

From Data-Driven Alloy Design to Characterisation: Machine Learning in Materials Science

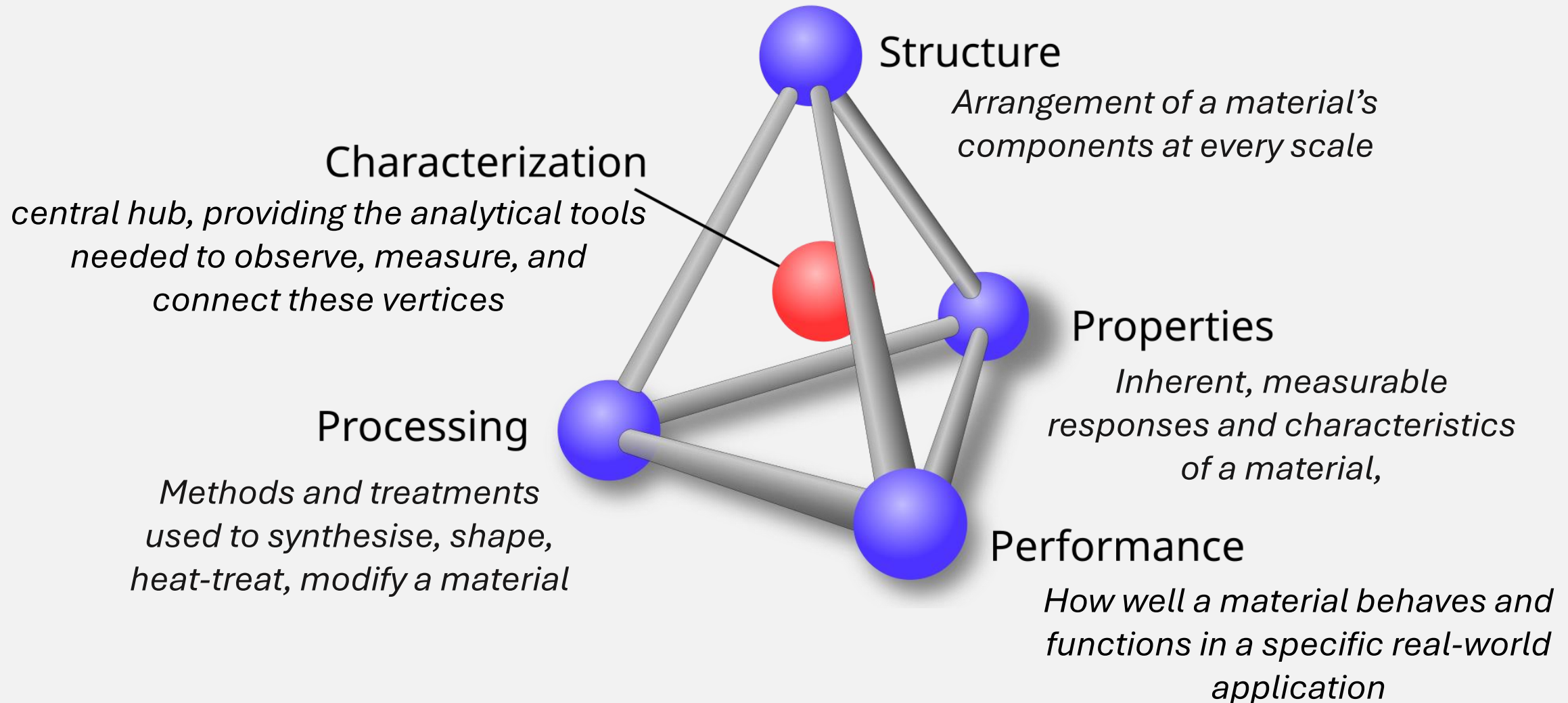
Swati Mahato
Postdoctoral Researcher

Erich Schmid Institute of Materials Science | Österreichische Akademie der Wissenschaften

swati.mahato@oeaw.ac.at
15 October 26

Materials Science Tetrahedron

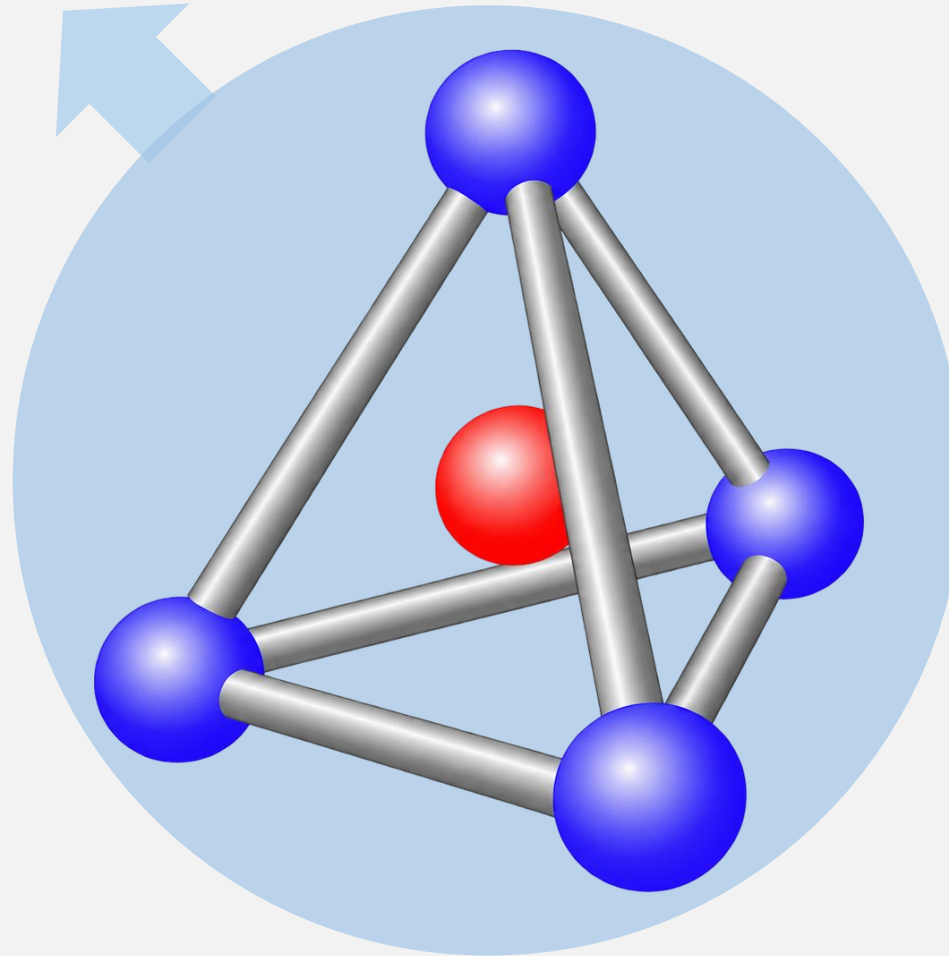
Foundational framework of materials science is the materials tetrahedron



Machine learning

Machine learning → overlay across the entire materials tetrahedron, accelerating every stage of materials development and optimisation overcoming hit and trial route

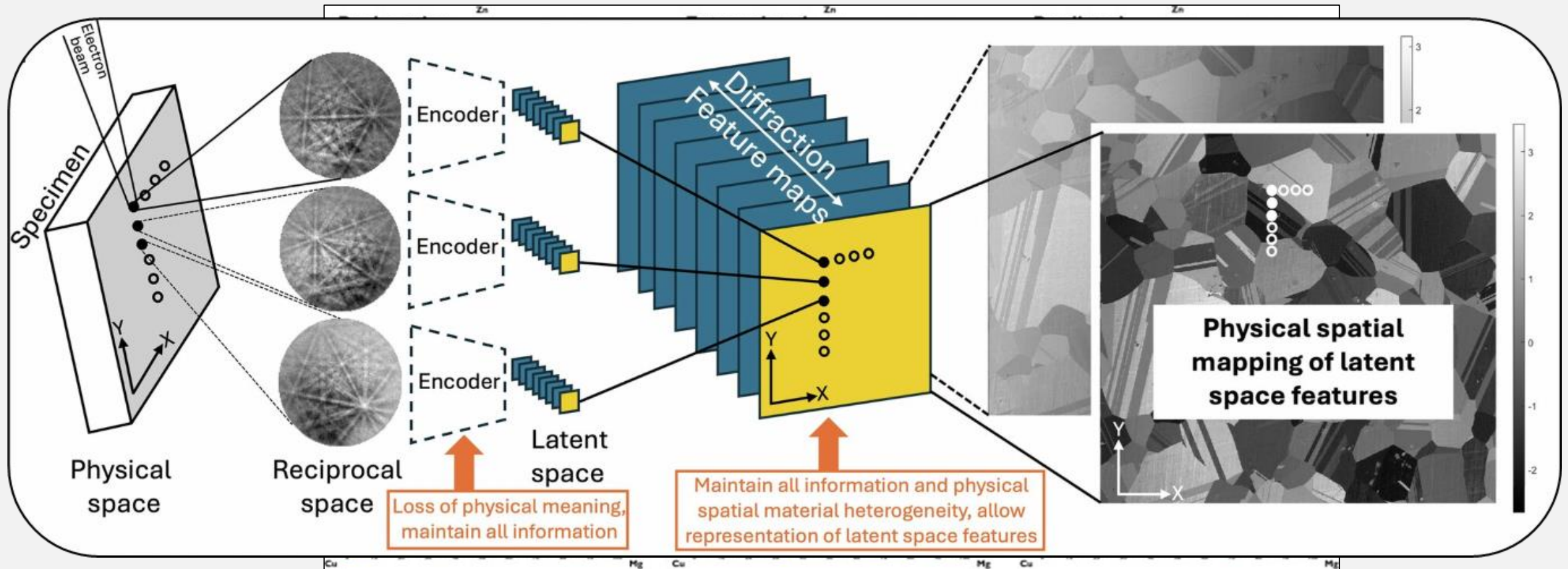
*Machine learning enable
to accelerate the
experimentation with
informed predictions*



Data: Experiments,
Simulations, large
literature databases

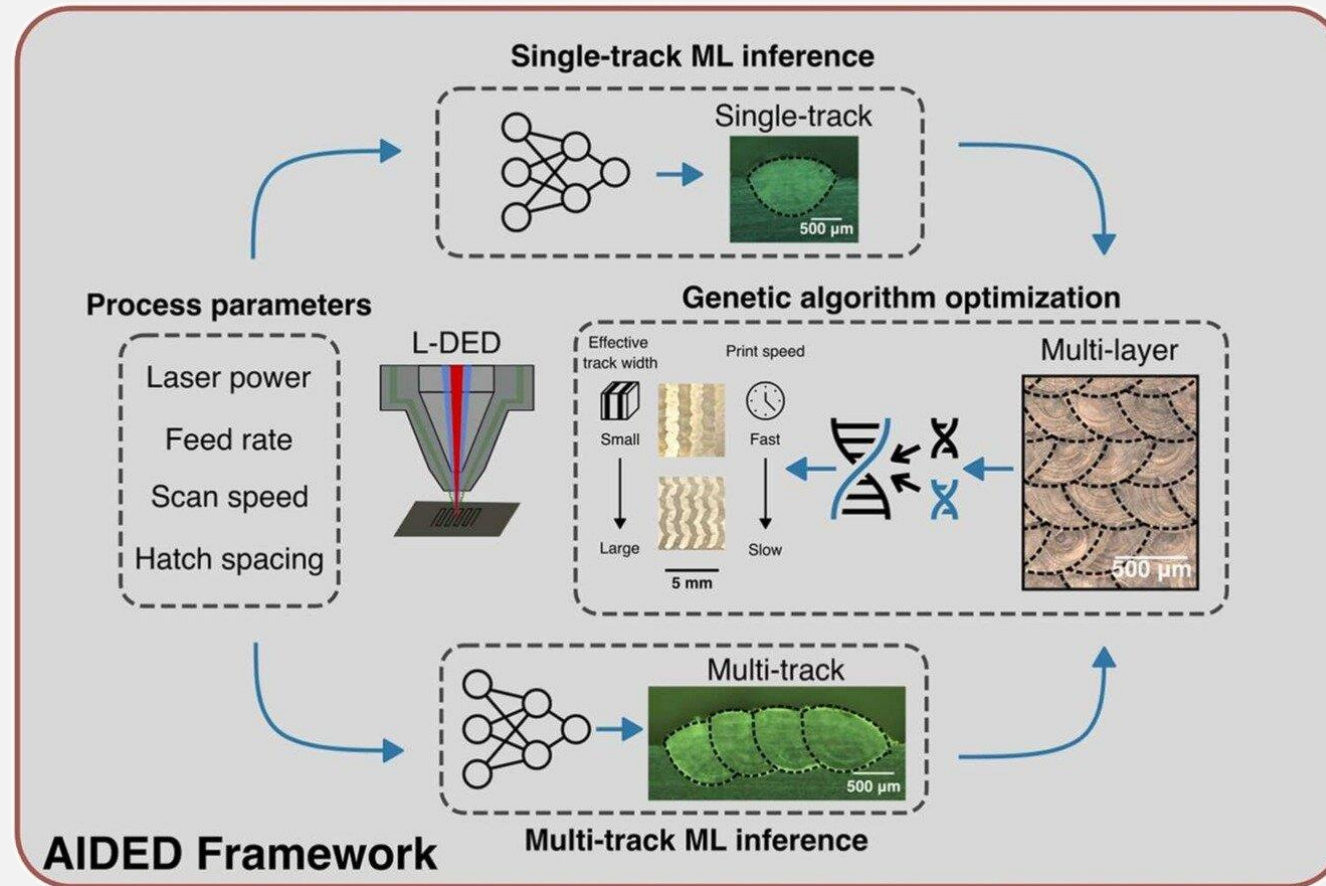
Structure

- *Phase prediction*
- *Microstructure reconstruction or analysis*



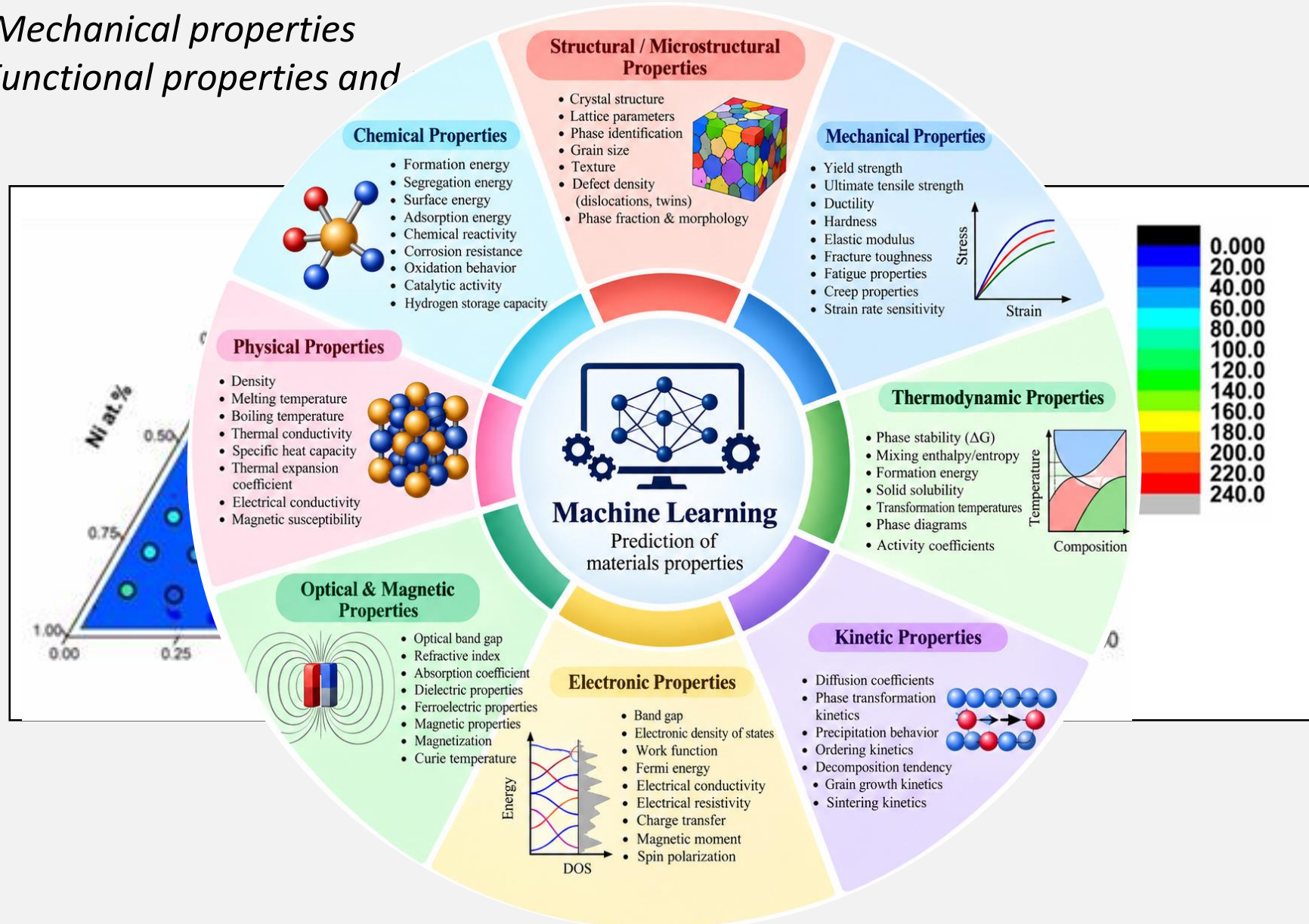
Processing

- *Optimising process parameters*
- *Defining heat treatment temperatures*



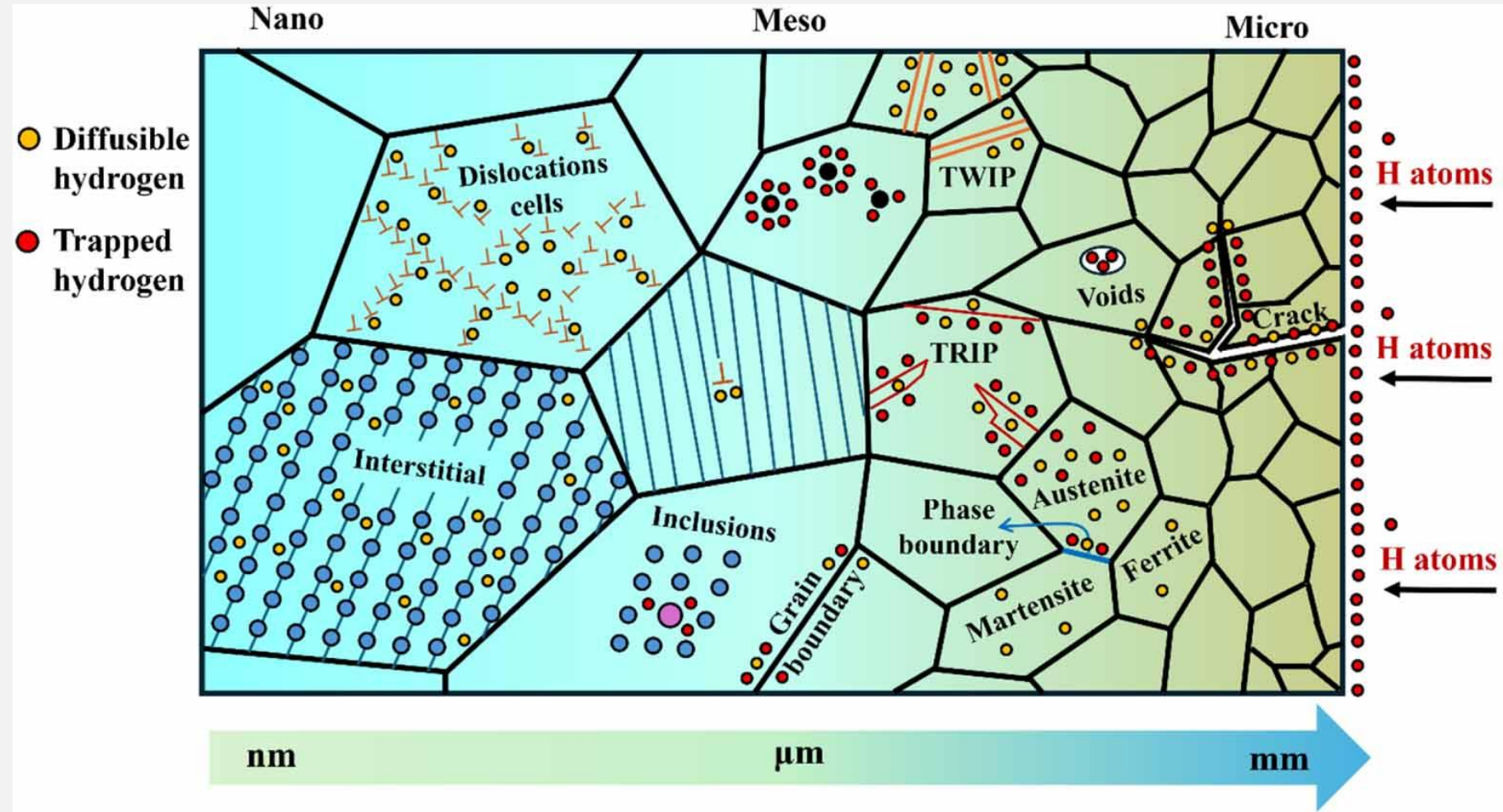
Properties

- *Mechanical properties*
- *Functional properties and*



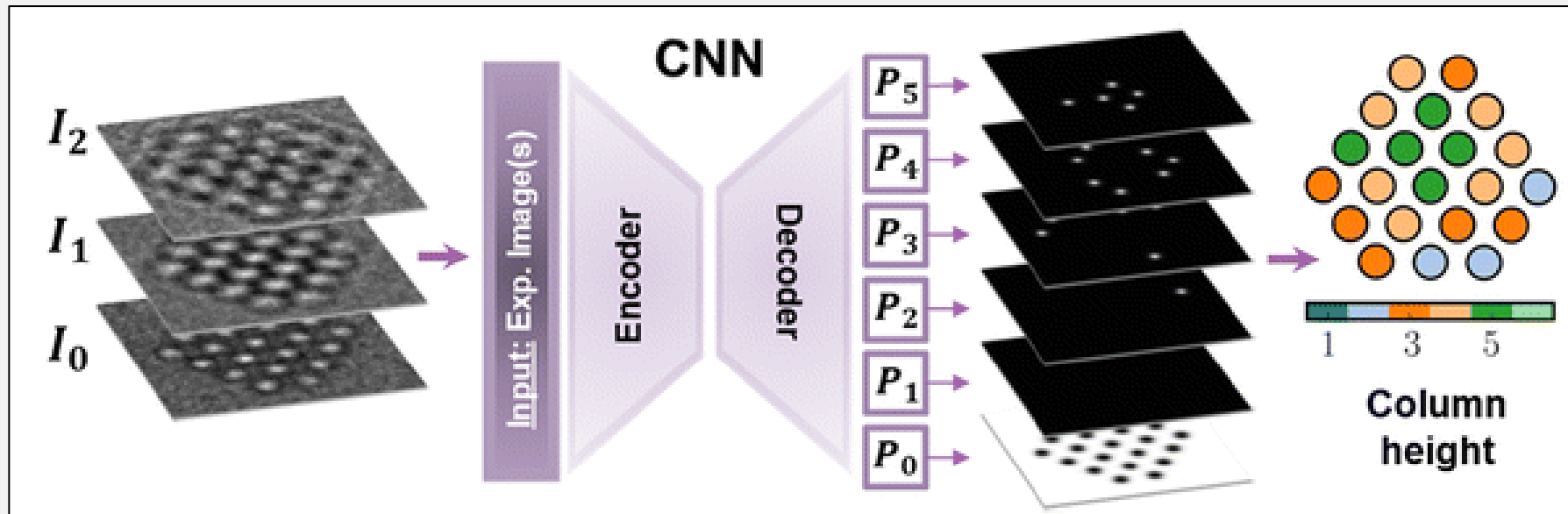
Performance

- life of the material under certain load and conditions*

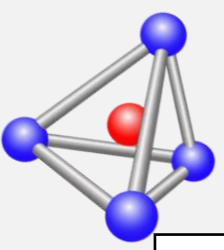


Characterisation

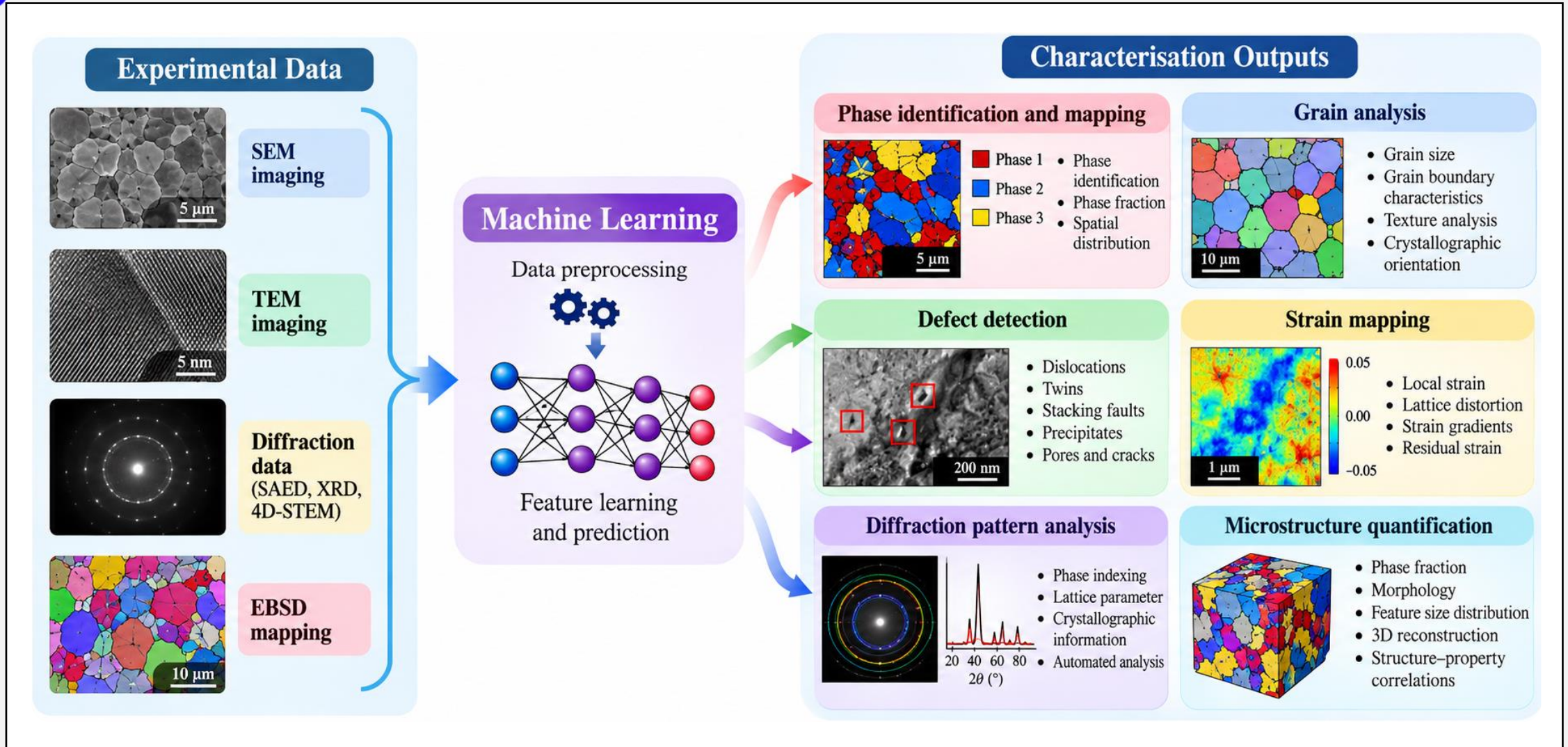
- *Advanced microscopes and detectors → Faster → Huge data*
- *Automated analysis of microscopy and diffraction data*



- *Trained CNN model on atomic resolution images to predict the column height*
- *Counts the atoms in each column directly from the images provided*
- *Faster and more efficient way to analyse this huge dataset collected*



Machine learning in Characterisation

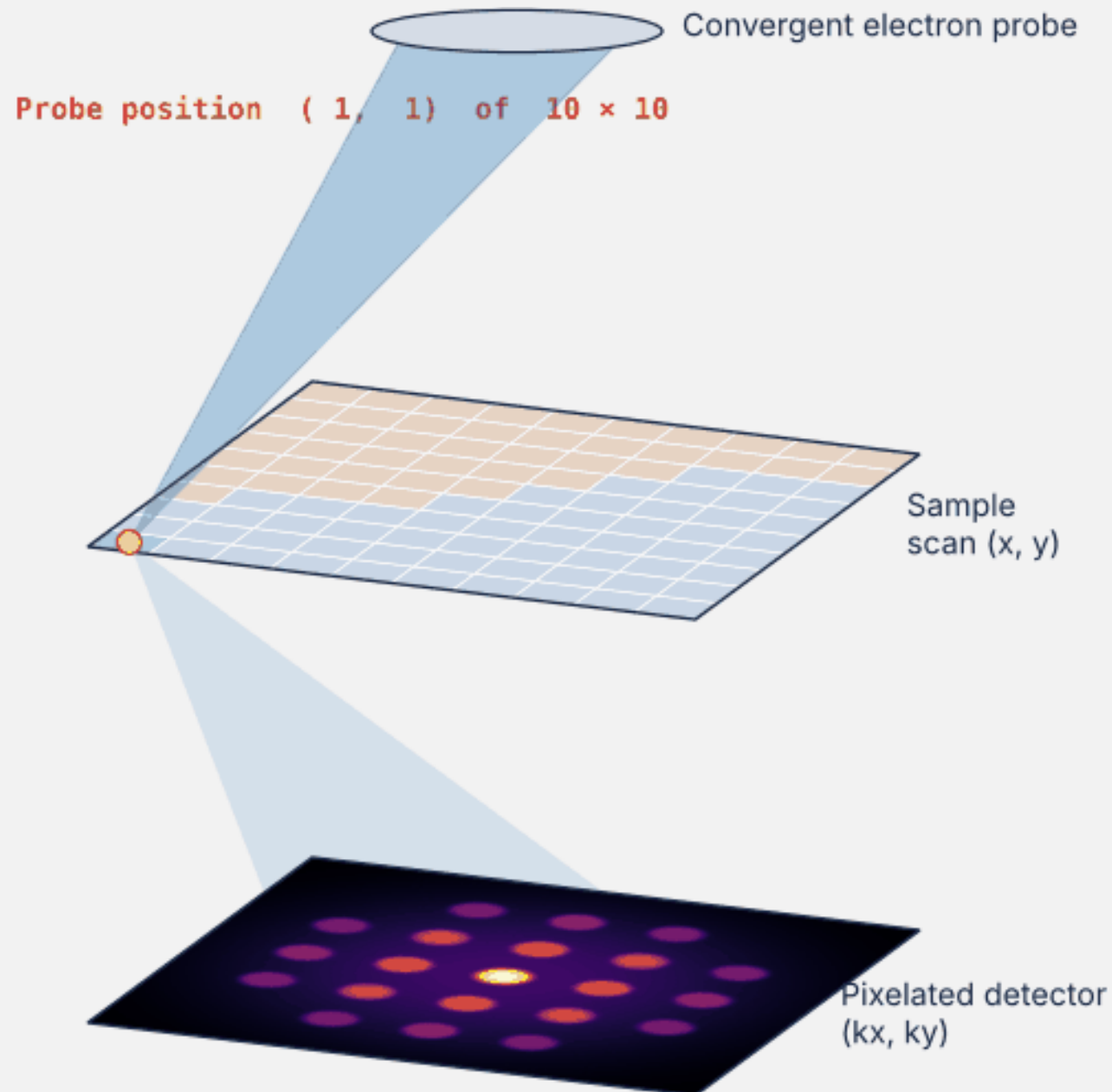




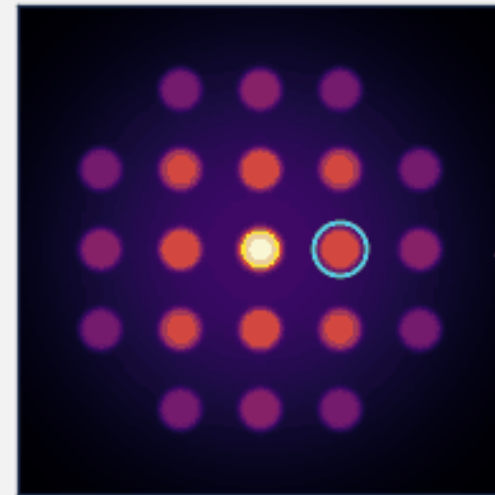
Machine learning in Characterisation

**Case Study: Physics- Guided Latent
Representation Learning for Nanobeam
Electron Diffraction via Strain- Conditioned
Convolutional Variational Autoencoder**

4D STEM Characterisation

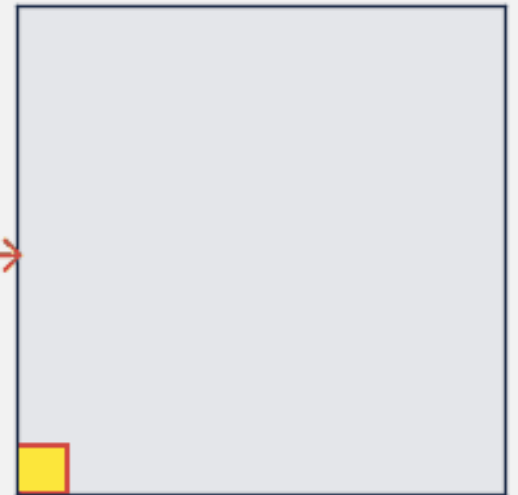


Diffraction pattern at (x, y)



cyan ring = virtual aperture

Virtual dark-field image



intensity inside aperture

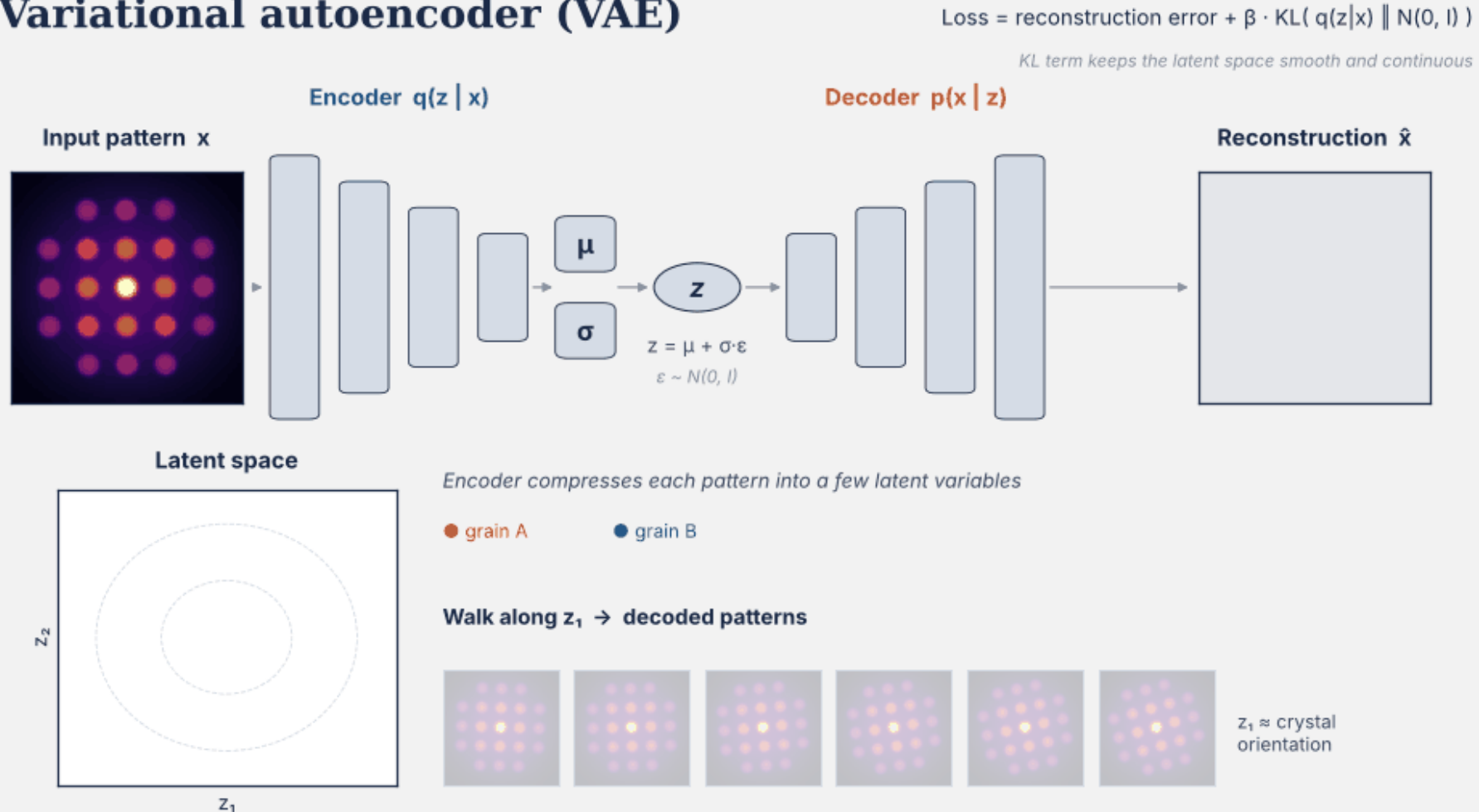
At each probe position a full 2D diffraction pattern is recorded: 2D scan × 2D pattern = 4D dataset

Orientation, phase, strain and thickness are encoded in every pattern; ML extracts them automatically.

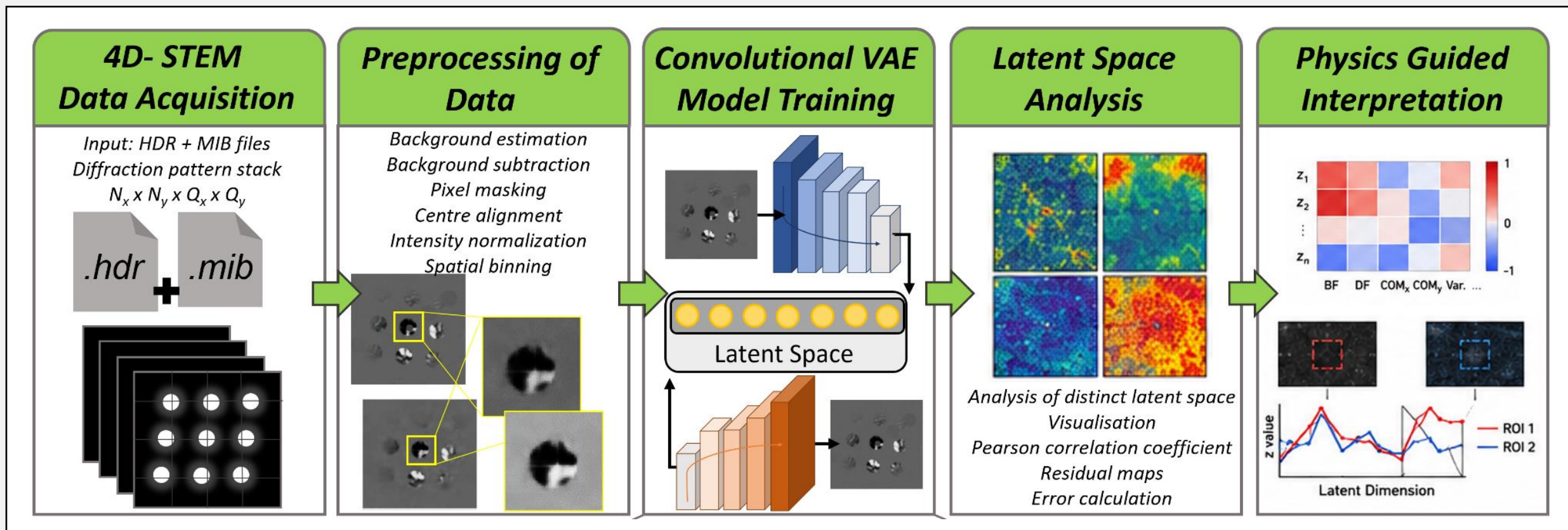
4D STEM Data Analysis

4D-STEM captures the full reciprocal-space signal at every probe position → Analysis still leans on conventional scalar descriptors: VBF, centre-of-mass, and sharpness

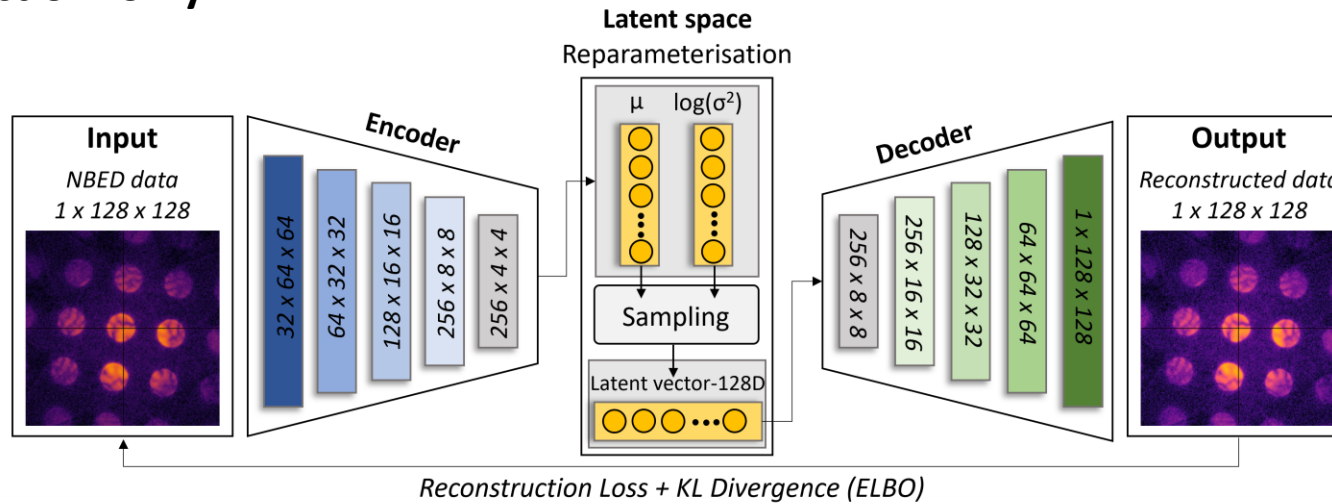
Variational autoencoder (VAE)



- 1 Can a generative model learn physically meaningful latent representations directly from experimental NBED data?
- 2 What reciprocal-space information do individual latent variables actually encode?
- 3 Can physics-informed supervision improve the organisation and interpretability of the latent manifold?



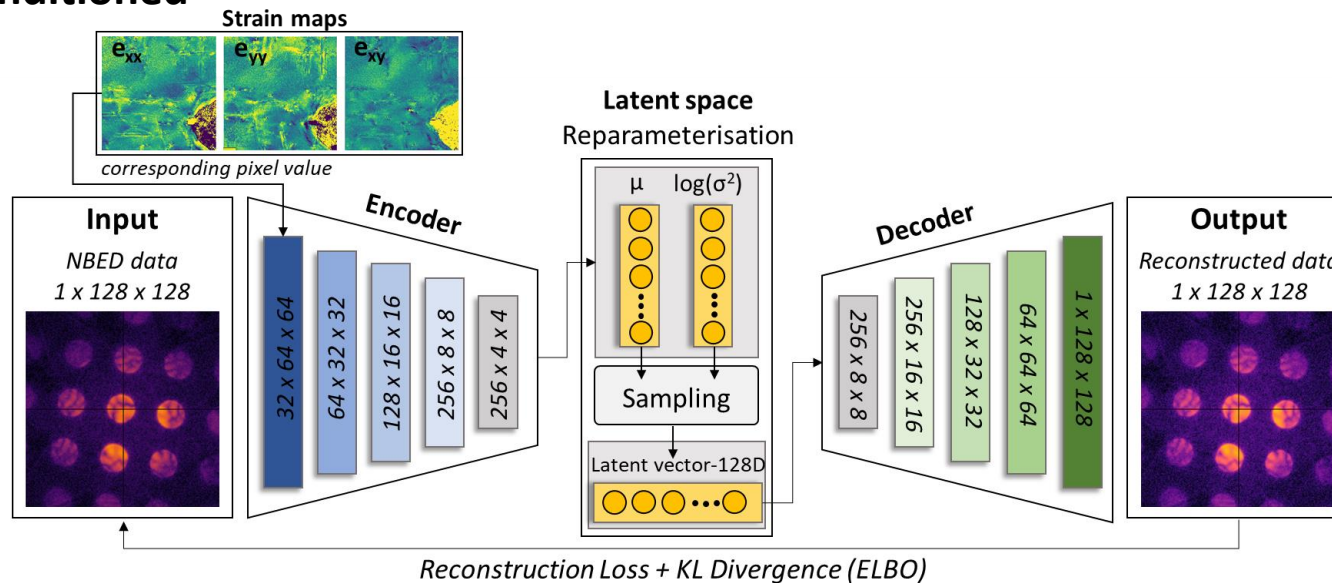
Reconstruction- only



Reconstruction-only

NBED pattern $\rightarrow$ 128-D latent code $\rightarrow$ NBED pattern $\rightarrow$ Trained purely to minimise reconstruction error

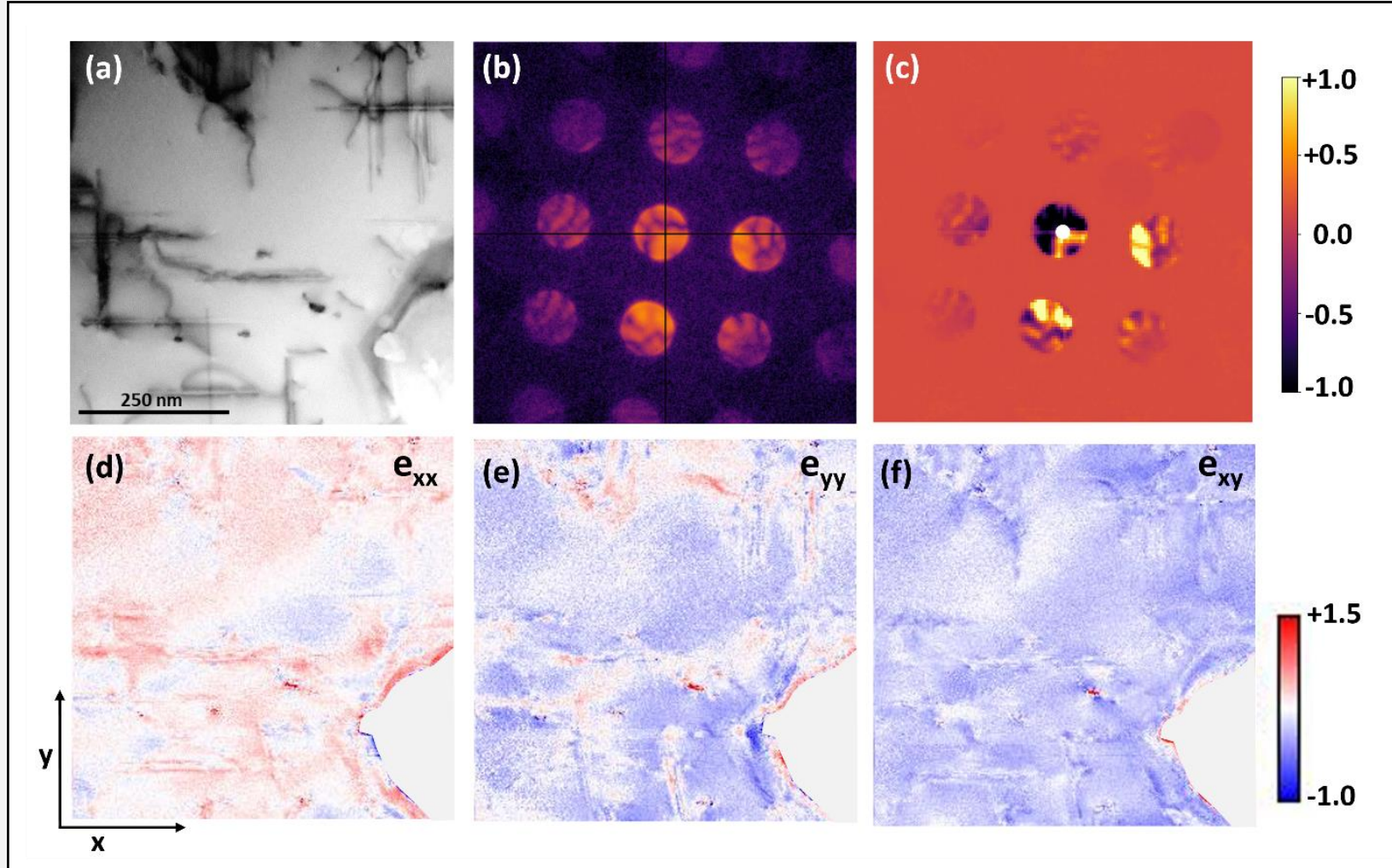
Strain- conditioned



Strain-conditioned

Same backbone, but e_{xx} , e_{yy} , e_{xy} strain values condition the encoder $\rightarrow$ as auxiliary input

Input Data



Material

Heat-treated Al-3.5Cu-
1.5Mg-1Si (T6)

Scan size

256 × 256 probe
positions = 65,536
patterns

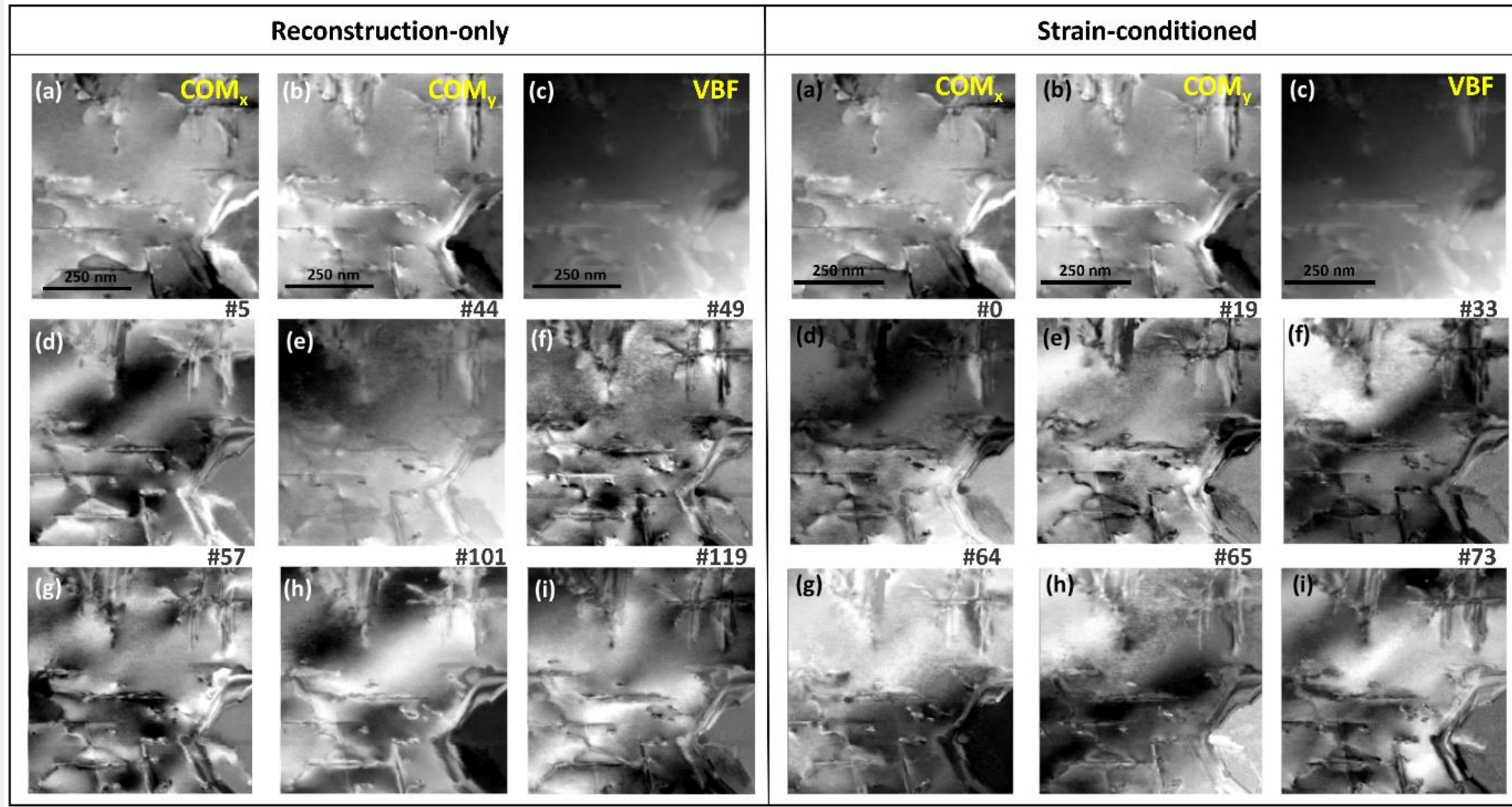
Detector

512×512, 12-bit → binned
to 128×128

Conditioning

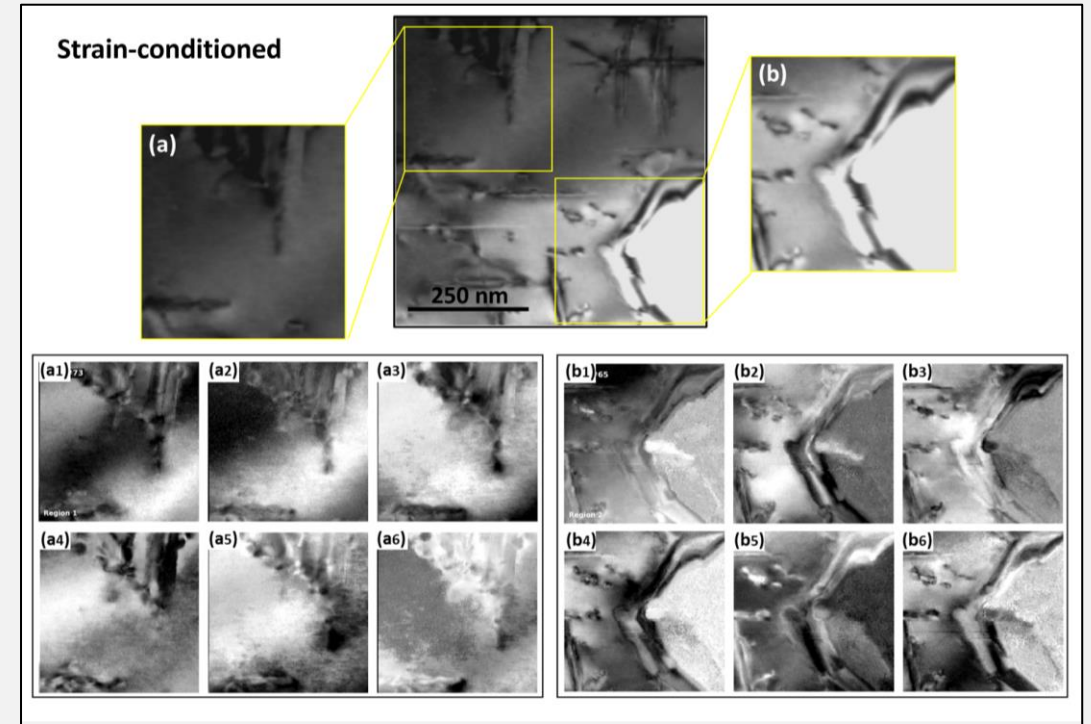
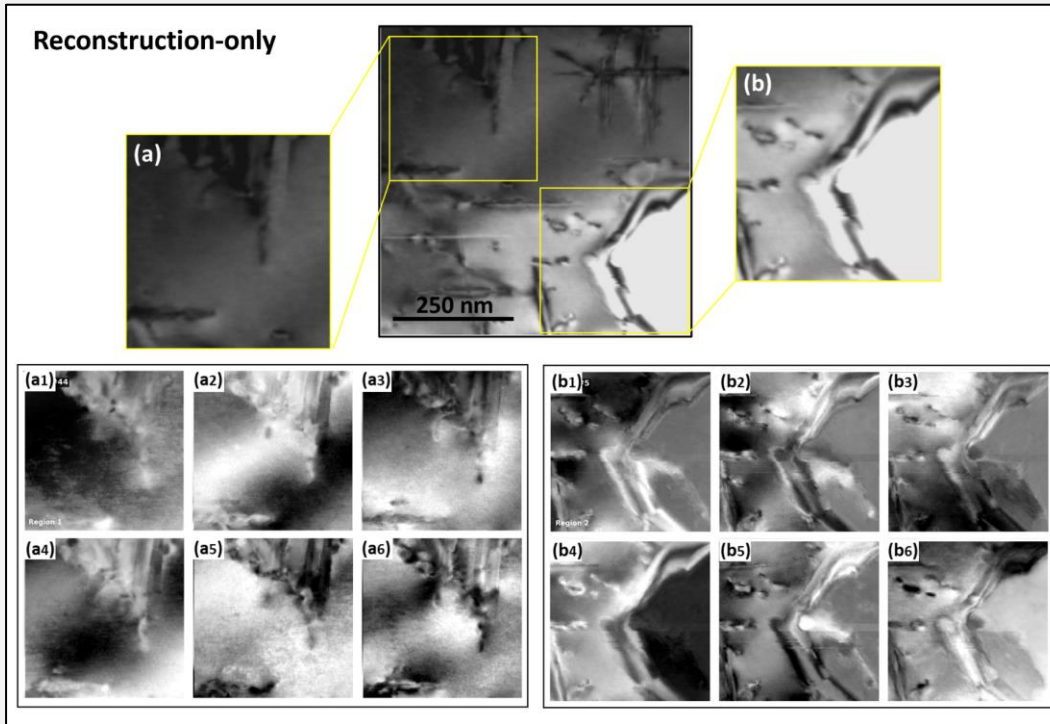
e_{xx} , e_{yy} , e_{xy} strain maps,
registered per-pixel

Latent Maps vs. Conventional Descriptors

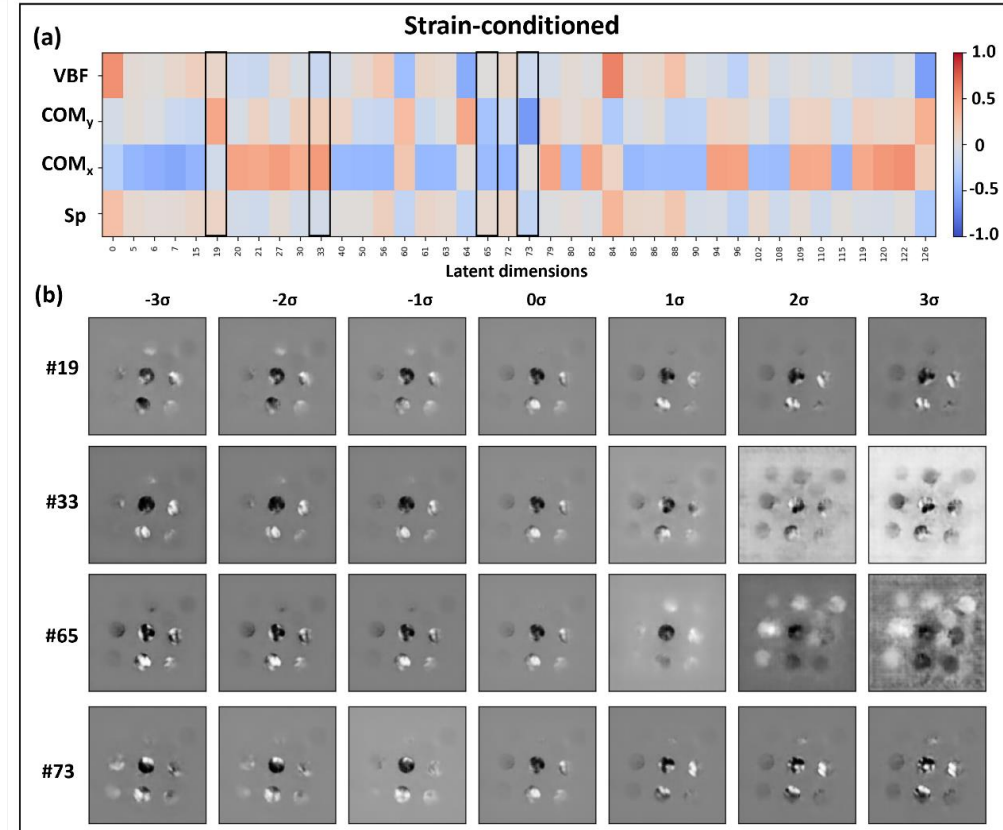
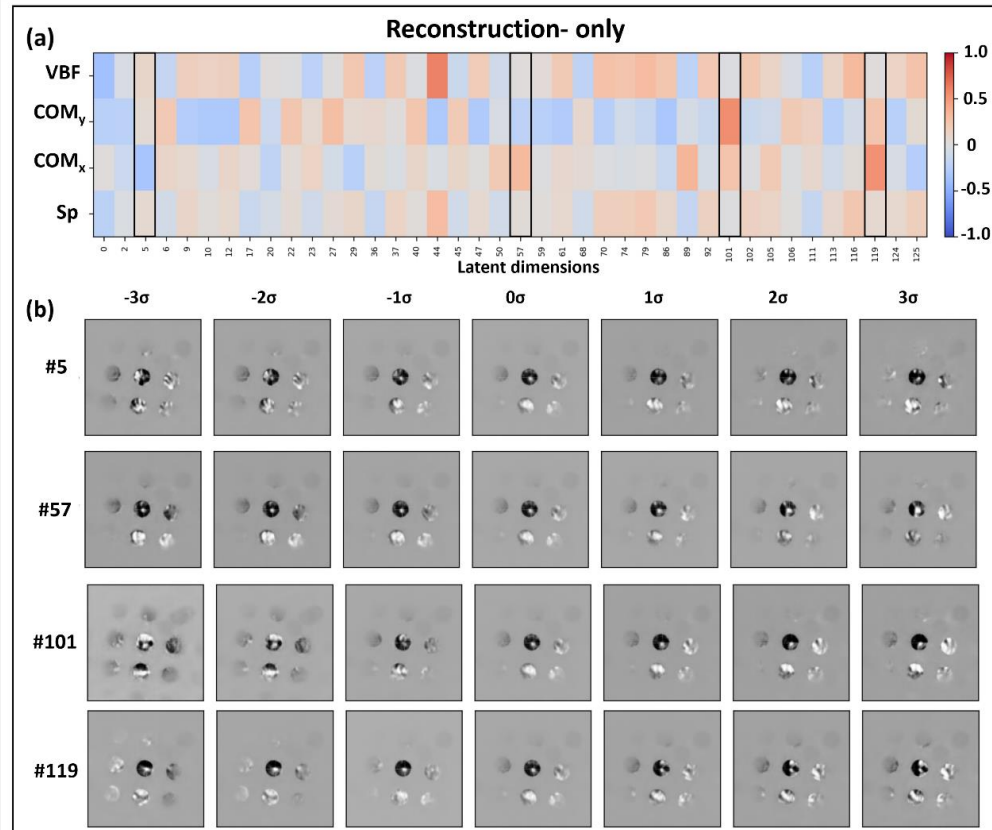


Both models recover microstructure without labels → strain-conditioned latent maps are more localised and complementary, sharpening precipitates, interfaces, and dislocations rather than repeating broad intensity contrast

Microstructural Heterogeneity Sensitivity

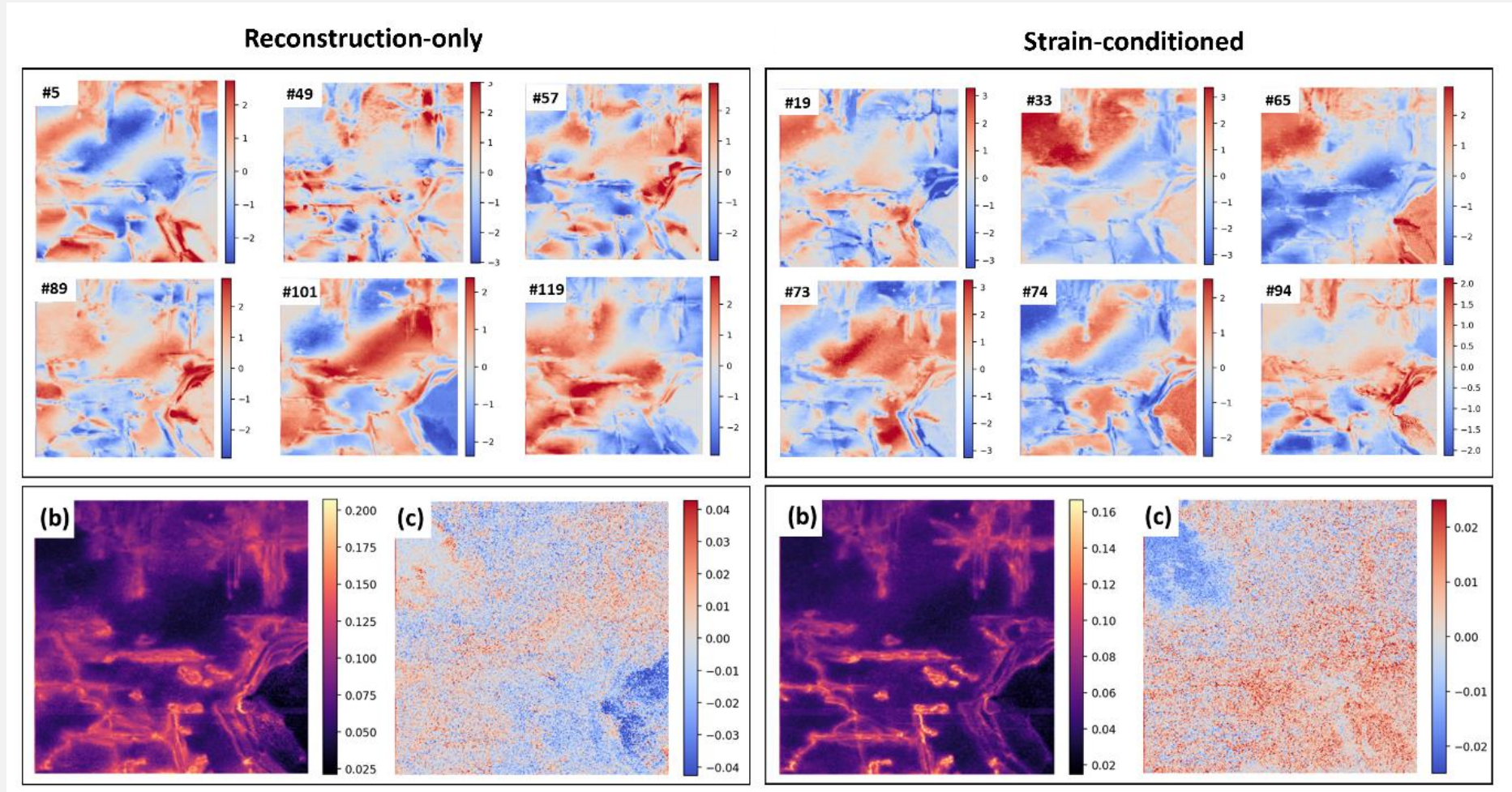


- Two regions of interest: a relatively homogeneous grain interior and an interface-rich region, compared across the same latent dimensions
- Reconstruction-only: several latent channels overlap, spreading reconstruction-related information across diffuse intensity gradients
- Strain-conditioned: individual dimensions selectively emphasise interfaces, dislocations, precipitates, and localised strain concentrations
- Diffuse background activation is markedly reduced : phase boundaries appear as narrower, higher-contrast features.



- Reconstruction-only latents show weak, broadly distributed correlation with VBF / COM/sharpness
- Strain conditioning concentrates correlation into specialised dimensions → without ever collapsing to a near-perfect match to any descriptor
- Reconstruction-only dimensions mainly redistribute intensity smoothly across the central disk
- Strain-conditioned dimensions show localised, reflection-specific, nonlinear changes → consistent with sensitivity to real lattice

RMSE and residual maps



RMSE and residual maps are comparable between the two models → errors concentrate at boundaries and precipitates in both

Strain conditioning redistributes latent capacity toward deformation features without sacrificing reconstruction fidelity¹⁹

Mahato et al. Small Str. (under revision), 2026

Conclusions

Strain conditioning fundamentally reorganises the latent space

Transforming it from a reconstruction-driven into a microstructure-aware representation of reciprocal-space scattering, with reduced redundancy and stronger localisation of precipitates, dislocations, and interfaces

Interpretability improves without sacrificing fidelity

Despite the added supervision, reconstruction quality remains as high as (or higher than) the reconstruction-only model, showing that the gain comes from smarter allocation of latent capacity, not added model complexity

latent variables encode real physics, not just statistics

Correlation analysis, latent traversals, and RMSE maps consistently show that learned dimensions track lattice distortion and diffraction-vector variation rather than merely reproducing conventional descriptors like VBF or COM

Establishes a general, physics-guided strategy for explainable AI in electron microscopy

Providing a robust foundation for quantitative 4D-STEM analysis and a pathway toward interpretable, AI-assisted microstructural characterisation



Thankyou

Any questions?