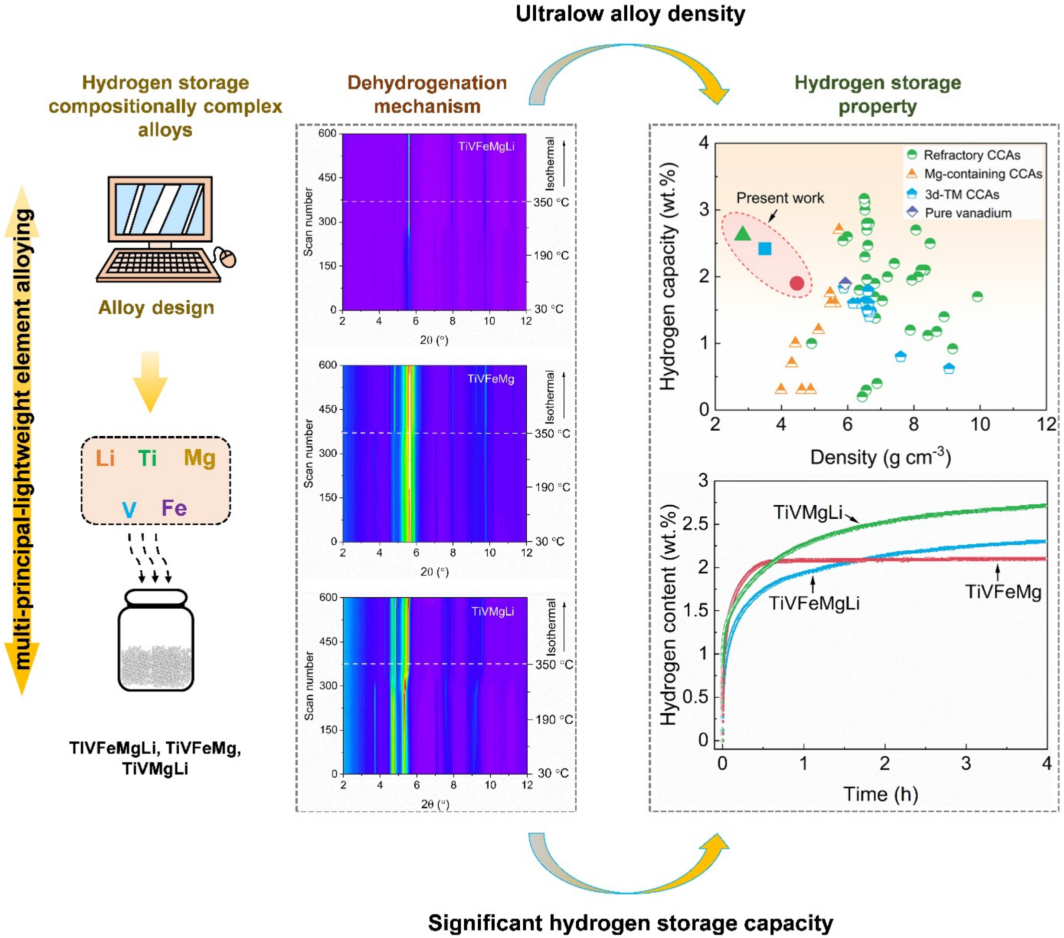
Le, T.T., Bordignon, S., Chierotti, M.R., **Shang, Y., Schökel, A., Klassen, T., Pistidda, C.** *Mixed Metal Amide-Hydride Solid Solutions for Potential Energy Storage Applications*. Inorganic Chemistry **2024** 63 (24), 11233-11241. **DOI: 10.1021/acs.inorgchem.4c01016**

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

Ultra-lightweight compositionally complex alloys with large ambient-temperature hydrogen storage capacity

New Hydrogen Storage Alloys: Lightest Hydrogen Storing High Entropy Alloys (HEA) so far

- ➔ CALPHAD thermodynamic modelling to identify promising composition
- ➔ in-situ Synchrotron experiments to analyse phase transformations
- ➔ Experimental verification of high hydrogen storage capacity
- ➔ Kinetic modelling shows hydrogen diffusion limited process



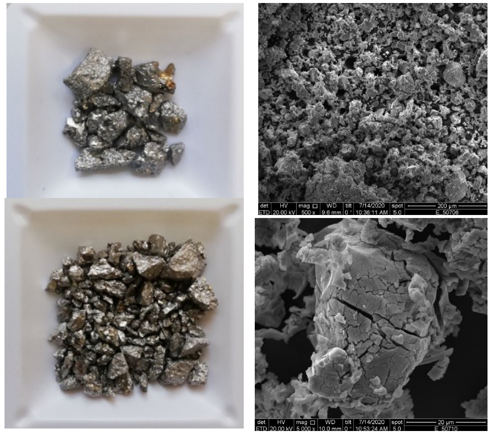
Yuanyuan Shang et al.,
Materials Today 67 (2023), 113-126

P3T4

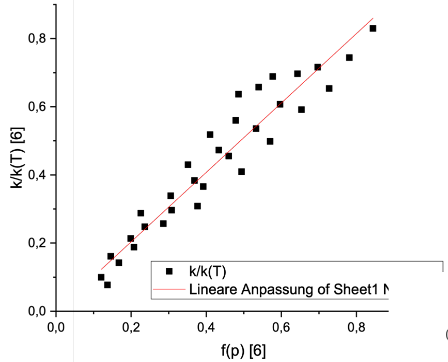
IF 26.9

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

Modelling of material for scaled-up Hydrogen storage tank including kinetics



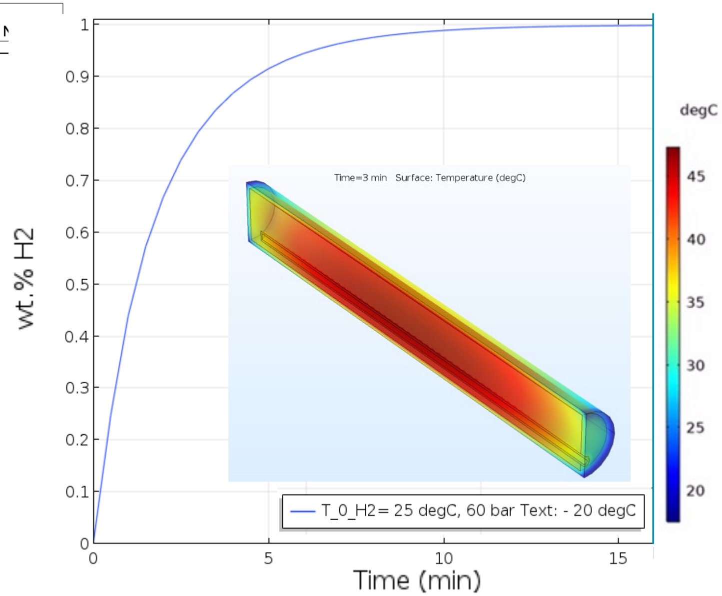
Modelling reaction kinetics



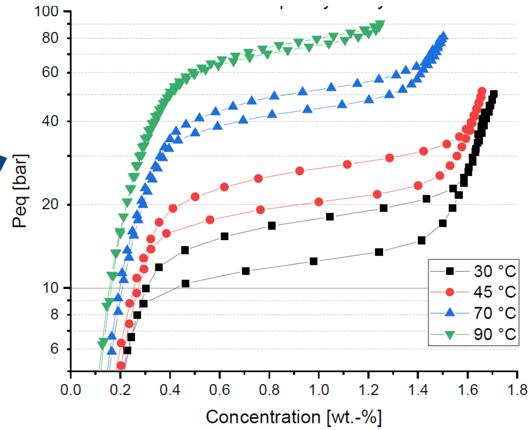
$$\frac{d\alpha}{dt} = K(T)\,F(p)\,G(\alpha)$$

$$\frac{d\alpha}{dt} = A\exp\left(\frac{-E_A}{R\,T}\right)\;\frac{(p-p_{eq})^{\frac{1}{2}}}{p_{eq}}\;\frac{3(1-\alpha)^{\frac{2}{3}}}{2\left(1-(1-\alpha)^{\frac{1}{3}}\right)}$$

80 % H_2 refueling in 3 min



Experimental data

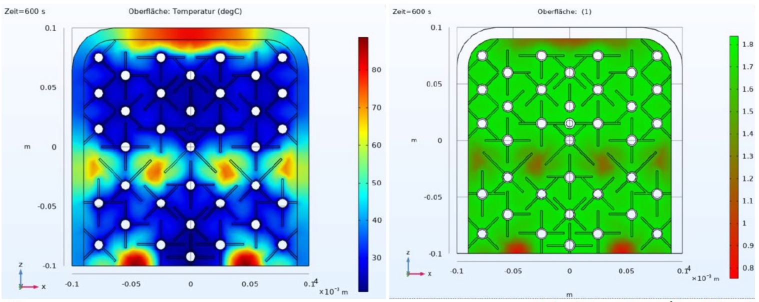


T4 Scale Bridging Designed Materials: From Fundamentals to Systems

thermo-chemical calculation and design of hydrogen storage tanks to fulfill requirements of application

Tailored storage tank design to perform WLTP-cycle

Temperature [°C] Hydrogen loading [wt-%]



Lasttabelle: A - 8

Schnitt z = 1 m / t = 20 min

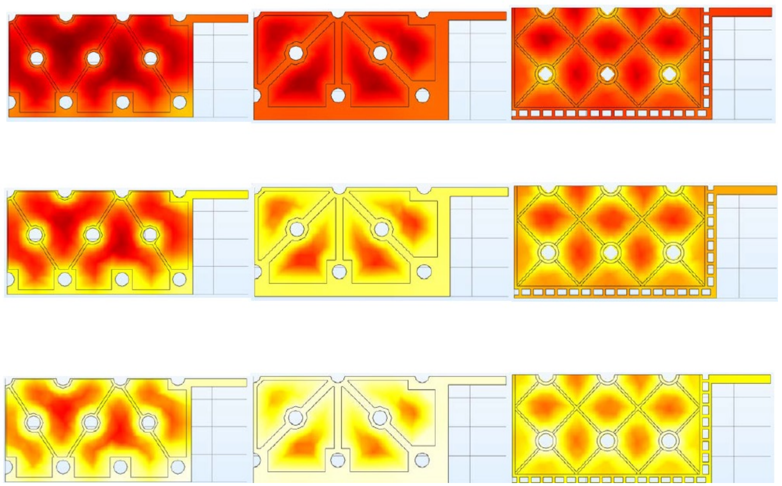
Temperatur [°C]
38 °C – 78 °C

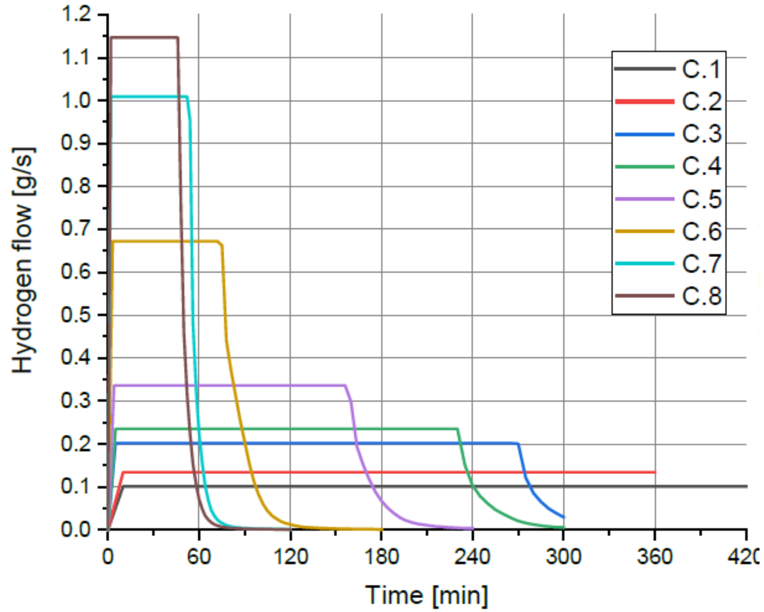
Variante 1 Variante 2 Variante 3

A.8: Originale Config.

A.8: Originale Config. – min. HX-Flow

A.8: Optimierte Config. – max. HX-Flow





T4 Scale Bridging Designed Materials: From Fundamentals to Systems

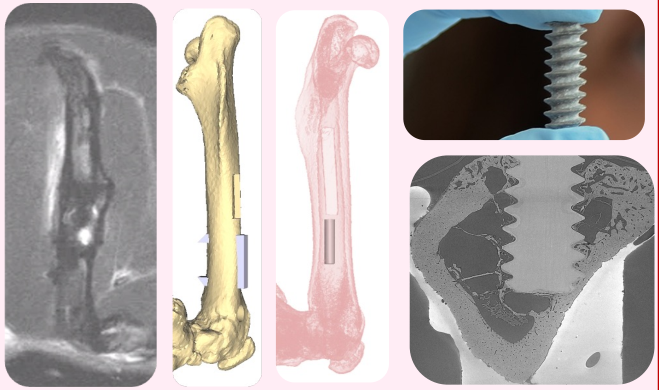
BMDV–NOW–Project: Green electricty for the research Vessel Coriolis: Living Hydrogen Lab

- **development and realization of a hydrogen lab on bord of a ship**
- **powering the Coriolis for 4 hours based on fuel cell and metal hydride storage**
- **data generation under real operation conditions for calibration of future system simulations**

T4 Scale Bridging Designed Materials: From Fundamentals to Systems

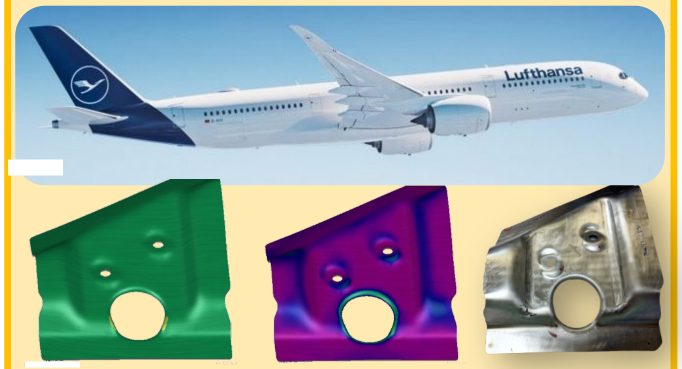
- from materials to components using in operando experiments & digital twins

Bio-Materials



biocompatible and resorbable implants

Light Weight Structures

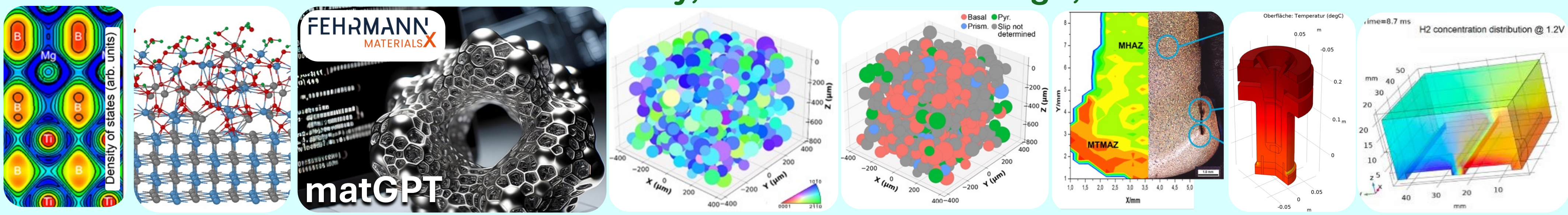


resource-efficient materials

Energy and Mobility

climate-friendly technologies

Information-Based Materials Discovery, Microstructure Design, Performance Prediction



from atomistic modelling to finite element simulation and property predictions

thank you!

Helmholtz-Zentrum hereon