Rethinking Nanoindentation toward Explainable Machine Learning and Open Science: In Situ Tip Radius Estimation and Advanced Property Mapping

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Nanoindentation has evolved into a high-throughput method for mechanical property characterisation. While the Oliver–Pharr approach remains standard for measuring elastic modulus and hardness, many studies have sought to estimate additional properties using dimensional analysis, finite-element simulations, and machine learning. However, most models assume perfectly sharp indenters and ignore tip wear, which introduces significant bias.

This talk presents a method to determine the radius of a Berkovich tip directly from the load-displacement curve. A Residual Multi-Fidelity Neural Network was trained on 2D and 3D simulations and experimental data. The study reveals that tips not only become blunt over time but can also sharpen under certain conditions. Features derived from the full curve enable accurate tip-radius prediction, and game-theory-based analysis confirms that normalised loading parameters are most influential.

The second part addresses property mapping and clustering. Conventional maps based on elastic modulus and hardness fail at disentangling nanoindentation data when the indentation response (elastic and plastic fields) begins to probe multiple phases. Using a curated High-Speed Steel dataset with 3,300 labelled indents, we show that unsupervised and supervised learning on full-curve features can separate materials constituents that *E*–*H* alone cannot. Explainable machine learning methods provide insight into model decisions, and all datasets and models are openly available.

This work introduces in situ tip monitoring, explainable multi-fidelity learning, and feature-rich clustering to improve nanoindentation analysis beyond traditional approaches.

Utilizing deep learning to study and predict the behaviour of biodegradable magnesium- and zinc-based implants

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Biodegradable alloys based on magnesium and zinc are heavily researched for their use to support bone healing or vascular repair. In initial *in vitro* tests, the mechanical properties and degradation dynamics of the implants depending on the alloy design are investigated. Once acceptable properties have been established, *in vivo* animal tests are performed, which will often be supplemented by *ex vivo* micro computed tomography (µCT) to assess osseointegration at high resolution in 3D in addition to the gold standard of histology. Deep learning is used across the different testing stages to accelerate experimental work. At the stage of *in vitro* testing, we have established a reproducible framework to predict the ultimate tensile strength (UTS) and degradation rate of Zn-Mg alloys based on processing, microstructural and environmental parameters. The UTS can be predicted with mean errors of 10.97%, while the error for the degradation rate is significantly larger and further optimization is required. At the stage of pre-clinical *ex vivo* research, we have established deep learning-based methods for digital volume correlation of time-resolved µCT imaging of push-out tests to accelerate the understanding of the quality of osseointegration of Mg-based implants. Additionally, we have implemented and tailored a CycleGAN, as well as diffusion models, to enable modality transfer between µCT and histology such that the biological information can be assessed independent of destructive sample preparation. The quality of the synthetic histology data is high and current work focusses on improving the resolution for further pathological assessment.

Data- and Physics-Driven Design of Defect-Tolerant TiN/MoN and TiN/TaN Superlattice Coatings

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Artificial intelligence and data-driven methods increasingly complement physics-based approaches in materials science by accelerating materials discovery and guiding microstructure design. In this contribution, we demonstrate how density functional theory, molecular dynamics, and data-assisted structure–property correlations can be combined to design defect-tolerant transition-metal nitride coatings, with a focus on TiN-based superlattices such as TiN/MoN, TiN/TaN, and doped architectures.

Advanced ceramic coatings exhibit exceptional hardness and thermal stability but typically suffer from limited plasticity and fracture toughness. Using DFT-derived ductility indicators and atomistic simulations, we identify the critical roles of bilayer period, chemical complexity, nitrogen content, and point-defect populations in controlling elastic anisotropy, dislocation nucleation, and interface stability. Guided by these insights, superlattices with tailored layer architectures, controlled vacancy concentrations, and targeted alloying were synthesized by reactive magnetron sputtering.

Micromechanical testing and advanced electron microscopy reveal that engineered defect populations can act as precursors for dislocation nucleation, enabling micro-slip and enhanced plastic deformability while preserving high load-bearing capacity. Pronounced superlattice effects are observed, with optimized architectures achieving simultaneous improvements in hardness and fracture toughness. This work demonstrates how integrating computational modeling, data-driven analysis, and targeted experiments enables efficient defect-by-design strategies to overcome the plasticity bottleneck in ceramic coatings.

DFT and MLIP study of solute segregation to coherent and semi-coherent α-Fe/Fe_3C interfaces

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Solute segregation to interfaces strongly affects material behavior. Most theoretical studies focus on grain boundaries and coherent interfaces, whereas semi-coherent interfaces remain largely unexplored due to structural complexity exceeding the practical capability of density functional theory (DFT) or chemical complexity constrained by the availability of classical interatomic potentials. Here, we investigate solute segregation to the coherent and semi-coherent α-Fe/Fe_3C interface and its mechanical impact using novel universal machine-learning interatomic potentials (uMLIPs). DFT calculated solution enthalpies, segregation energetics, and cohesion changes at the coherent interface serve to benchmark several state-of-the-art uMLIPs, identifying GRACE-2L-OAM and GRACE-2L-OMAT as most consistent with quantum-mechanical predictions. Among the studied tramp and trace elements, Cu shows the strongest segregation energy to the coherent interface of ≈ -0.3 eV. However, at the semi-coherent interface, all elements exhibit significantly stronger segregation energetics, reaching below ≈ -1.5 eV, with the deepest traps near the misfit dislocation core. Sb, Sn, P, and As strongly reduce the coherent interface cohesion, Cu mildly, while Ni has a negligible influence, and Cr and Mo slightly enhance cohesion. At the semi-coherent interface, all solutes except P promote embrittlement, with Sn and Sb showing the strongest effect. These results underscore the importance of realistic interface structures for predictive materials design.

How to predict friction: A tale of surface topography and machine learning

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Friction is ubiquitous in daily life, from nanoscale machines to large engineering components. By probing the intricate interplay between system parameters and frictional behavior, scientists seek to unveil the underlying mechanisms that enable prediction and control of friction—an essential step toward carbon neutrality. Yet, reproducing frictional behavior in experiments is notoriously difficult. We will present that this difficulty arises from the extreme sensitivity of tribological systems to tiny variations, typically presumed well-controlled. Even after meticulously minimizing surface topography variations to semiconductor-industry standards and curtailing misalignment-induced oscillations, the influence of lingering variations in both remains subtly intertwined. In turn, minute initial differences lead to statistically significant variations in friction and wear, giving rise to system-level chaotic behavior. Nevertheless, by leveraging features of surface topography and oscillations, we identified a pioneering physical model that accurately predicts high-friction regions in vastly different lubrication conditions, with its performance further improved through machine learning.

Artificial intelligence and data-driven design of materials

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Recent advances in materials science have introduced novel compositionally and structurally complex materials, which have opened up a vast configuration space for discovery. These innovative materials have the potential to transform industries related to energy storage, transportation, and medicine. However, traditional methodologies are not well-suited to dealing with the high-dimensional configuration spaces involved. This presentation addresses the application of artificial intelligence and data-driven strategies as an emerging solution to this problem. These strategies combine artificial intelligence approaches with physical laws and advanced simulation techniques to improve the predictability of AI models, while automated digital workflows facilitate the efficient exploration of materials and their discovery. This synergy accelerates the design pipeline and effectively supports the navigation of the newly opened vast material space. Real-world case studies will demonstrate the potential of these methodologies.

Modeling the segregation of intermetallic phases in Pb-free microelectronic solders

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Driven by environmental and legislative requirements, the microelectronics industry has transitioned toward Pb-free solder materials. Sn–Ag–Cu solder balls used in microelectronics tend to segregate intermetallic phases at elevated temperatures, predominantly along grain boundaries. The formation of these phases is governed by Gibbs energy potentials, with mechanical contributions playing a crucial role due to the significant transformation eigenstrains associated with the lower specific volume of the intermetallics. This work is based on the principle of minimum entropy production while ensuring conservation of energy and mass of the diffusing species. The governing equations are formulated within a variational framework and solved in an automated fashion using an open-source finite element package. The results demonstrate that mechanical contributions to the chemical potential are non-negligible at grain boundaries, providing a substantial additional driving force for intermetallic phase formation. Conventional variational formulations for reactive diffusion generally fail to enforce continuity of species flux across interfaces and are therefore prone to instability. To address this limitation, the flux is introduced here as an additional degree of freedom. Simulations show that the intermetallic product phase evolves predominantly from triple junctions of the parent grains, in agreement with in-situ ageing experiments on cold-formed Sn–Ag–Cu solder balls observed using scanning electron microscopy.

Experimental Investigation and Simulation Validation of Friction Stir Welding of thick Aluminium 6082-T651

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Friction stir welding (FSW) is a well-established solid-state joining process for aluminium alloys, but its industrial application is still largely limited to relatively thin sections. This project aims to extend FSW to aluminium EN AW-6082-T651 thick-walled profiles using a bobbin tool.

A numerical simulation model is being developed and validated using experimental data. In a first step, experiments are conducted to generate input data for model development, including system stiffness characteristics, process forces determined from preliminary tests, and boundary conditions defined by the clamping setup. In a second step, independent welding experiments are used to validate the model by comparing simulated results with measured process temperatures and the microstructure of weld cross-sections.

The experimental program employs three tool concepts: a pinless tool, a conventional FSW tool, and a bobbin tool. In this contribution, results obtained with the pinless tool are presented as the first stage of the investigation. Based on these results, the simulation model will be extended stepwise as the tool complexity increases.

The main objective of this work is to establish a calibrated friction and heat generation model based on experimental data using a pinless tool to reduce complexity. The model provides a basis for subsequent extension to a conventional FSW tool and ultimately a bobbin tool, thereby supporting the systematic advancement of the simulation framework toward more complex process scenarios.

Workflow for Automated Information Extraction from Materials Science Literature Using Ontology-Guided Reflective AI Agents: A γ-TiAl Creep Case Study

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Recent advances in natural language processing have made text mining a powerful tool for extracting knowledge from scientific literature. In materials science, large volumes of experimental data remain untapped in the literature, which could be utilised for inverse materials design. However, reliable extraction of structured information is hindered by ambiguous terminology and the interleaving of multiple datasets within individual articles. This work presents a fully automated workflow that addresses these challenges through agent-based named entity disambiguation (NED) and dataset-level segmentation, guided through a formally defined ontological data model. Autonomous AI agents, supported by both proprietary and open-source large language models, analyse textual content using ontology-defined entity classes, relations, and constraints to extract and link fragmented information, yielding coherent composition-process-structure-property (CPSP)-aware datasets. To further improve reliability, the workflow employs continuous reflection loops that iteratively evaluate and refine extracted information. The workflow is applied to a γ-TiAl creep case literature study, where extracted datasets from >100 most relevant publications are analysed to identify interdependent relationships between alloy composition, heat-treatment–induced microstructures, and reported creep rates. Benchmark evaluation using vanilla settings of general language models as the baseline demonstrates improvements in both entity disambiguation and dataset segmentation. The workflow also supports ad-hoc data model creation and dynamic prompt generation for scalable information extraction across diverse materials science domains.

From Spectra to Insight: Multivariate Analysis of NIR Data for Early Degradation Detection in Photovoltaic Materials

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Photovoltaic (PV) modules are subjected to long-term environmental stressors such as thermal cycling, ultraviolet radiation, and moisture. These conditions cause physical and chemical degradation in polymeric-based PV components (such as encapsulants and backsheets) along with electrical performance losses for the whole product [1]. Near-infrared (NIR) spectroscopy is used as a non-destructive and non-invasive tool to assess the chemical state of PV packaging materials directly in the field. However, NIR measurements generate high-dimensional spectral datasets with multiple overlapping absorption features (bands), limiting direct interpretation of degradation trends. To overcome this challenge, unsupervised data-driven techniques are applied. Principal Component Analysis (PCA) is used to identify dominant variance and associate them with degradation features of PV materials, while Uniform Manifold Approximation and Projection (UMAP) captures subtle, nonlinear differences between material types. Twelve PV modules from a PV plant in central Italy, in operation for 13 years, were selected to assess long-term degradation of polymers. The analysis identified spectral patterns linked to degradation, shifting exposed from unexposed modules and differentiating the two encapsulant types. PCA loadings indicate that the main differences occur in spectral regions reflecting variations in vinyl acetate content and additive composition. While UMAP provides clearer separation by capturing non-linear patterns, these observations are confirmed through laboratory chemical analysis. This approach is intended for integration with robotic platforms for in-field polymer monitoring and PV lifetime estimation enabling predictive maintenance to preserve efficiency, and reduce energy losses.

References

[1] A. Omazic, G. Oreski, M. Halwachs, G. C. Eder, C. Hirschl, L. Neumaier, G. Pinter, and M. Erceg, “Relation between degradation of polymeric components in crystalline silicon PV module and climatic conditions: A literature review,” *Sol. Energy Mater. Sol. Cells*, vol. 192, pp. 123–133, 2019.

Bayesian Optimization of Laser-aided Fracture Toughness Specimen Preparation

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Reliable lifetime prediction of ceramic components requires fracture toughness measurements supported by sharp, reproducible artificial defects. Conventional notching techniques often lack consistency, are time-consuming, and are particularly limited for fine-grained ceramics and geometrically complex specimens. This study investigates a modified femtosecond-laser vaporization approach that targets an ablation area rather than a single line. To efficiently explore the complex, material-dependent parameter space, Bayesian optimization was employed for zirconia and both conventionally and additively manufactured alumina. The method rapidly identified suitable parameters for zirconia, achieving sharp, smooth notches within only a few experimental iterations. In contrast, alumina exhibited unsuitable fracture behavior, with failure initiating at notch flanks rather than roots. Overall, laser notching demonstrated clear advantages in speed, reproducibility and geometric flexibility, including applicability to complex designs such as the CharAM specimen. Further research is required to ensure consistent root-initiated fracture and to expand understanding across a wider range of materials.

On the thermo-acoustoelastic effect of Rayleigh waves and its metal physical interpretation

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The acoustoelastic effect describes the relationship between the propagation velocity of ultrasonic waves and the stress state of a material. In addition to mechanical stresses, this effect is influenced by several other factors, including temperature, plastic deformation, microstructure, and material damage. From a physical perspective, the acoustoelastic effect arises from the strain dependence of the components of the effective elasticity tensor in the prestressed configuration.

In our work, the coupled influence of temperature and mechanical stress on the propagation velocity of Rayleigh waves is investigated using numerical simulations. While these effects have typically been considered independently in previous studies, thereby neglecting any mutual interaction between temperature- and stress-related influences, the present approach enables a consistent analysis of their interaction. The results demonstrate that the acoustoelastic effect becomes more pronounced with increasing temperature. Furthermore, the temperature dependence of the acoustoelastic constant is analysed.

The numerical results are subsequently validated against experimental measurements and show a high level of agreement. In addition, the simulations allow for a more detailed investigation of individual effects that cannot be fully resolved in experimental studies due to measurement uncertainties.

Digitalization of Materials, the Basis for Machine Learning Applications and Advanced Materials Technologies

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Advanced materials form the central basis for innovations concerning practically all of our social challenges, from the energy transition to a resilient circular economy. The effective application and efficient use of advanced materials enables both optimal performance outcomes and resource conservation in engineering projects. However, this is only possible with digital images/models of the material based on reliable materials data. FAIR materials data must therefore be available – throughout the entire life cycle and across company boundaries. In particular, such data is needed for machine learning applications and the creation of related materials models. In the talk, I will give a few examples concerning microstructure classification, the evaluation of cast components, and machine learning prediction of fatigue damage initiation.

FAIR – Findable, Accessible, Interoperable, Re-usable

Advanced materials are engineered materials whose structure and composition are carefully designed to deliver enhanced performance for specific applications.

AI-assisted image analysis as a powerful tool to accelerate materials development for solid oxide electrolyzer cells

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Solid oxide electrolyzer cells (SOECs) represent a promising future technology for highly efficient electrochemical storage of surplus electrical energy in chemical energy carriers such as H_2 or syngas (H_2/CO). The material development of SOEC air electrodes is currently pushing the limits of cell efficiency and lifetime, with the performance depending in a complex way on various compositional and morphological features. This study provides a proof of concept for a knowledge-based AI-assisted design of SOEC air electrodes, which could circumvent the conventional time-consuming and cost-intensive workflow. Electrochemical impedance spectra of symmetrical cells with $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$ (LSCF) − $Ce_{0.9}Gd_{0.1}O_{1.95}$ (GDC) composite air electrodes with different phase ratios indicated a pronounced minimum in the polarization resistance at 50:50 wt.%. The morphological features of the electrodes were extracted with an accuracy >96% by using AI-assisted segmentation of SEM images. This allowed the peak performance of the 50:50 wt.% electrode to be linked to several key morphological features. To validate the derived relationships, the two best electrode designs were transferred to full cells. As predicted, the 50:50 wt.% LSCF-GDC electrode delivered an exceptionally high current density of −2.37 A cm^{-2} at 1.2 V and 800°C, while the cell with the 70:30 wt.% electrode exhibited a significantly lower current density. Finally, a long-term electrolysis test of a 5×5 cm^2 cell with 50:50 wt.% LSCF-GDC electrode was conducted for 220 h. The excellent performance demonstrates that AI-assisted image analysis is a powerful tool to accelerate and improve the development of SOEC electrodes and cells in the future.

AI-driven multiscale modeling of thermal transport in $LiCoO_2$ cathode materials

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Photothermal (photonic) sintering is a promising route to rapidly process solid-state battery components such as $LiCoO_2$ (LCO) cathodes, but rational tuning of experimental conditions requires knowledge of the temperature evolution during millisecond-scale heating. The current process design relies heavily on simulated temperature profiles. Commercial software typically assumes 1D heat conduction with constant material properties; for LCO, reported room-temperature thermal conductivities span almost an order of magnitude and are essentially unknown for amorphous phases. To address this, a foundational neural network potential (Matlantis) is used to sample crystalline and disordered LCO configurations, which are recomputed with DFT+U+vdW to build a curated dataset of 999 structures. A dedicated Allegro E(3)-equivariant neural network potential is then trained and Pareto-optimized, achieving near *ab initio* accuracy with excellent strong and weak scaling on multi-GPU architectures. The potential reproduces structural, elastic and vibrational properties of layered LCO and enables Green–Kubo calculations of thermal conductivity in both crystalline and amorphous phases. Amorphous LCO is found to have low, weakly density-dependent thermal conductivity and is incorporated as an effective grain-boundary phase in a thin-interface model that reproduces grain-size–dependent heat transport consistent with experiments. Finally, atomistically derived thermal properties are combined with measured optical data in 1D multiphysics simulations, showing that amorphous LCO films reach higher surface temperatures than crystalline films under identical photothermal loading, and thus providing physics-based guidance for tuning photonic sintering conditions.

Under pressure – AI usage for faster simulations of Li-Ion cells

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The steady increase in commercially used lithium-ion batteries over the last decades has allowed for smaller, more powerful batteries but has also increased their volatility, leading to an increased risk of thermal runaway [1]. To counter this risk, a deep understanding of material behaviour and safety tests on cells are necessary. However, real crush tests are expensive, complex, and involve high risk. Elaborate simulation models can decrease the risk involved but are still complicated and time-consuming, especially for detailed component-level simulations. Here, AI-based support tools can help, facilitating the necessary simulations and therefore reducing the computation time and resources required.

For this work, components of a commercial prismatic lithium-ion battery were tested under compressive load using a novel cylindrical flat-top indenter capable of applying up to 2000 N of force. The results from the compression testing rig were used to calibrate material models through Finite Element Method simulations, in which the indentation process on single- and multi-foil samples was modelled. The data generated using the single- and multi-foil models will then be used to train a neural network-based material model. This material model will enable the simulation of the complex structure of a lithium-ion battery cell.

References:

[1] Y. Chen, Y. Kang, Y. Zhao, L. Wang, J. Liu, Y. Li, Z. Liang, X. He, X. Li, N. Tavajohi und B. Li, „A review of lithium-ion battery safety concerns: The issues, strategies, and testing standards,“ Journal of Energy Chemistry, pp. 83-99, 2021.

AI-Accelerated Multiscale Design of Permanent Magnets

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Permanent magnets are a key enabling technology, yet their performance often relies on critical rare-earth elements. To mitigate supply risks, we target magnet concepts that eliminate terbium/dysprosium (Tb/Dy) and reduce neodymium (Nd) content while maintaining high coercivity. Achieving this requires simultaneous control of composition and three-dimensional microstructure—an ideal use case for Artificial Intelligence (AI) coupled to physics-based modelling. I will present an AI-driven multiscale workflow that couples models across length scales for magnet design. The workflow starts with uncertainty-aware prediction of intrinsic properties from composition, providing fast estimates of saturation magnetisation and anisotropy field together with a confidence measure. These predictors are used during objective-function evaluation in a genetic algorithm that maximises coercivity and magnetisation while minimising cost. Microstructure is incorporated by constructing 3D synthetic grain structures from scanning electron microscopy images, by minimising the mismatch between power spectra computed from images and those obtained from slices through the synthetic structures. To generate training data efficiently at a fraction of the computational cost of full micromagnetic simulations, we employ a reduced-order model of magnetisation reversal for large-grained magnets, enabling rapid yet physically grounded demagnetisation (B–H) curve calculations. We represent the granular topology as a graph and train graph neural networks to predict demagnetisation curves from the 3D grain structure. These coupled surrogates enable rapid screening and cost-aware inverse design of chemistry and microstructure for rare-earth-lean magnets.

Foundational GRACE: Towards quantum accuracy in atomistic modeling of materials

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The emergence of foundational machine learning interatomic potentials (MLIPs) has catalyzed a paradigm shift in atomistic materials simulations, offering a scalable bridge between first-principles accuracy and large-scale molecular dynamics. Unlike models specific to a particular task or chemistry, these universal potentials achieve generalization across diverse chemical spaces and out-of-distribution robustness in various simulated conditions.

This presentation focuses on the Graph Atomic Cluster Expansion (GRACE), a framework which provides a complete and efficient description of atomic interactions and unifies many current MLIP approaches. We will demonstrate the robustness of GRACE for simulations of thermodynamic, functional and mechanical properties for a wide range of multicomponent materials. We will also address the incorporation of magnetism and other material properties and discuss the systematic generation of comprehensive training datasets for creating transferable and accurate foundational MLIPs.

Machine learning model for predicting grain boundary enrichment in ferrite

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Grain boundaries (GBs) play a key role in the design of high performance materials. A variety of experimental and theoretical methods exist to explore GB chemistry and structure. From the theoretical side, atomistic simulations provide a direct access to segregation energies, which are key fundamental GB properties and allow estimation of the GB enrichment via thermodynamic models. On the experimental side, the most commonly applied technique to address GB excess are Auger electron spectroscopy (AES) or, nowadays, Atom Probe Tomography (APT). There are, however, many systems in which theoretically and experimentally measured predicted GB enrichment do not match, one of which is P segregation in ferrite [1]. Alternatively, one can use experimental data to train machine learning models for the prediction of GB segregation, which requires large databases. While for APT large databases are currently not available, AES has provided segregation for many alloys [2].

In this talk we will present our approach of using the GB enrichment data from a comprehensive AES database to train machine learning models. While this database is composed of over 50 publications and therefore consists of numerously different laboratory setups and ways of analyzing GB segregation, we are able to predict GB enrichment with high accuracy. In addition, the expected dependency of the GB enrichment on the aging temperature and bulk concentration of the solute could be replicated and the model is also able to correctly identify site-compensation effects. The extrapolation capability of this model is discussed together with the efforts that would be related to calculating segregation based on a pure ab-initio approach.

Our results show that efforts into sharing and storing data openly should be a priority of the scientific community. This is a prerequisite to establish machine learning as a useful tool, even applicable for complex phenomena, such as solute enrichment at grain boundaries.

[1] A. Reichmann et al., *Grain boundary segregation for the Fe-P system: Insights from atomistic modeling and Bayesian inference*, Acta Materialia, 279, 15, 2024

[2] P. Lejček, *Grain Boundary Segregation in Metals*, Springer Berlin Heidelberg, Berlin, 2010

Machine-Learned Potentials as Efficient Surrogates for First-Principles Modeling of Organic Semiconductors

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Crystalline molecular semiconductors present significant challenges for computational modeling. Their structures are often anisotropic, composed of relatively large unit cells with low symmetry, and their molecular packing is governed by weak non-covalent interactions. Traditional first-principles methods, such as density functional theory (DFT), provide accurate insights but are computationally prohibitive for large-scale simulations of lattice vibrations, elastic moduli, and thermal transport.

We demonstrate that machine-learned interatomic potentials, trained via active-learning molecular dynamics, offer an efficient and highly accurate alternative. Here, the potentials are specifically designed for lattice dynamics, aiming to reproduce DFT-level accuracy at a fraction of the computational cost. This approach enables simulations that would otherwise be infeasible, including calculations based on the Boltzmann transport equation, and yields results in excellent agreement with experimental phonon band structures as well as thermal conductivities of acene-based crystals.

By unlocking simulations beyond the reach of DFT, machine-learned potentials offer deeper insight into the structure–property relations of complex organic crystals, ultimately paving the way for organic semiconductors tailored for thin-film electronics resilient to thermal degradation, or for thermoelectric applications.

Moving from Algorithmic to Agentic Computing in Materials Research

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In this talk, you'll get an inside look at atomistic modeling at Empa—highlighting how simulation software has evolved rapidly over the past decade and how it is now delivering tangible impact in real materials research. A key inflection point has been the rise of machine-learning interatomic potentials (MLIPs), which bring ab initio accuracy to large-scale atomistic simulations and enable truly quantitative agreement with experiment. At the same time, the explosive growth of ab initio training datasets has catalyzed a new generation of foundational MLIPs, capable of describing interactions across nearly the entire periodic table.

In parallel, foundational large language models (LLMs) have introduced a new kind of capability: robust reasoning over tasks and tools. This marks a shift toward agentic computing in materials research – systems that can plan, execute, and iterate within complex computational workflows.

To bring these advances together in a single, accessible platform, we developed OptiMat Chat (www.optimat.chat): a conversational AI agent framework for materials research designed to democratize access to advanced computational tools and techniques. Looking ahead, we aim to extend this approach across the full research pipeline – from knowledge mining and processing for direct and inverse materials design to embodied AI systems that enable autonomous experimentation in the real world.

Large Language Models in Materials Science

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Large language models (LLMs) are increasingly recognized as a transformative class of models in machine learning. This talk highlights how they are reshaping modern materials science in particular, focusing on two complementary and mutually reinforcing roles: as intelligent orchestrators of complex computational workflows and as surrogate models for the prediction and optimization of challenging materials problems. In their role as orchestrators within multi-agent systems, LLMs can coordinate complex simulation workflows (such as DFT and related first-principles simulations), converting high-level scientific intent into structured, executable workflows. Acting as central controllers, LLMs manage communication between specialized agents, generate and validate simulation inputs, monitor convergence and failure modes, and adaptively steer calculations based on intermediate results. Beyond orchestration, LLMs can function directly as surrogate models that approximate complex structure-property and process-performance relationships. This is illustrated with use cases drawn from corrosion science and gradient-free optimization problems in mechanics. Taken together, these roles suggest a shift toward hybrid, agentic materials design frameworks in which LLMs unify simulation, learning, and optimization, either handling parts of the workflow themselves or delegating tasks to specialized modules such as multiphysics codes.

Accelerated pathways to discover and apply novel sustainable materials solutions with AI

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Insights gained from experimental characterisation and theoretical modelling drive materials science, providing a deep understanding of the process-structure-property (PSP) relationships at its core. These insights are integral to the four paradigms of materials science, which describe how research on materials has evolved from empirical science, to model-based theoretical science, to today's computational science, and finally to data-driven science. The fourth paradigm was only recently introduced and, to fully exploit its potential, several key integrations are required to address the current challenges in developing advanced materials.

This talk will outline the needs and implications of the fourth paradigm of materials science, and its application in topics such as digitalisation, interoperability, the integration of multi-scale modelling with machine learning, and materials acceleration platforms. These platforms allow for the accelerated design and development of sustainable and advanced materials, and their application. This will be demonstrated using several use cases that focus on understanding the underlying mechanisms to enable knowledge-based design. These use cases include the predictive, multi-scale modelling of impurities in recycled steel, the probabilistic modelling of phase transformation in steels with uncertainty propagation and quantification, the application of machine learning to industrial production data and the Bayesian optimisation of the mechanical properties of bainitic steels based on high-throughput experiments. All of these use cases are integrated into the *ALPmat* platform, which will be expanded this year to include material use cases for hard magnets, sustainable aluminium alloys and a self-driving laboratory for solder materials.

Bypassing Trial-and-Error: From 1000 Hours to Rapid Prediction of Recycled PP Blends

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The qualification of polypropylene (PP) non-pressure pipes made with post-consumer recyclate is increasingly governed by product-level performance tests, such as the EN 1852-1 "1000-hour" internal pressure test. While such long-term testing was historically acceptable for comparatively tough virgin grades, it becomes economically and environmentally inefficient once recyclates are introduced: post-consumer streams and derived batches exhibit pronounced variability, and even minor changes in polymeric or non-polymeric impurities can shift slow crack growth (SCG) performance dramatically. Consequently, manufacturers face a practical dilemma: First, they must identify a feasible virgin/recyclate blend that passes the 1000-hour requirement. Second, even after a "successful" formulation is found, batch-to-batch variations can force repeated trial-and-error product testing to avoid unexpected failures.

This paper presents a data-driven approach that replaces large parts of this trial-and-error workflow by predicting EN 1852-1 performance from short-term laboratory data. The approach combines accelerated material characterization with SCG-based modelling to estimate the probability for a given blend of passing the 1000-hour pressure test. It explicitly accounts for recyclate batch variation, enabling reliable assessments and reducing the need to re-run extensive product-level testing for every incoming batch. Across the investigated datasets, the proposed models forecast test outcomes with an accuracy of over 90 %, demonstrating a practical route to faster qualification, lower testing effort, and more sustainable use of recycled PP in sewer pipe applications.

Bayesian optimization applied to the parameterization of Crystal Plasticity models

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Predicting material behavior under various loading conditions is a key challenge in Engineering and Materials Science [1]. In this context, predictive models capable of evaluating microstructural evolution can accelerate material development for a wide range of applications [2]. Accordingly, Crystal Plasticity Modelling (CPM) emerges as a powerful predictive tool by combining constitutive equations that describe the mechanical response with deformation kinetics at the microstructure scale, and intergranular interactions [1, 2]. However, the accuracy of these models is highly dependent on parameter tuning of the constitutive laws governing elastoplastic behavior [2], which is often performed through manual calibration, a time-consuming and iterative process involving numerous simulations [1]. In this work, an automated calibration workflow based on Bayesian Optimization (BO) was developed to determine the optimal parameter set, aiming to minimize the discrepancy between simulated tensile results and experimental data. Calibration outcomes were compared using statistical metrics (R^2, RMSE, and MSE), indicating that the developed workflow can achieve low errors relative to the expected deviations associated with microstructural variations. Furthermore, it calibrates the model using a relatively small number of simulations, thereby significantly reducing computational costs and time to solution.

[1] CHOI, J. et al. Multi-objective surrogate-assisted calibration of CPFEM models using macroscopic response and in situ EBSD measurements of grain reorientation trajectories. Acta Materialia, [S.L.], v. 305, p. 121809, fev. 2026. Elsevier BV. http://dx.doi.org/10.1016/j.actamat.2025.121809.

[2] CUPPARI, Marcio Gustavo di Vernieri; MENDES FILHO, Aníbal de Andrade; VEIGA, Roberto Gomes de Aguiar. Simulated annealing global optimization of crystal plasticity parameters and modeling of polycrystalline α-titanium. **Mrs Communications**, [S.L.], v. 15, n. 2, p. 235-239, 24 fev. 2025. Springer Science and Business Media LLC. http://dx.doi.org/10.1557/s43579-025-00697-x.

Constitutive Modeling of Anisotropic Elasto-Damage Materials – A Data Driven Machine Learning Approach

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A data driven machine learning based approach is presented to model the constitutive response of anisotropic elasto-damage materials such as wood and fiber reinforced composites. Adopting principles of continuum damage mechanics, the nonlinear constitutive response is formulated by recourse to damage variables or damage tensors. The knowledge of the damage tensor and the undamaged (initial) linear elasticity determines the nonlinear relation between the stress and stain tensors. Instead of analytically expressing the relation between damage and strain state, an artificial neural network (ANN) is employed.

For training, testing, and validation of various ANN architectures data sets are generated by Finite Element Method simulations. Monotonous increasing, radial strain loads are applied to sample the strain space with sufficient resolution. Complementary to the strain–stress and strain–damage response given by the trained ANNs, physics principles are considered outside the ANN to handle unloading and reloading scenarios. Tension-compression asymmetry and mesh size dependence are addressed.

Examples are shown for plane stress states for which the nonlinear tensorial constitutive relation is captured by a surrogate model, i.e. a trained ANN. The latter is implemented as constitutive material law into a Finite Element Method program to run structural analyses.

Linking Grain Boundary Segregation to Embrittlement: Experimental and First-Principles Analysis of Tramp Elements in 51CrV4 steel

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The growing use of recycled scrap in steelmaking can lead to increased levels of residual elements such as Sn, Sb, Cu, and Ni in commercial alloys. These tramp elements tend to segregate to grain boundaries, where they can alter the interface cohesion, ultimately affecting the macroscopic mechanical performance. A profound understanding of their joint segregation behavior is therefore critical for maintaining toughness in modern steels.

In this work, tramp element segregation in a model 51CrV4 steel was examined using a coordinated atom probe tomography (APT) and density functional theory (DFT) strategy under processing conditions representative of industrial practice. Steels containing different residual element concentrations (Sn, Sb, Ni, and Cu) were quenched and subsequently tempered at 450 °C and 650 °C. Nanoscale chemical information obtained by APT was compared to DFT segregation energies to evaluate how accurately DFT captures experimentally observed enrichment at random high angle grain boundaries. APT reveals substantial accumulation of Sn, Sb, and Cu at grain boundaries, which coincides with impact toughness reductions of up to 60%. The DFT results support these findings, showing that the simultaneous presence of Cu, Sn, and Sb leads to a pronounced decrease in grain boundary cohesion that exceeds the effect of each element independently. Direct comparison between measured enrichment factors and calculated segregation energies shows strong consistency at the dilute solute levels typical of tramp elements (<1 at.%), demonstrating that ab initio simulations can reliably reproduce segregation tendencies in multicomponent systems. Noticeable discrepancies occur mainly when segregation is dominated by interstitial boundary sites for example when P or C are concerned. The close agreement between APT observations and DFT predictions establishes a consistent mechanistic picture of tramp element induced embrittlement and underscores the predictive value of first-principles modeling for the development of scrap-tolerant steel grades.

From Process to Product: Structured Flow Data as a Foundation for AI Applications

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The effective use of AI methods in materials science requires consistent, high-quality, and context-rich production data as well as corresponding quality data. This talk presents a process-flow system that digitally captures the complete lifecycle of an individual product throughout manufacturing. Each product begins in a defined initial state (flow object) and is transformed step by step through successive processes. Every process produces a new flow state, creating a continuous sequence of *process – flow – process – flow*.

This structured chain enables the aggregation of data along the entire production route, supports the identification of relationships between process parameters and material properties, and allows large, coherent datasets to be generated. These datasets form a reliable foundation for AI applications such as predictive modeling or process optimization in metallurgical and materials-engineering environments. The presentation demonstrates how systematically linking heterogeneous data sources creates a scalable, industry-ready data backbone for future AI use cases.

Multiphysics simulations and machine learning of thermal fields and mass transport in SiC crystal growth in PVT furnaces

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The physical vapor transport (PVT) method is key for producing large, high-quality, SiC single crystals. Despite its widespread use, challenges remain, notably with temperature distribution affecting the growth rate and crystal quality. Temperature gradients, for instance, cause thermal stresses, the primary source of dislocation formation. Direct observation is hardly possible since the process operates at extreme temperatures in a semi-closed system. Therefore, numerical modeling is essential for understanding and optimizing SiC bulk crystal growth.

In this study, COMSOL multiphysics simulations based on the finite element method are conducted to investigate heat transfer and mass transport. The importance of accurate radiation modeling and the ability to control thermal gradients in SiC crystal growth simulations is investigated in detail. Bayesian inference utilizing experimental data and a machine learning (ML) model is used to calibrate the material properties of the hot-zone in the PVT simulation[1]. Crystal growth rate and shape are explored via mass transport simulations incorporating a physical growth model with chemical reactions, vapor species transport, and the kinetics of etching and deposition. This approach accurately describes the growth rate process. The results demonstrate that flux distribution within the growth chamber directly influences both the growth rate and the resulting boule shape. Therefore, precise control of the thermal field and species flux is essential to achieve an optimized SiC boule shape. The optimization of the thermal field was conducted by using a ML model in combination with an optimization algorithm to efficiently determine optimal process parameters and geometric configuration for a specific PVT reactor design[2] . This ML-based approach enables PVT optimization regardless of the operation principle (resistive or inductive) and seed crystal diameter (6-inch, 8-inch, etc.).

In its entirety, our work provides improved insight into SiC crystal growth and generates computational data that can be closely compared to experimental observations of the crucible and boule after the growth process. Finally, the implications of our results for targeted improvements of the crystal growth process will be discussed.

References

[1] L. Taucher, Z. Ramadan, R. Hammer, T. Obermüller, P. Auer, L. Romaner, Machine learning assisted calibration of PVT simulations for SiC crystal growth, CrystEngComm 26 (2024) 6322–6335.

[2] L. Taucher, Z. Ramadan, R. Hammer, S. Defregger, P. Auer, L. Romaner, Efficient thermal field optimization of PVT simulations for SiC single crystal growth, J. Cryst. Growth 679 (2026)

128490.

Effects of tramp elements in recycled steels supported by AI-assisted microstructural analysis

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The shift toward increased scrap utilization in steelmaking is a key strategy for reducing CO_2 emissions. However, this transition elevates tramp element concentrations in steels and introduces additional challenges for microstructural control and performance. This study examines how tramp elements affect the microstructural evolution with implications for the design of robust and recyclable alloys.

Grain size development and thermally induced transformations are characterized via dilatometry and high-temperature laser scanning confocal microscopy. Additionally, AI methods are used to explore grain sizes and the characteristics of pearlite formations from scanning electron microscopy images. Segregation and nanoscale precipitation behavior are investigated by means of atom probe tomography and correlative transmission electron microscopy. The results are subsequently correlated to those obtained from notch impact testing.

The findings reveal that tramp elements accelerate the martensitic transformation and promote refinement of the austenite grain structure. Observations obtained using AI-based methods further suggest that tramp elements located at GBs impede the continuous growth of ferrite and cementite lamellas, as well as overall grain growth. Moreover, segregation of Mo can increase grain boundary cohesion leading to increased toughness, while co-precipitation of Cu and Sn at ferrite-cementite interfaces highlights complex solute interactions.

These insights advance the understanding of impurity-driven mechanisms in recycled steels, enabling alloy and process design for sustainable and circular metallurgical systems.

Advancing AI-Driven Microstructure Analysis through Correlative Microscopy Approaches

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AI-based microstructure analysis has become increasingly important in recent years and is now a key topic at scientific conferences. While AI can already automate standard tasks, its greatest potential lies in the analysis of complex microstructures for which no reliable evaluation methods currently exist. A major challenge is the creation of a reliable ground truth for such microstructures. This process is labor-intensive and susceptible to subjective expert opinions. Correlative microscopy makes a decisive contribution here by combining different microscopy techniques, thus enabling robust, AI-ready data sets.

This talk is positioned at the intersection of traditional metallography and the emerging field of digital materials analysis: Using examples of grain size and phase analysis in steels, we demonstrate how correlative images from light microscopy, scanning electron microscopy, and electron backscatter diffraction are used to enable data annotation for AI training in the first place or to even generate automatic annotations, thereby significantly reducing the need for manual labeling. In general, the increased effort involved in correlative microscopy serves primarily to build high-quality training and reference datasets with the aim of transferring subsequent routine analyses to the simplest available microscopy method.

Beyond Load-Displacement: Leveraging Computer Vision for *In Situ* Micromechanical Testing Experiments

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In situ micromechanical testing inside the scanning electron microscope is a valuable tool for accessing mechanical properties and investigating deformation and failure mechanisms at small length scales. However, the quantification of such experiments is typically limited to load-displacement data, treating the acquired series of electron microscopy images merely as a qualitative information channel. In this work, we present a framework utilizing state-of-the-art computer vision models to perform image segmentation, deformation tracking, and object detection on *in situ* micromechanical testing data. Thanks to the generalization capabilities of current foundational models, precise tracking of specimen deformation is widely possible without the need for application-specific fine-tuning of models. We demonstrate that continuous shape tracking of microsamples during deformation, enables the calculation of quantities otherwise not easily accessible, such as Poisson's ratio via lateral contraction, as well as viscoelastic relaxation after rupture. Furthermore, it allows for compliance correction of the measurement chain, significantly improving the accuracy of Young's modulus determination in uniaxial tests. Additionally, a meshing and relaxation algorithm of the tracked shape of microcantilever samples is presented, in order to resolve the strain gradient within the bending geometry and compare bending stress levels to the failure stresses observed during uniaxial loading of the same material.

Hybrid segmentation model for detecting Fe-rich intermetallic phases in secondary aluminium alloys

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The rising use of recycled aluminum content in alloy production leads to an accumulation of certain tramp elements like Fe, Si, Cu, Mn and thus to an increasing content of brittle intermetallic phases (IMPs). The Fe-rich IMPs can exert either beneficial or detrimental effects depending on their size, type and morphology and the intended application. For wrought alloys, fine and homogenously distributed Fe-rich IMPs show favourable effects on the mechanical properties, due to an enhanced strain-hardening potential and overall smaller grain size. The phase fragmentation during the rolling process is strongly influenced by the IMPs morphology in the as-cast state. Various morphologies have been reported in literature for the Fe-rich IMPs. The β-AlFeSi phase often form thin plates, whereas the α-Al(Fe,Mn)Si phases often exhibits blocky structure or complex branched morphologies, also known as "Chinese script". Detecting the latter, often-disconnected structures in the 2D cross section as entity is not feasible with conventional segmentation models leading to a misleading impression of their actual size and fragmentation behaviour. Thus, a hybrid segmentation approach is established, in which a specially trained AI model is applied in a first step to segment Chinese script and blocky phases, followed by conventional thresholding to identify fine platelets. This allows for a high-throughput segmentation of BSE-SEM mappings without the need for run-time-intensive measurements or time-consuming and complex sample preparation.

Automated microstructure analysis through image segmentation using a neural network

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Microstructure analysis of silicon nitride is valuable for linking grain features to mechanical properties like the fracture toughness. Using image processing does not work well for silicon nitride, because image colours or their gradients are not always easily distinguishable. Hence the automation of this workflow through a neural network to achieve satisfactory quantitative microstructure characterisation is of high interest.

A U-Net–based approach was used to train a model with micrographs and their ground truths that performs encoder–bottleneck–decoder segmentation with skip connections. The training dataset is comprised of seven scanning electron microscopy images of three different silicon nitride materials which were manually labelled. For training, the images were tiled to 512 pixels × 512 pixels, and data augmentation via 90° rotations was used to artificially expand the dataset. Training applied an intersection over union metric to track accuracy. On validation, the model achieved 94 % accuracy, compared to the manually labelled ground truth. Using the trained model on raw micrographs produces binarised outputs that can be directly used to compute comprehensive microstructural statistics. The application of the trained model to different silicon nitrides shows the potential of this approach.

While accurate labelling and model training are time- and computationally-intensive, expanding the dataset under consistent imaging conditions and evaluating advanced U-Net variants are promising directions to further improve performance and generalisation.