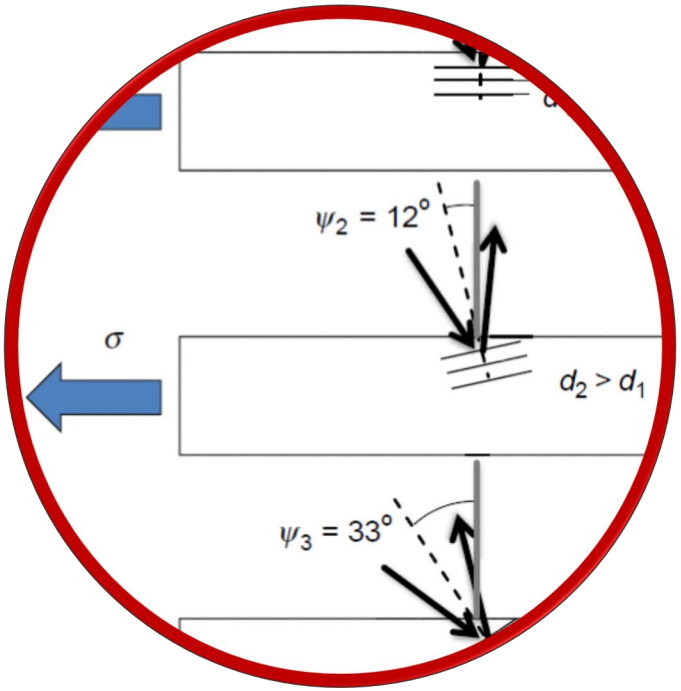
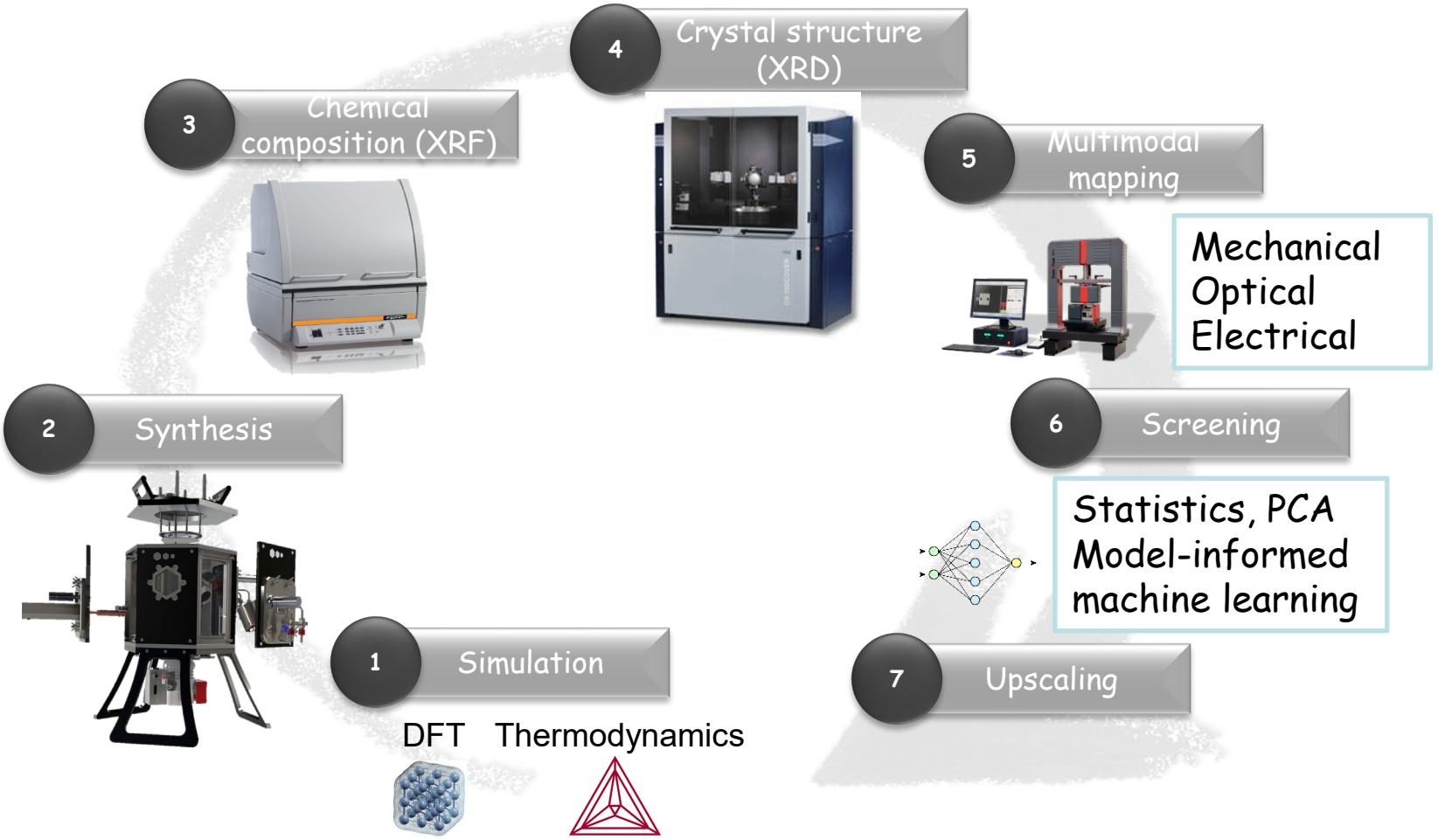
7. Outlook

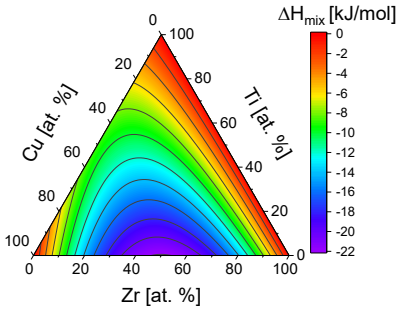


Outlook: Accelerated materials discovery through combinatorial thin film libaries

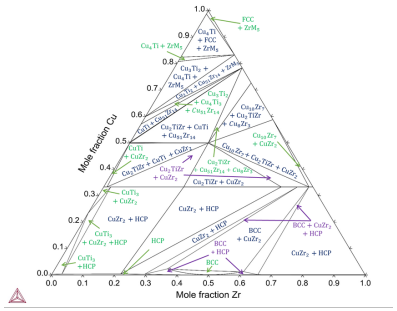


Simulation - preselection of elements

Empirical rules

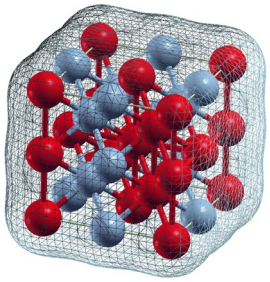


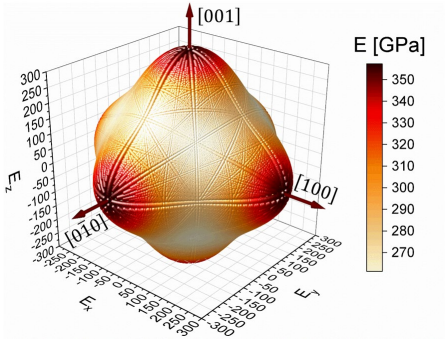
Thermodynamical modelling



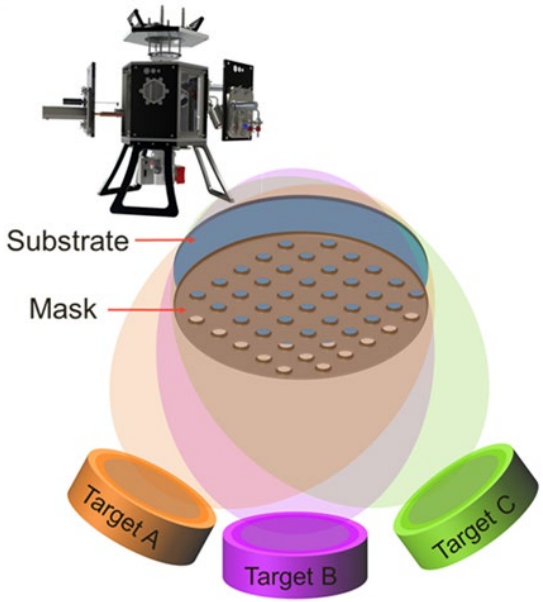
600°C

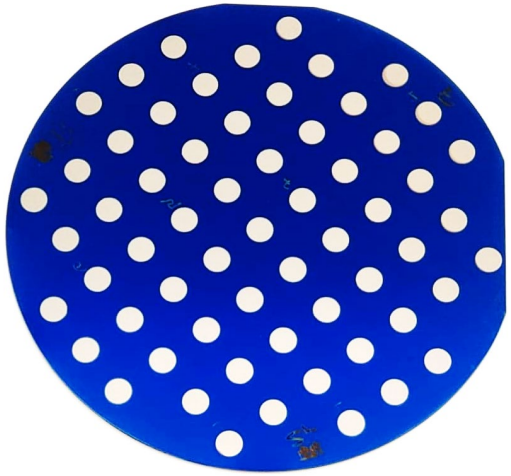
Density functional theory

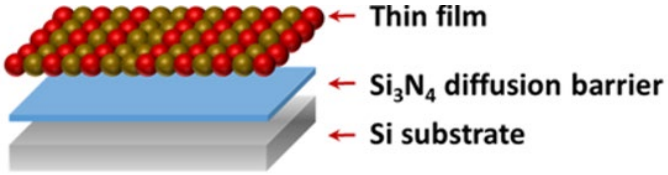




Deposition – combinatorial thin film libraries

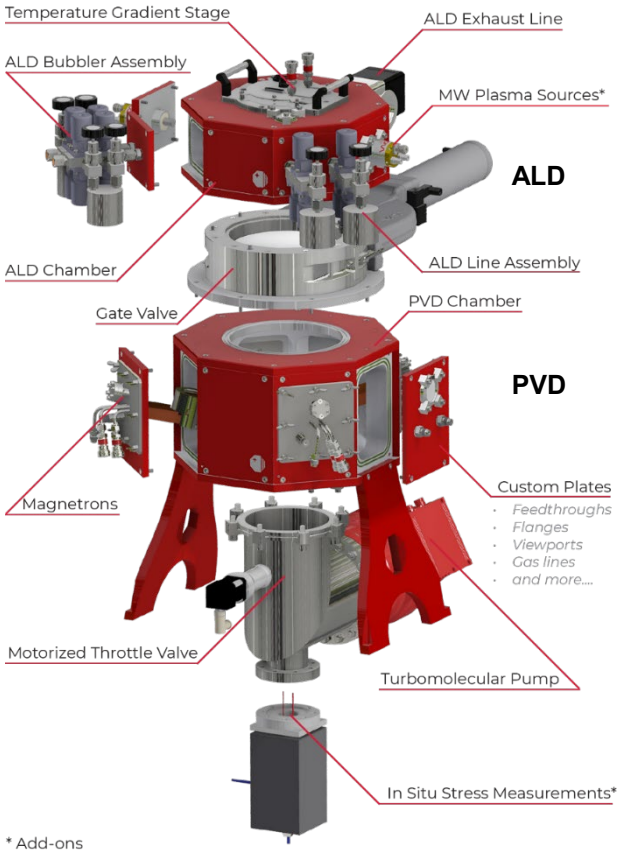


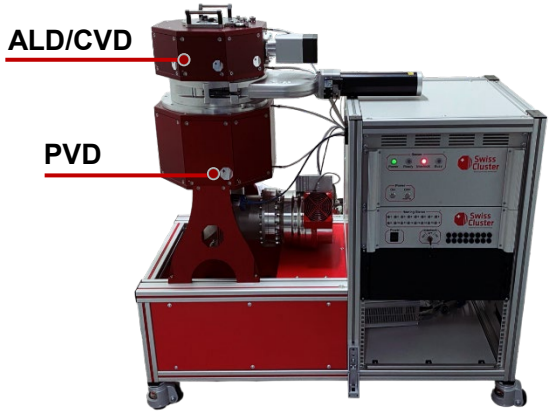




- 4in wafer with 69 patches
- Si_3N_4 interlayer for diffusion barrier, chemical inertness, electrical isolation
- Composition gradient: ±20at%

Deposition – novel equipment

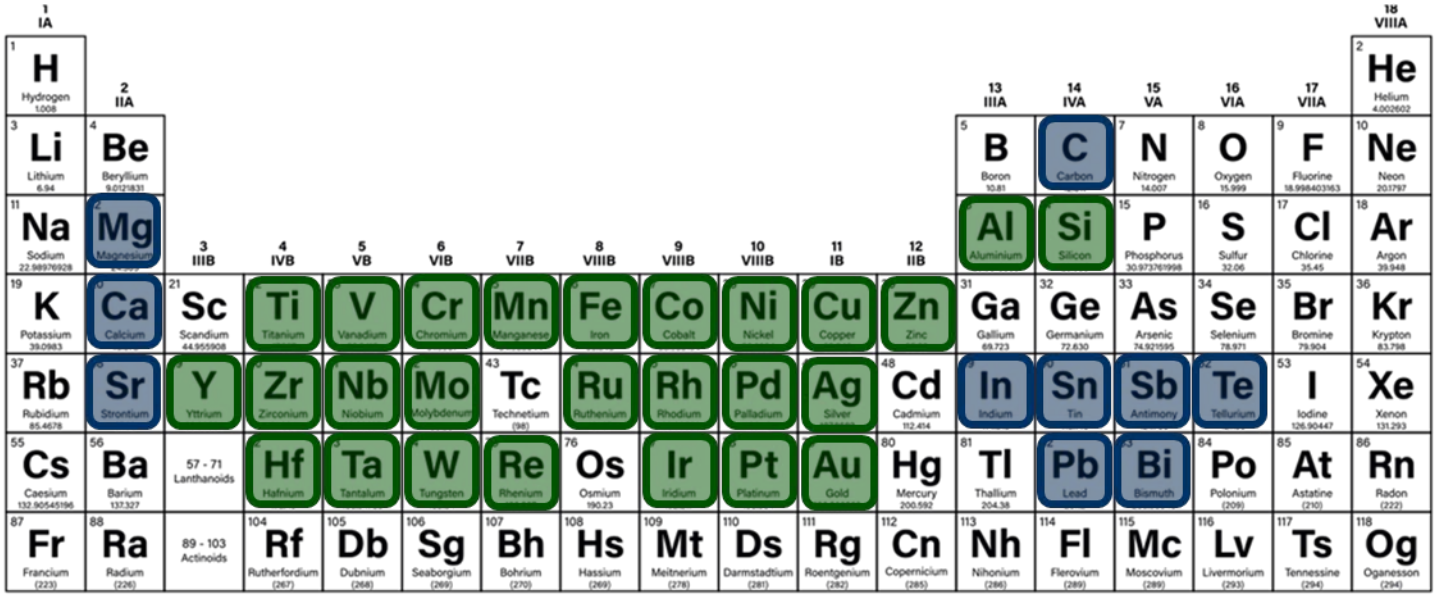




Swiss Cluster

- Laboratory cluster system
  - combines PVD and ALD
- Up to 8 magnetrons
- Temperature gradient stage (RT to 400°C)
- HIPIMS compatible
- 4 inch wafer substrates

PVD possible targets



Can be deposited

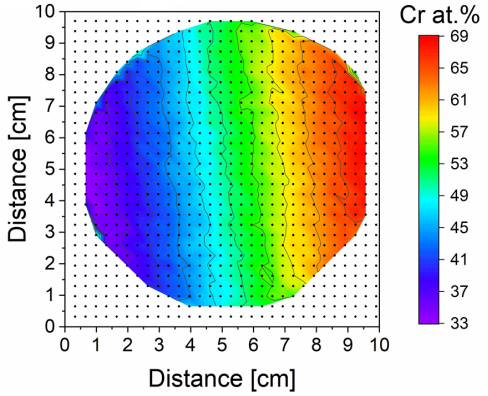
Can be deposited, but we prefer to avoid (chamber contamination or health concerns)

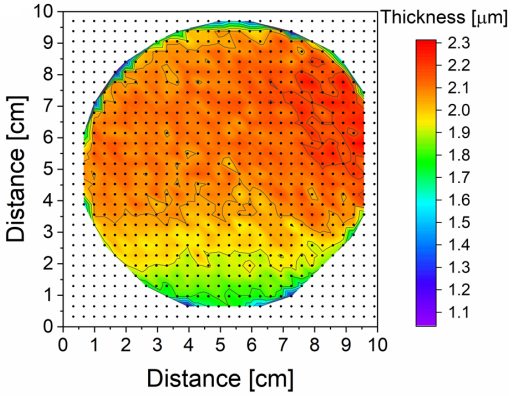
Composition mapping

Fischerscope X-Ray XDV-SDD

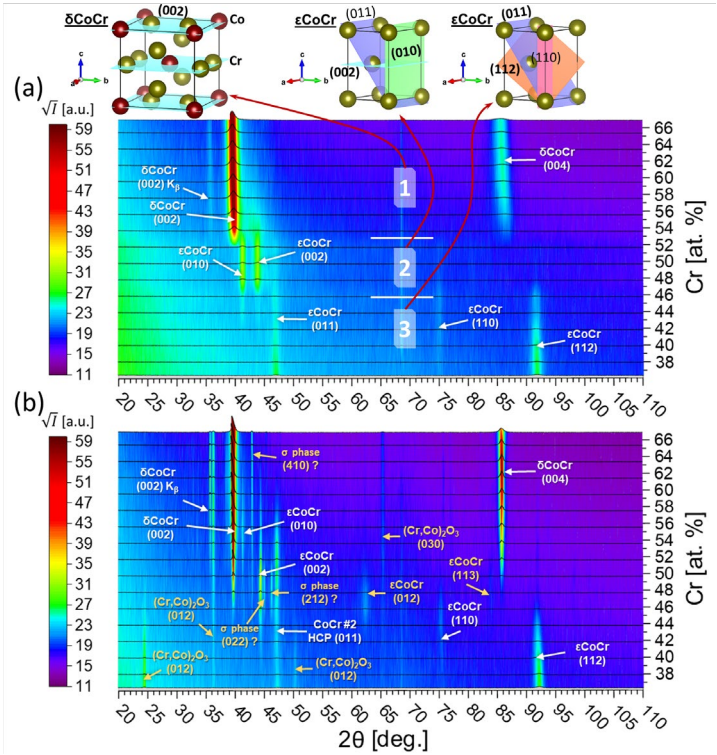
XRF mapping on each patch:

- Chemical composition
- Coating thickness





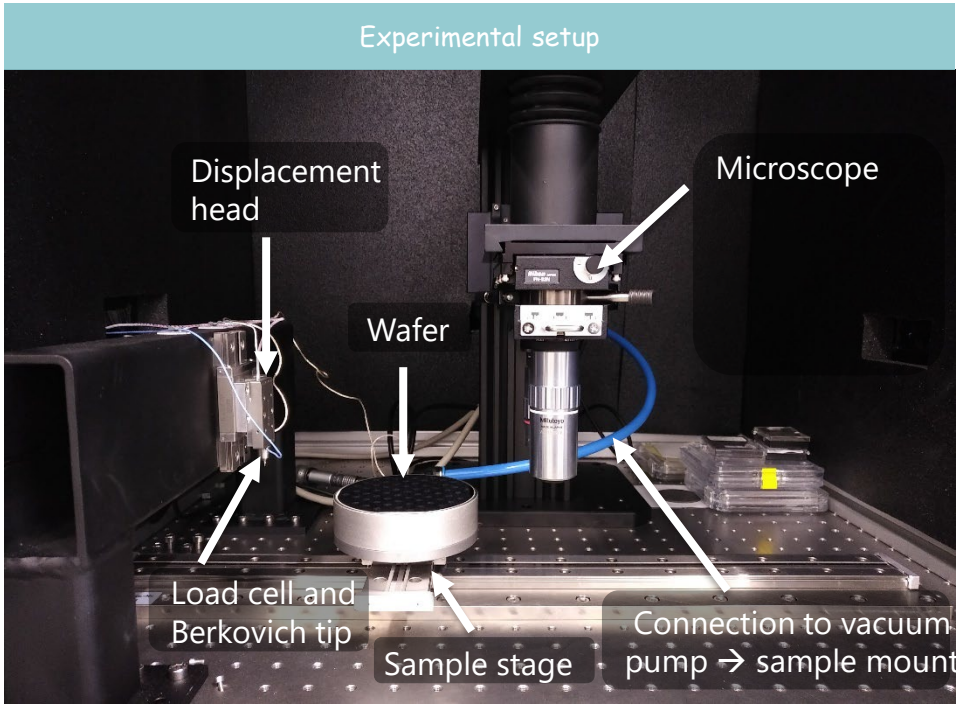
Microstructure mapping



XRD mapping on each patch:

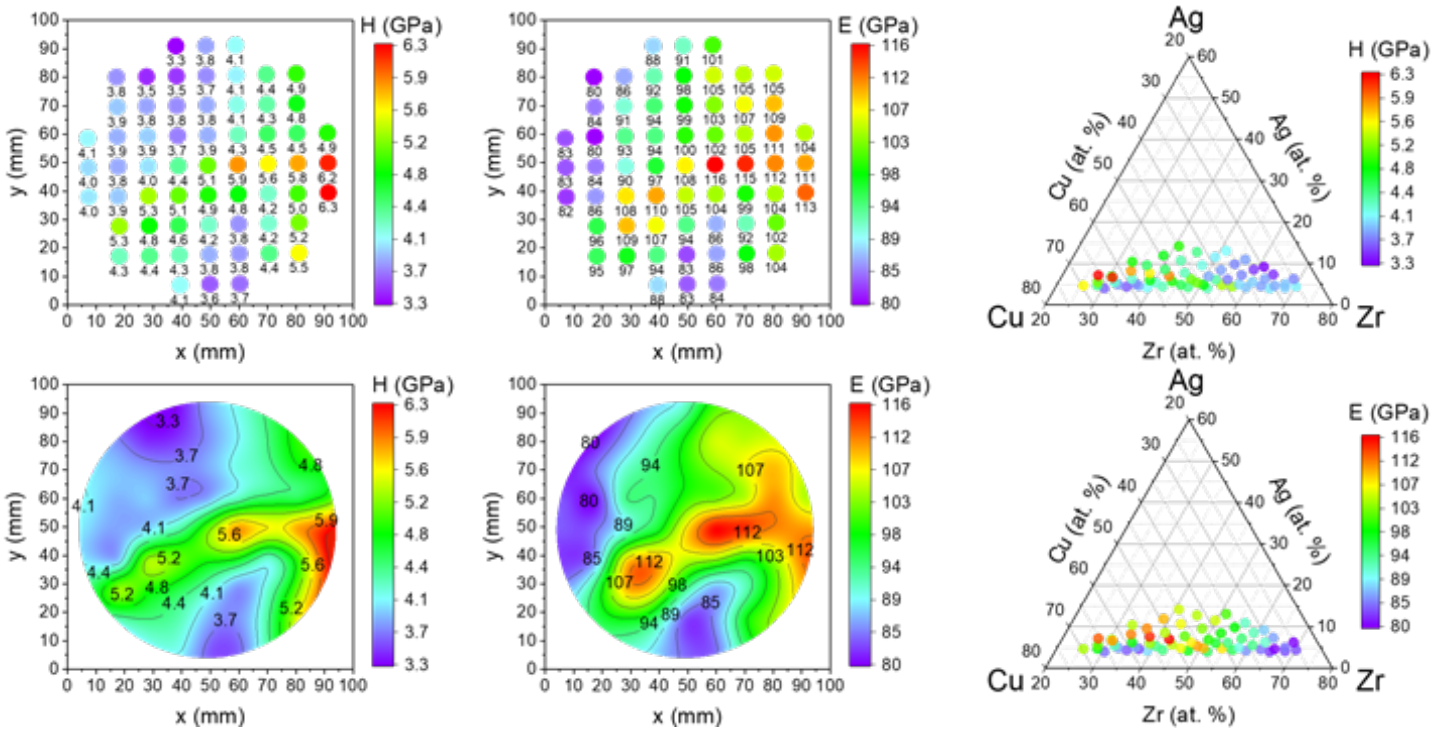
- Identification of phases
- Grain size analysis
- Correlation with composition

Mechanical property mapping



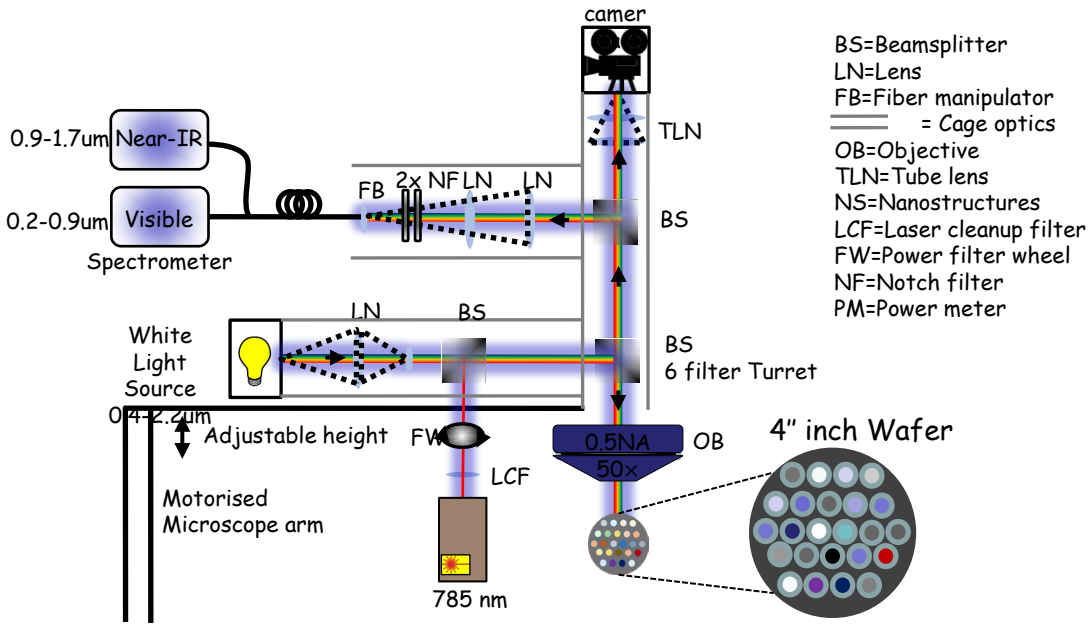
- High accuracy, low noise for thin film mechanical property measurements
- Automatic mapping of mechanical properties on 4in wafers
- Constant machine compliance
  - Guarantees consistent results over whole wafer
- Nanoindentation for measuring hardness, modulus, coating adhesion
- Scratch testing

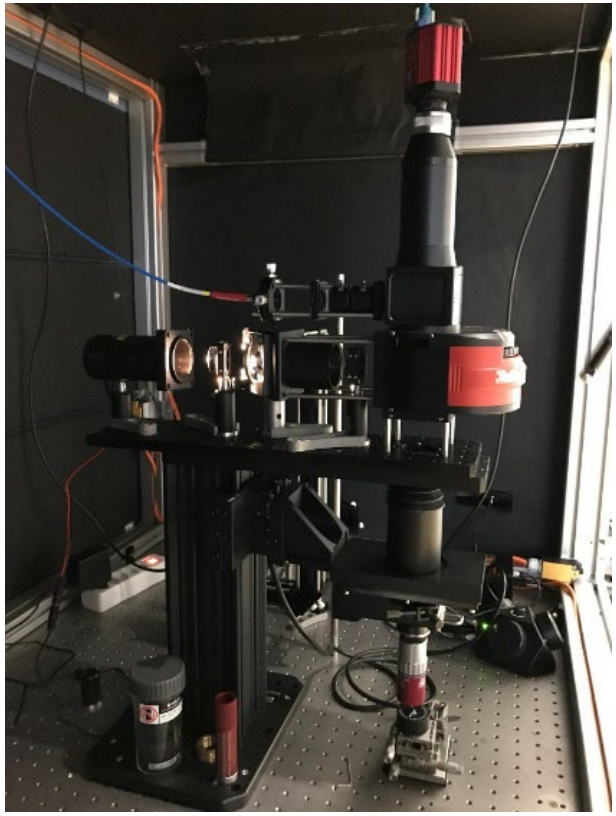
Mechanical property mapping - CuZrAg



Hardness and modulus correlated to composition

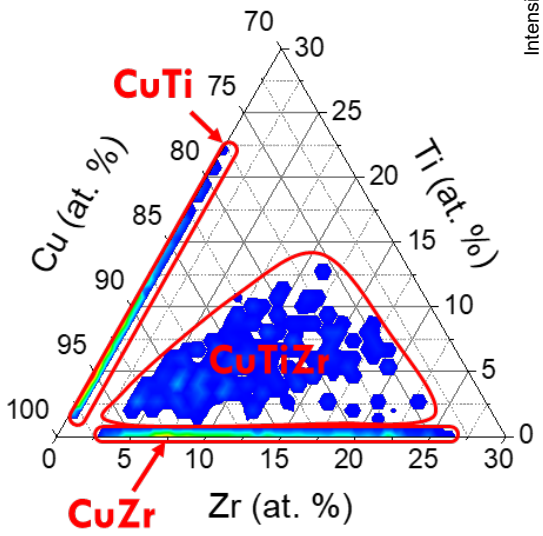
Optical property mapping

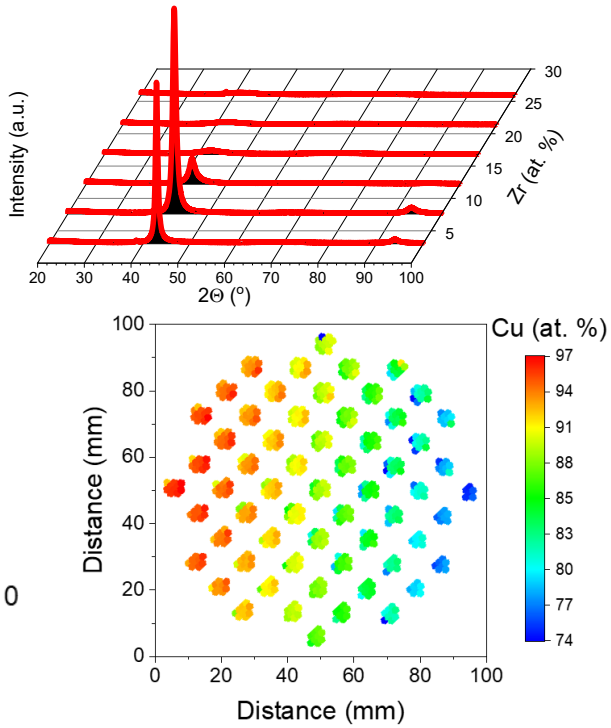




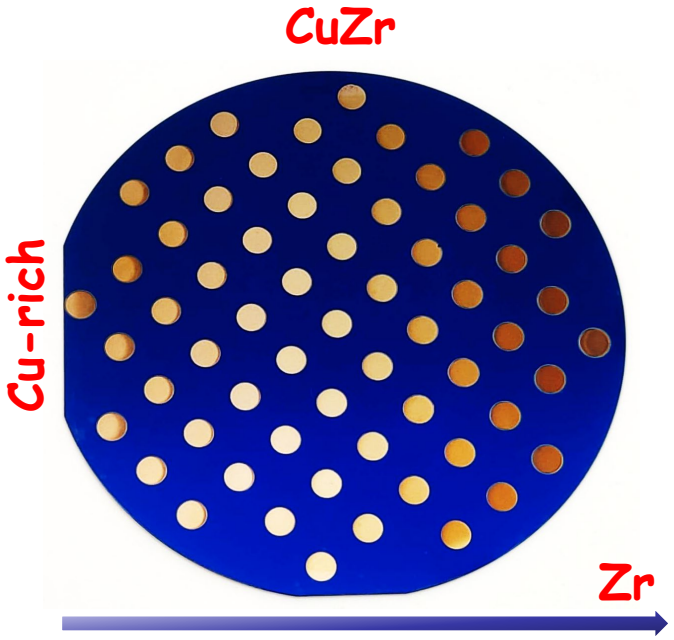
- **Reflectivity: 300nm to 1800nm**
- **Raman spectroscopy (785nm laser)**

Optical property mapping - CuZrTi





Heat treatment: 200°C / 10 min
Atmosphere: air

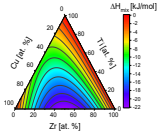


Note: Colour of the thin film changes significantly with the gradient of the chemical composition

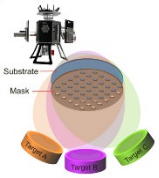
Combinatorial materials discovery – outline

Biological properties

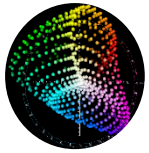
Theoretical approach



Deposition



Optical properties

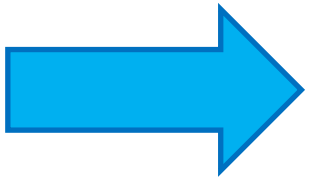


Composition

Mechanical properties

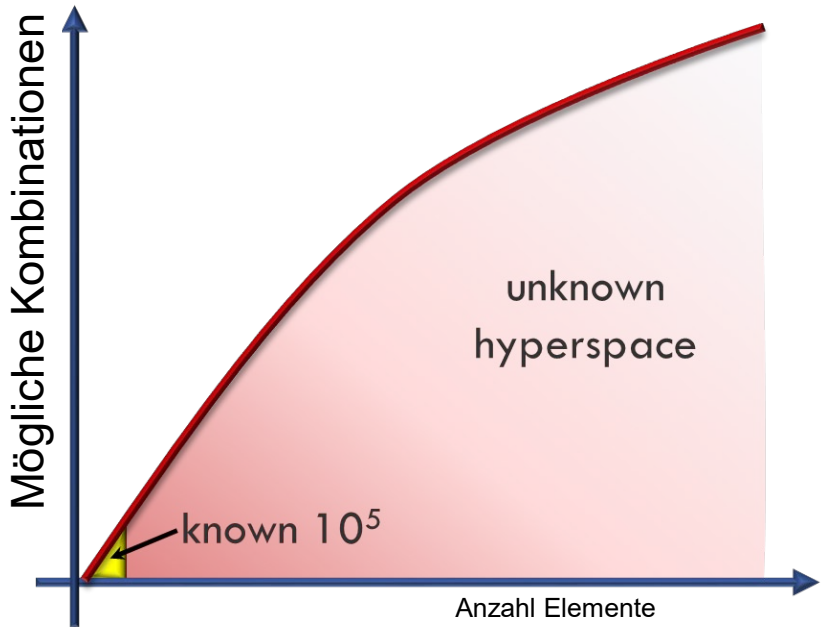
Microstruct

Upscaling



Applications

Motivation – Warum Hochdurchsatz?



Method – combinatorial thin film libaries

4 Microstructure (XRD)

3 Composition (XRF)

5 Multimodal mapping

Mechanical
Optical
Electrical

2 Synthesis

6 Screening

Statistics, PCA
Machine
Learning

1 Simulation

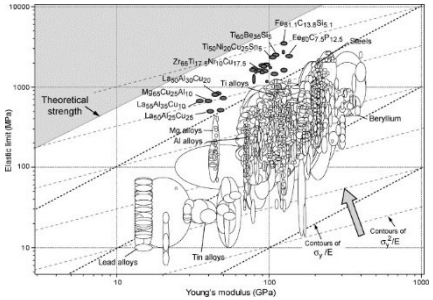
DFT Thermodynamics

7 Scaling up

Metallic Glasses for medical applications

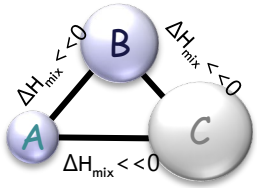
Advantages:

- High hardness and strength
- High wear resistance
- High corrosion resistance



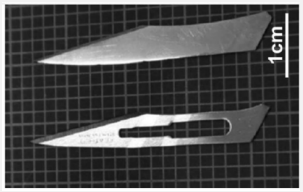
Design rules:

- At least 3 elements
- Highly negative enthalpy of mixing
- Atomic radii >12 % difference

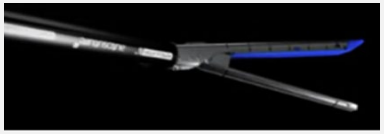


Applications:

Instruments for minimally invasive surgeries



Surgical steel blade with BMG coating

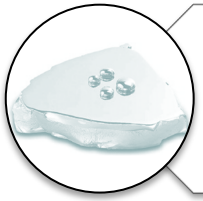


Medical instrument

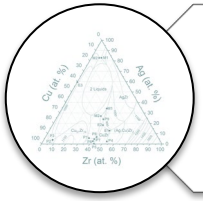
Dental laser system

K. Wieczerzak et al.: Unlocking the potential of CuAgZr metallic glasses: A comprehensive exploration with combinatorial synthesis, high-throughput characterization, and machine learning, Adv. Sci. (2023).

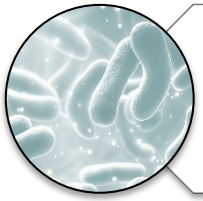
Why CuZrAg?



High glass forming ability



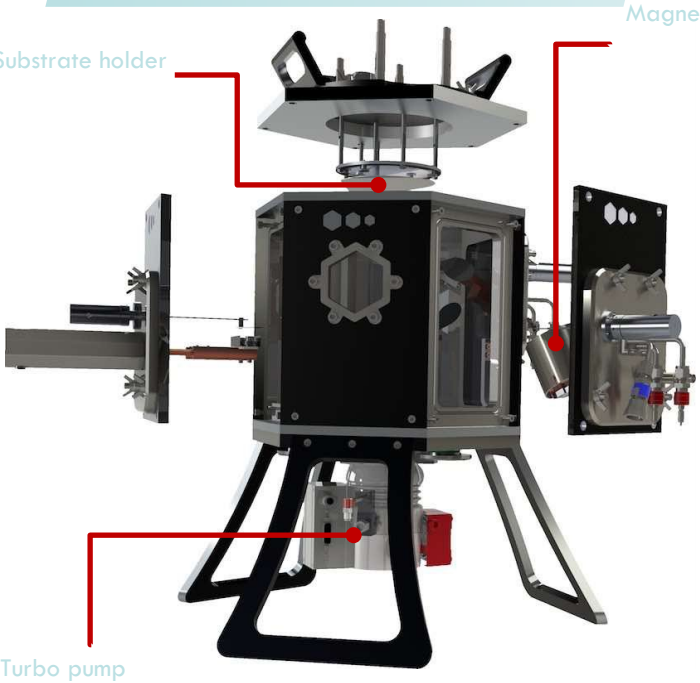
Portion of the phase diagramm where glasses are forming is known

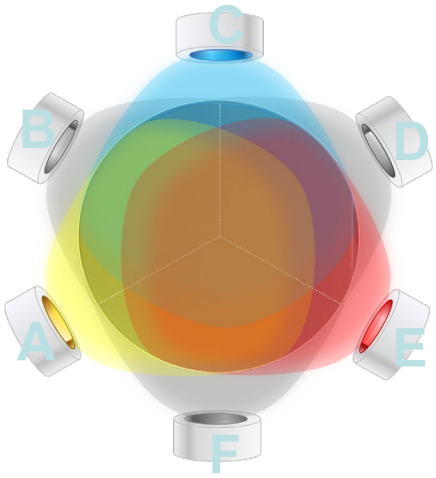


Cu and Ag possess antimicrobial properties

Deposition of thin film libraries

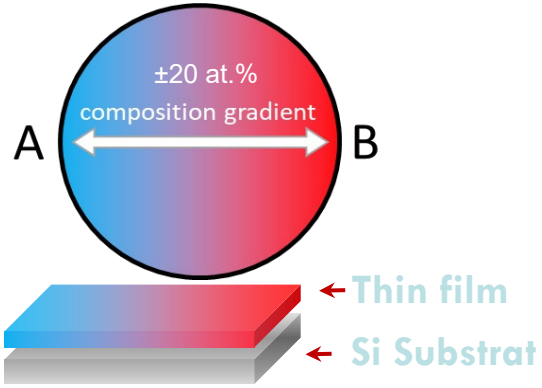
PVD deposition

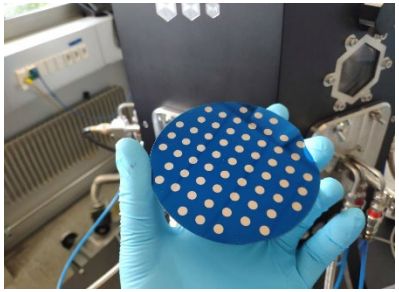




Deposition process

Material library

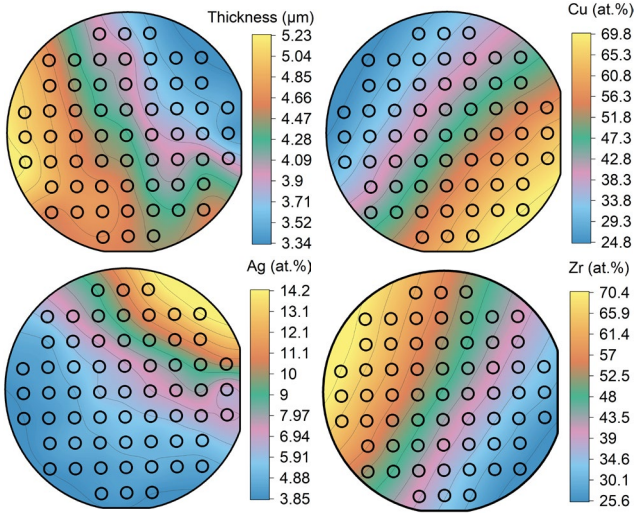


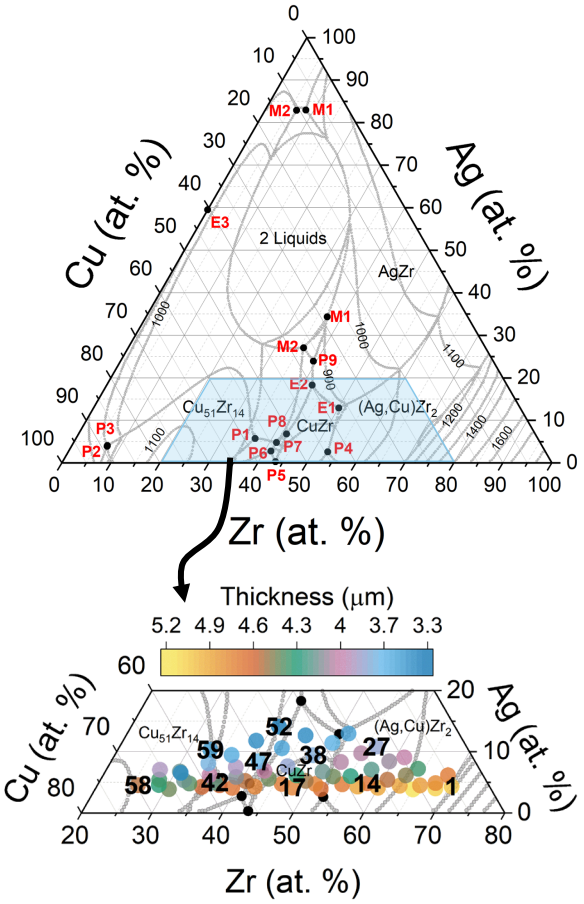


Thin film library

Chemical composition

Fischerscope X-Ray XDV-SDD

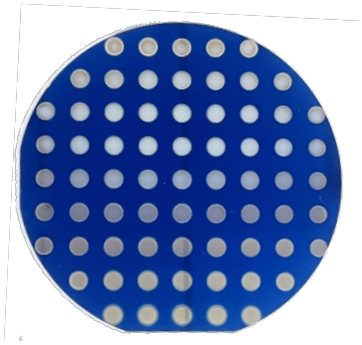


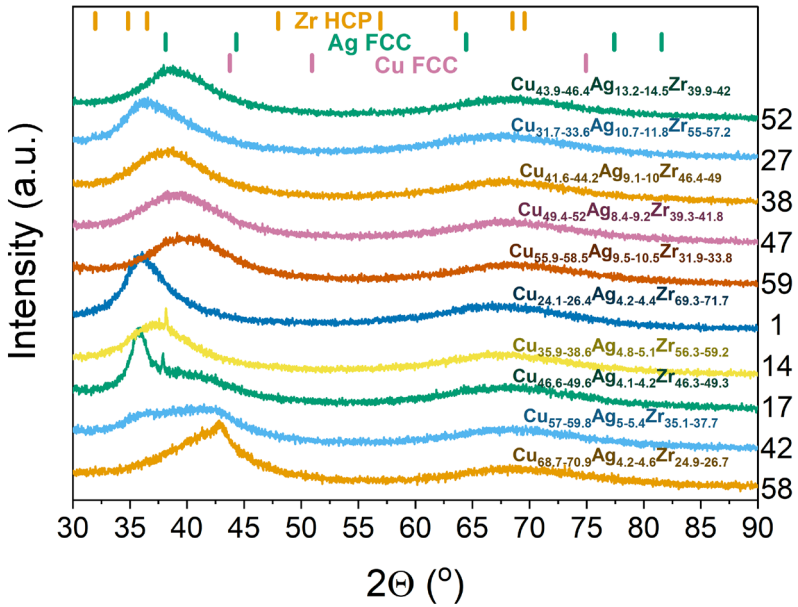


XRF mapping on every patch:

- Chemical composition
- Film thickness

Microstructure

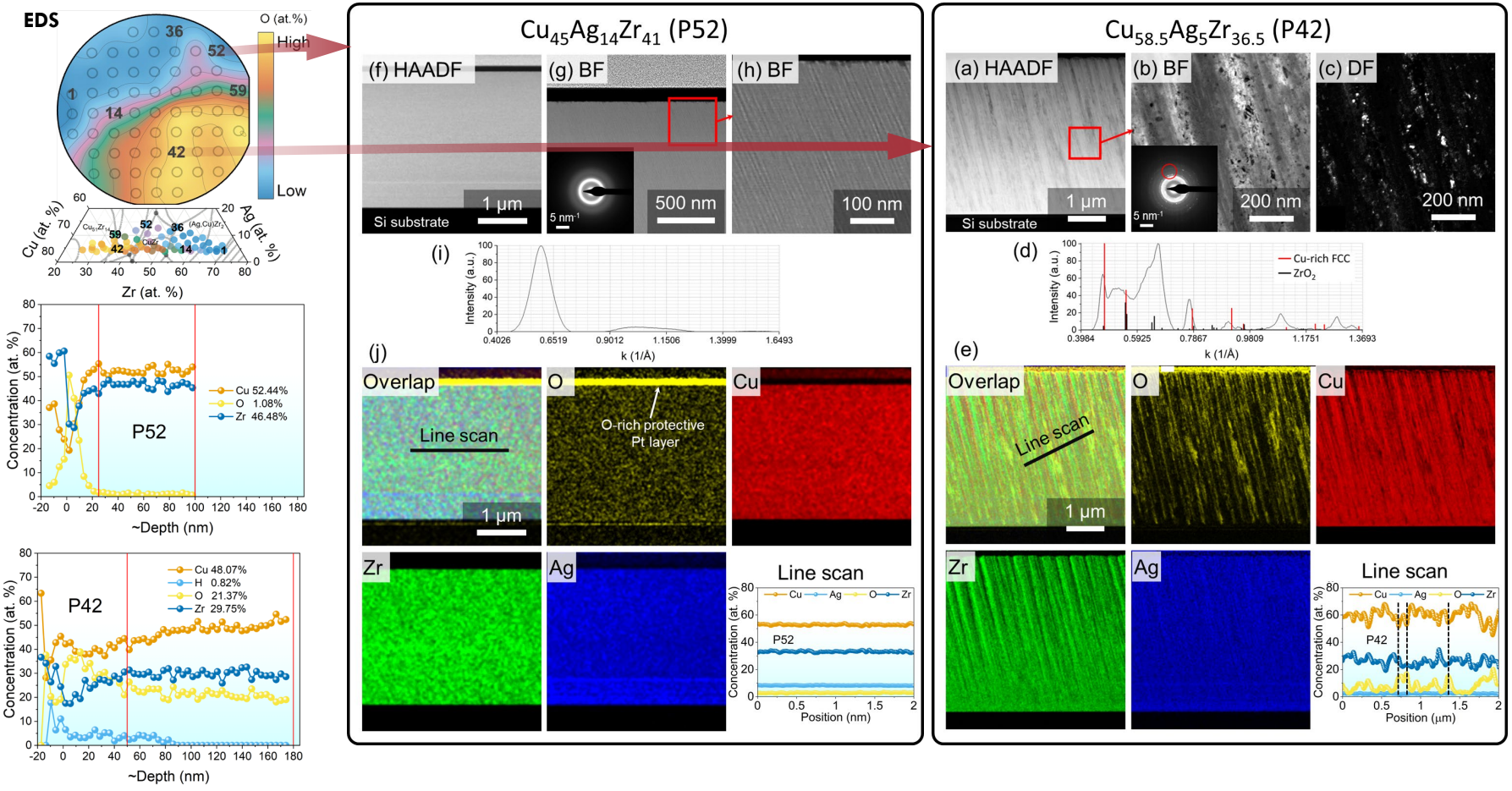




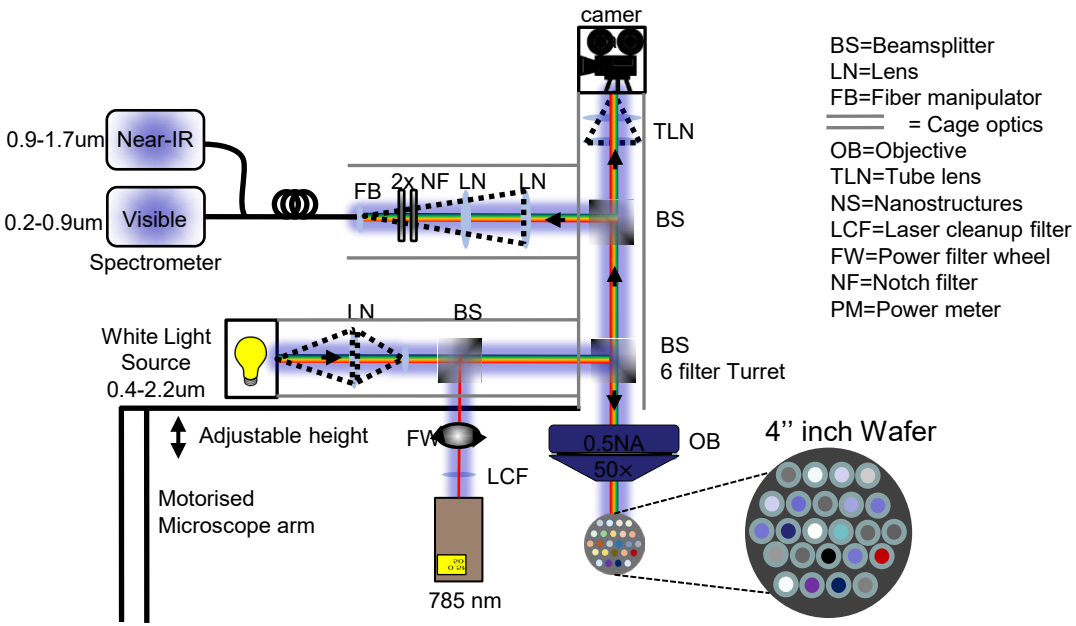
XRD on each patch:

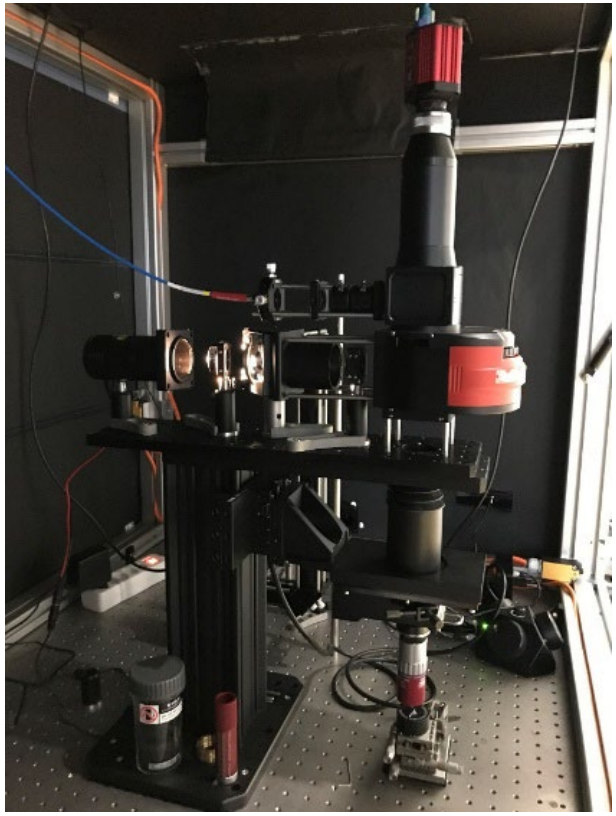
- Amorphous structure

Defects and oxygen content



Instrument development: optical properties

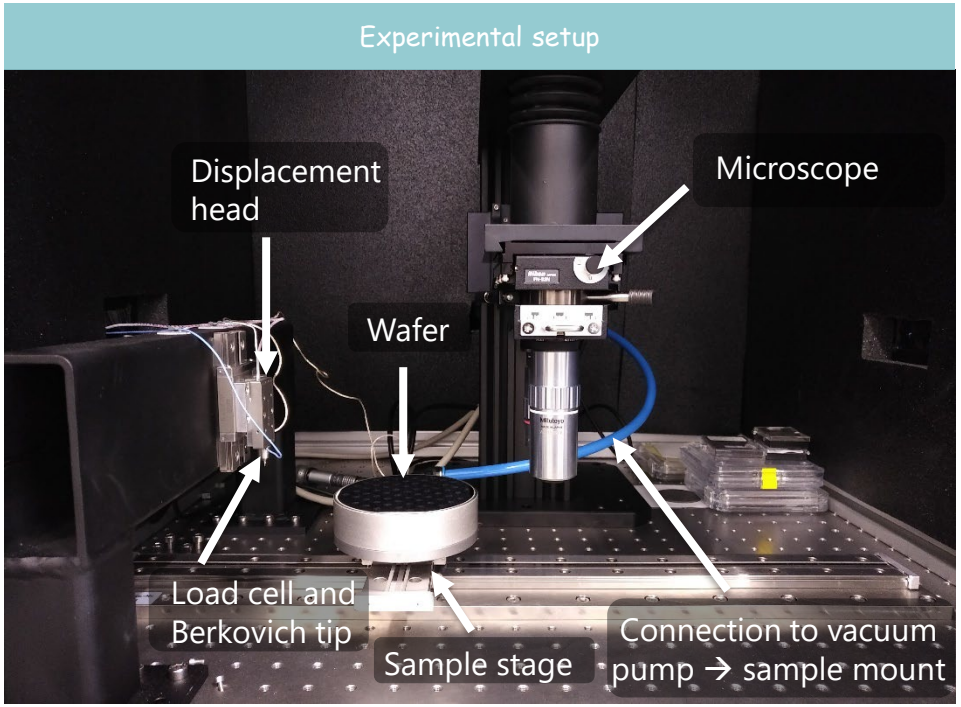




- Reflectivity: 300nm to 1800nm
- Raman Spectroscopy (785nm laser)

Instrument development: Nanoindentation

alemnis
engineering your ideas

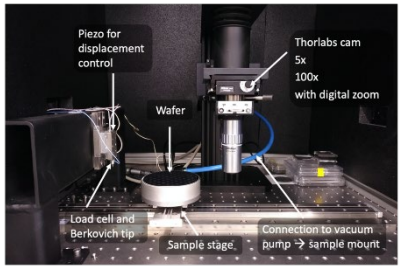


- High accuracy, low noise for thin film mechanical property measurements
- Automatic mapping of mechanical properties on 4in wafers
- Constant machine compliance
  - Guarantees consistent results over whole wafer
- Nanoindentation for measuring hardness, modulus, coating adhesion
- Scratch testing

Nanomechanical properties

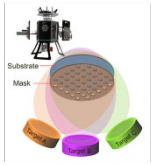
Scanning Indenter

Automatische Messung auf 4 in Wafern

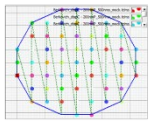


\+

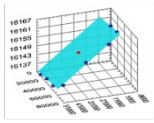
Chemische Gradienten



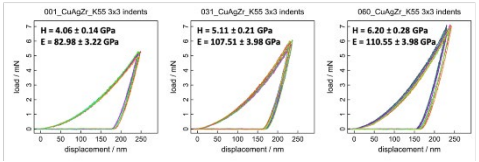
Automatisiertes Mapping

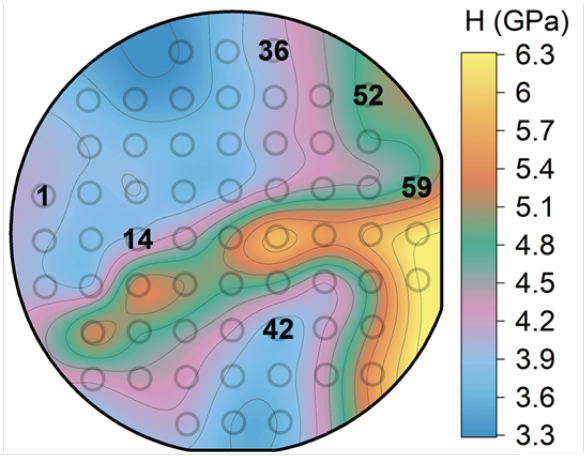


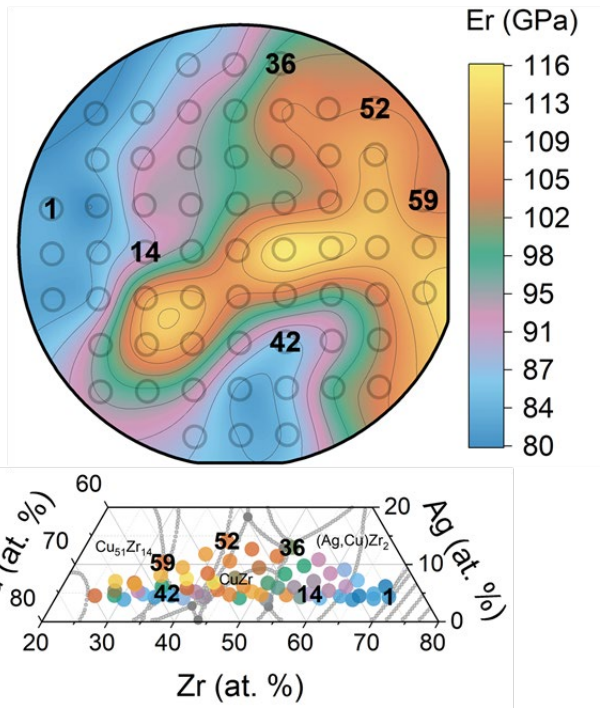
Oberflächendetektion



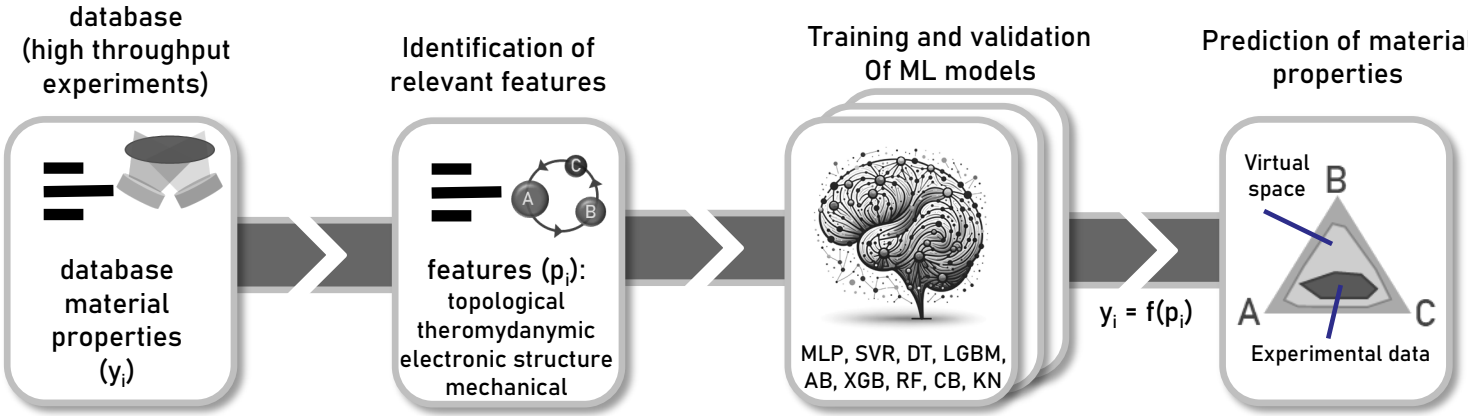
Messung von Härte und Modul der 61 Kompositionen



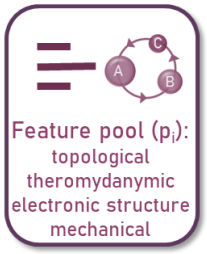




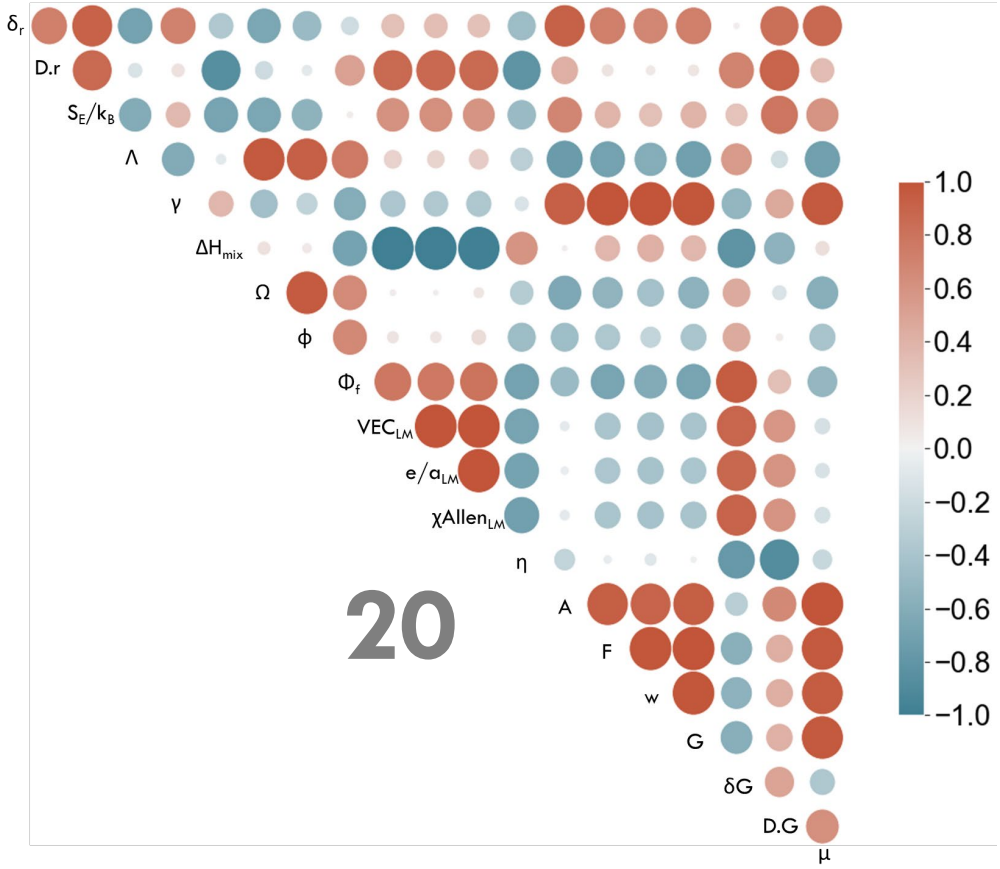
Data analysis using machine learning



Data analysis using machine learning



Feature pool (p_i):
topological
theromydanymic
electronic structure
mechanical



Correlation
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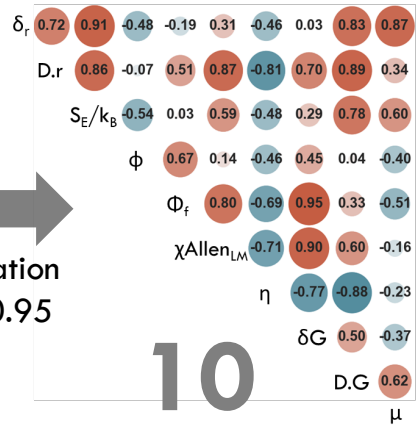
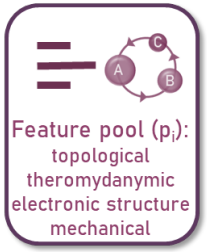
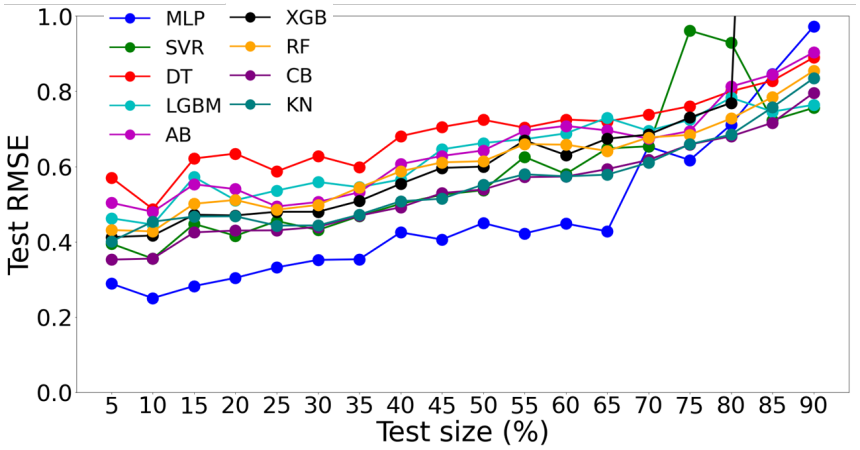
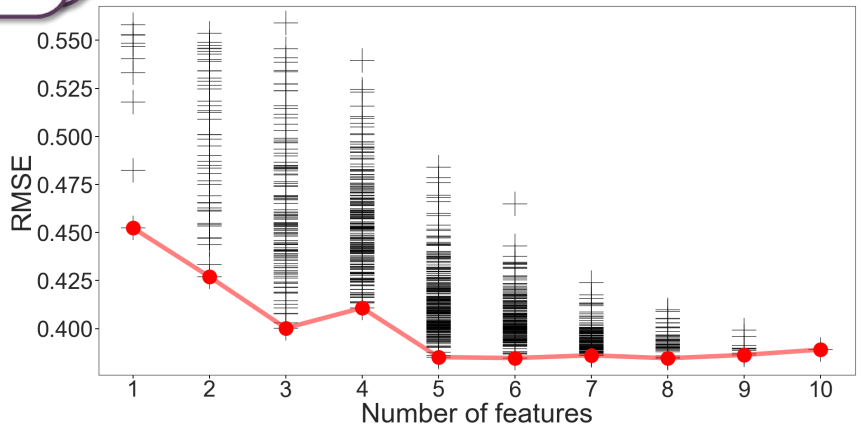


Data analysis using machine learning



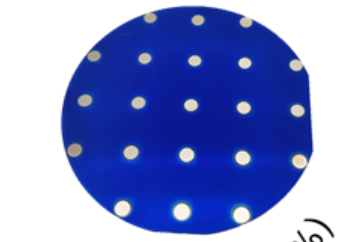


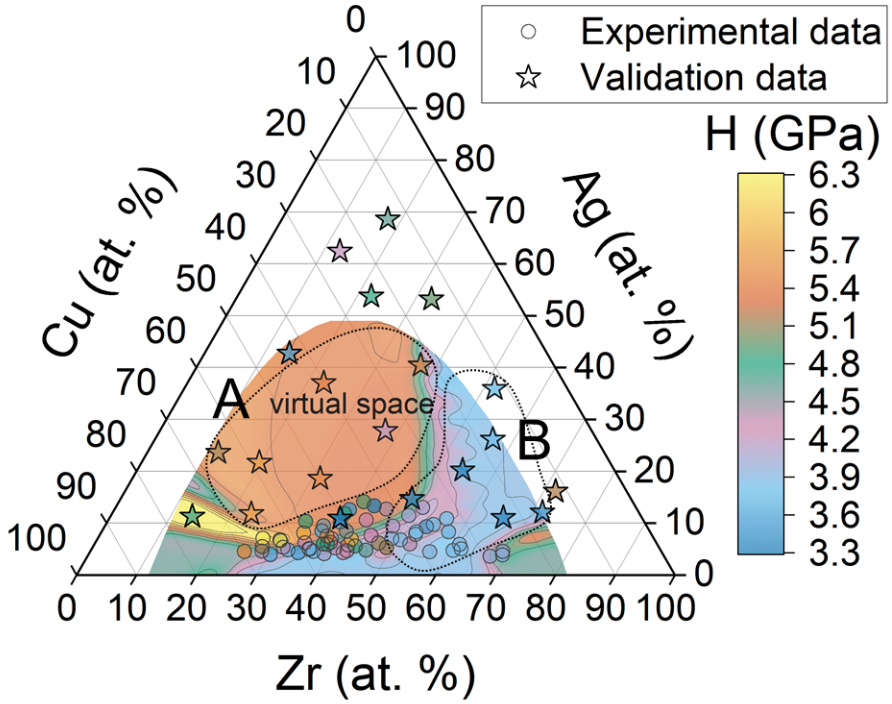


# feature	Best set of features	RMSE
1	μ	0.4524
2	Φ_f, μ	0.4270
3	Φ_f, η, μ	0.4002
4	Φ_f, χAll_{LM}, D.G, μ	0.4108
5	Φ_f, χAll_{LM}, η, D.G, μ	0.3851
6	δ, Φ_f, χAll_{LM}, η, D.G, μ	0.3847
7	δ, D.r, φ, Φ_f, χAll_{LM}, D.G, μ	0.3861
8	δ, D.r, Φ_f, χAll_{LM}, η, δG, D.G, μ	0.3846
9	δ, D.r, SE/kB, Φ_f, χAll_{LM}, η, δG, D.G, μ	0.3863
10	δ, D.r, SE/kB, φ, Φ_f, χAll_{LM}, η, δG, D.G, μ	0.3891

Data analysis using machine learning

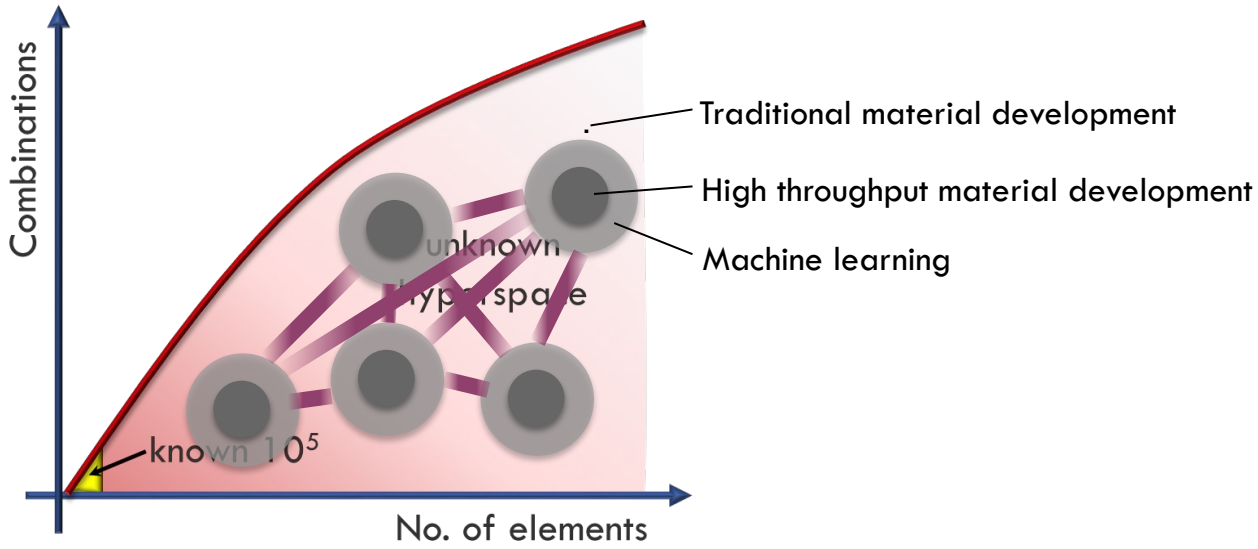
Machine learning





Summary

- ✓ Combination of combinatorial material libraries, high throughput experiments, and machine learning can significantly speed up the material development process
- ✓ The methods used in this study can be generalized and used for other material systems.
- ✓ The investigation of the CuAgZr system using our methods allows identifying compositions with high potential for biomedical applications.



K. Wieczerzak et al.: Unlocking the potential of CuAgZr metallic glasses: A comprehensive exploration with combinatorial synthesis, high-throughput characterization, and machine learning, Adv. Sci. (2023).