UNIVERSITY OF CAMBRIDGE

Probabilistic neural network design of an alloy for direct laser deposition

Gareth Conduit

Theory of Condensed Matter group

Neural network algorithm to

Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

Accelerate materials and drugs discovery

Generic with proven applications in materials discovery and drug design

A black box

Train with complete data

Materials design

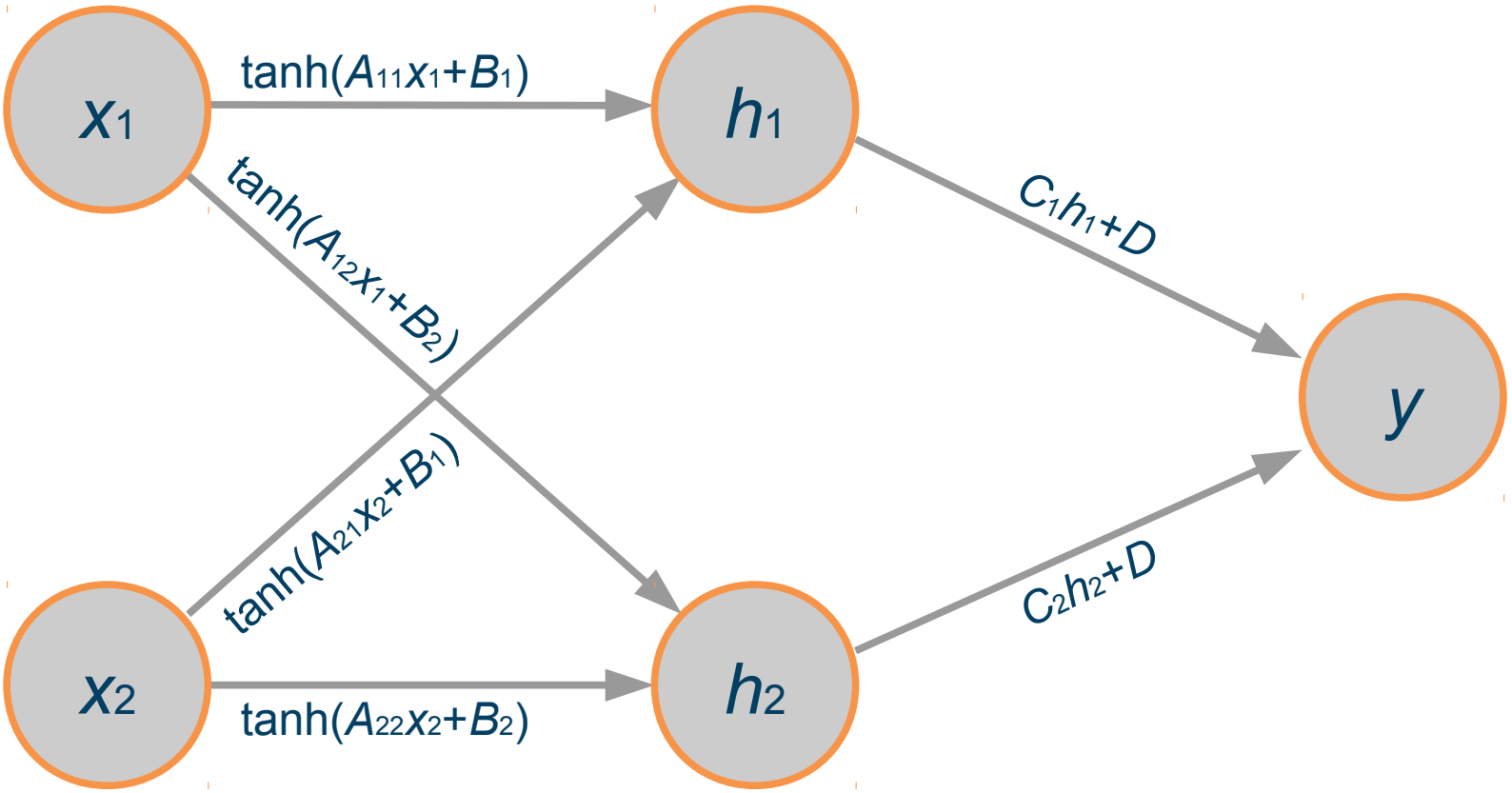
Materials design

Predict with complete data

Crystal structure

Crystal structure

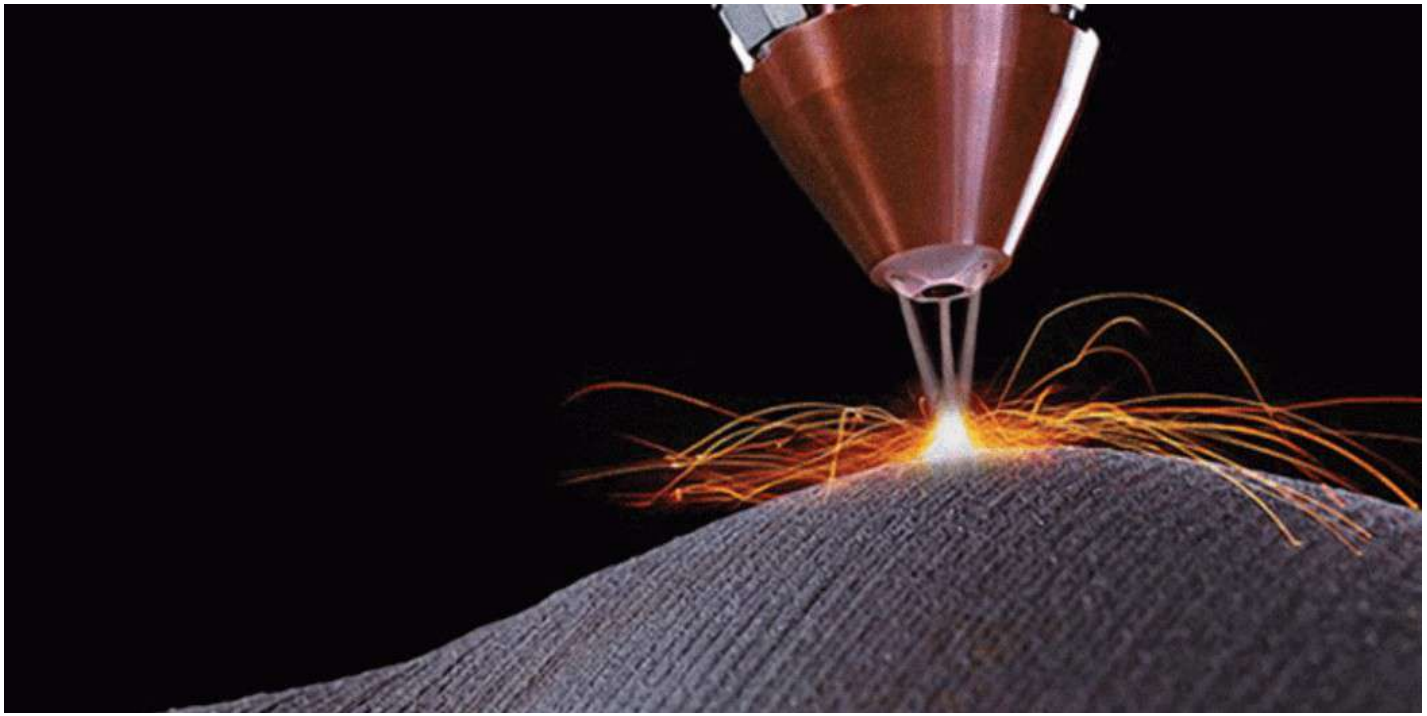
Architecture



Train with fragmented data

Predict with fragmented data

Direct laser deposition requires new alloys



Neural networks for materials design

Composition

Properties

Process

Fatigue

Welding

Neural networks for materials design

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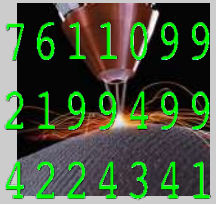
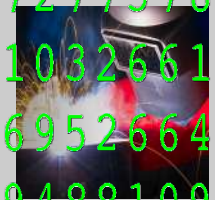


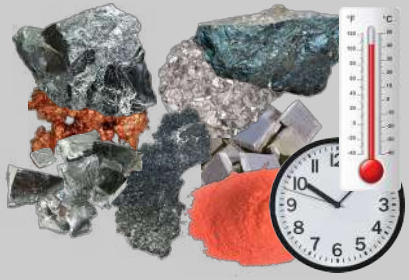
Fatigue

Welding



Neural networks for materials design

Composition



Properties

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Neural networks for materials design

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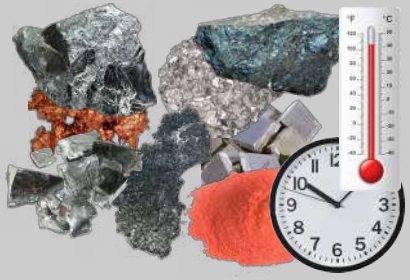

Properties

Process

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Composition

Properties

Process

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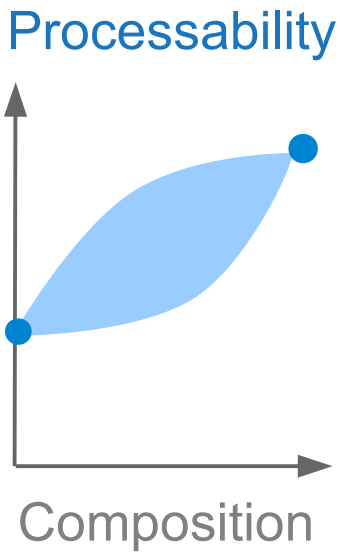
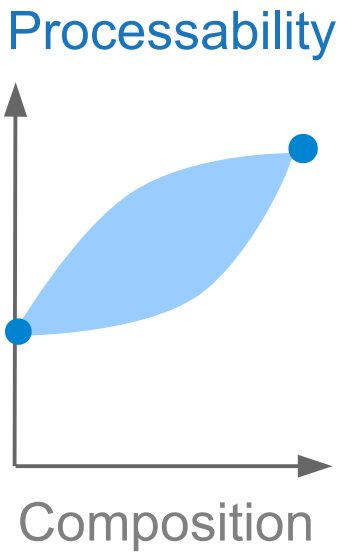
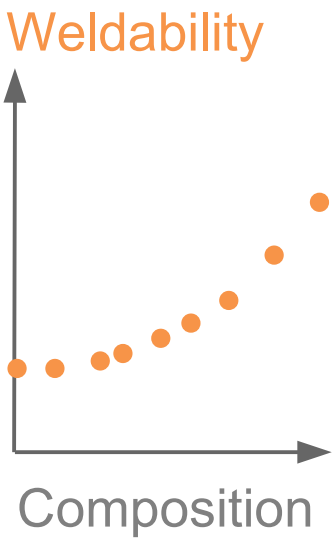
Insufficient processability results

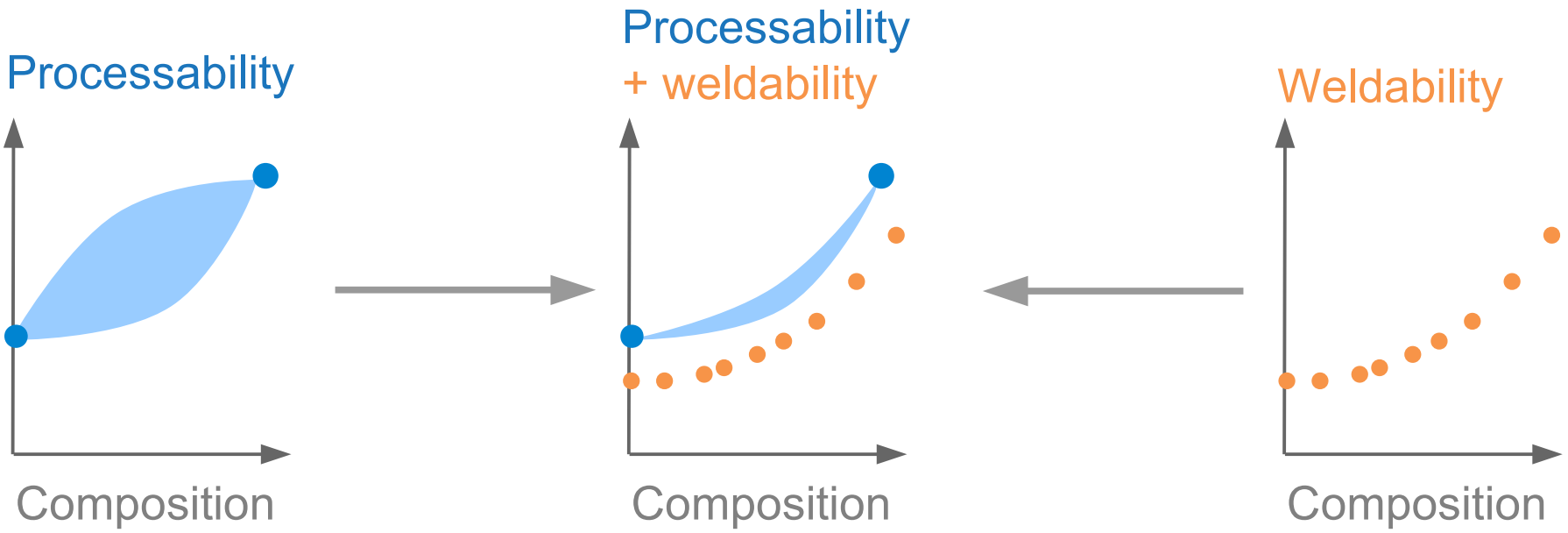


Welding is analogous to direct laser deposition

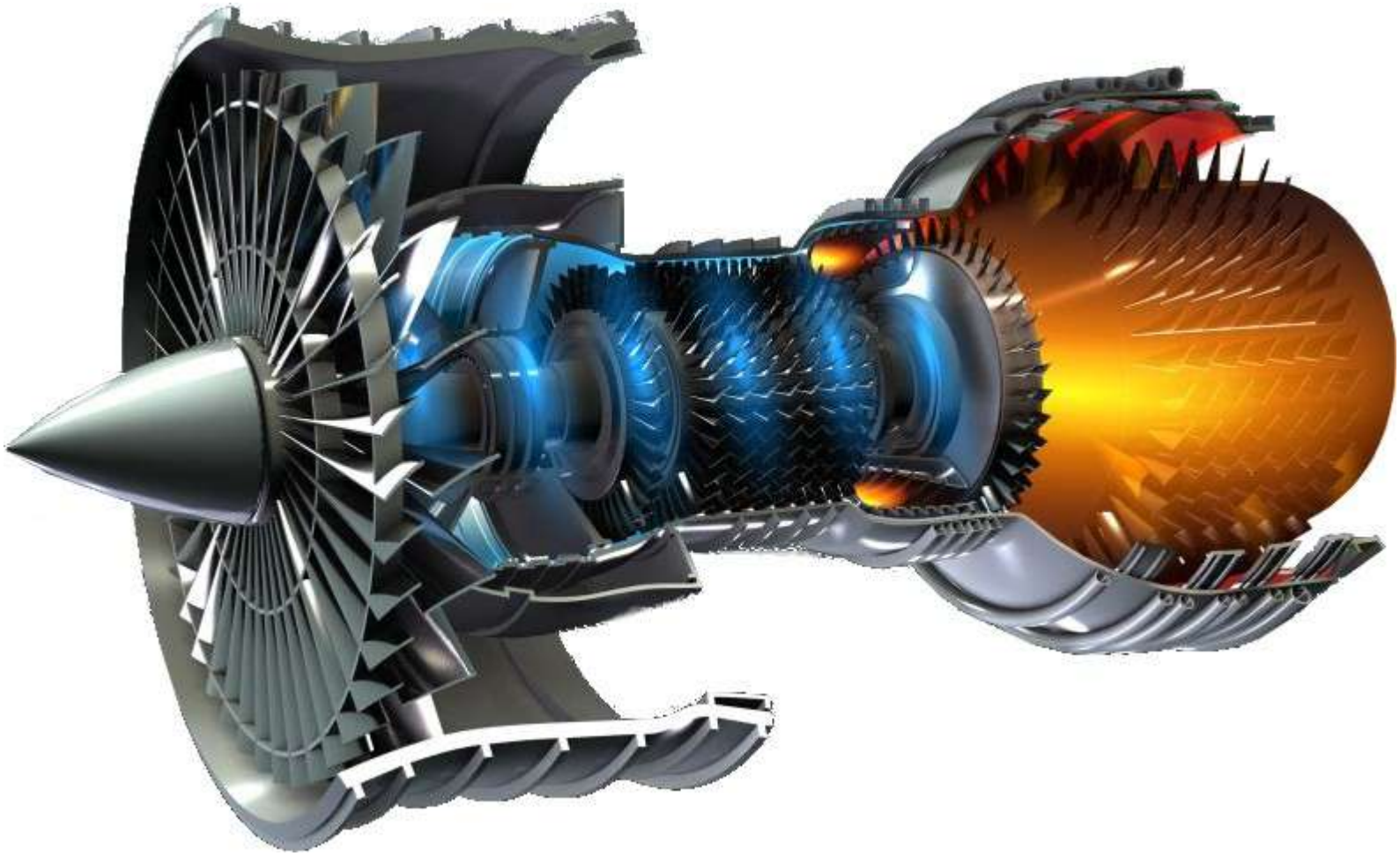




Merging properties with the neural network



Schematic of a jet engine



Target properties

Elemental cost	< 25 $\$kg^{-1}$
Density	< 8500 kgm^{-3}
γ' content	< 25 wt%
Oxidation resistance	< 0.3 $mgcm^{-2}$
Processability	< 0.15% defects
Phase stability	> 99.0 wt%
γ' solvus	> 1000˚C
Thermal resistance	> 0.04 $K\Omega^{-1}m^{-3}$
Yield stress at 900˚C	> 200 MPa
Tensile strength at 900˚C	> 300 MPa
Tensile elongation at 700˚C	> 8%
1000hr stress rupture at 800˚C	> 100 MPa
Fatigue life at 500 MPa, 700˚C	> 10^5 cycles

Composition

Cr: 19%

Co: 4%

Mo: 4.9%

W: 1.2%

Zr: 0.05%

Nb: 3%

Al: 2.9%

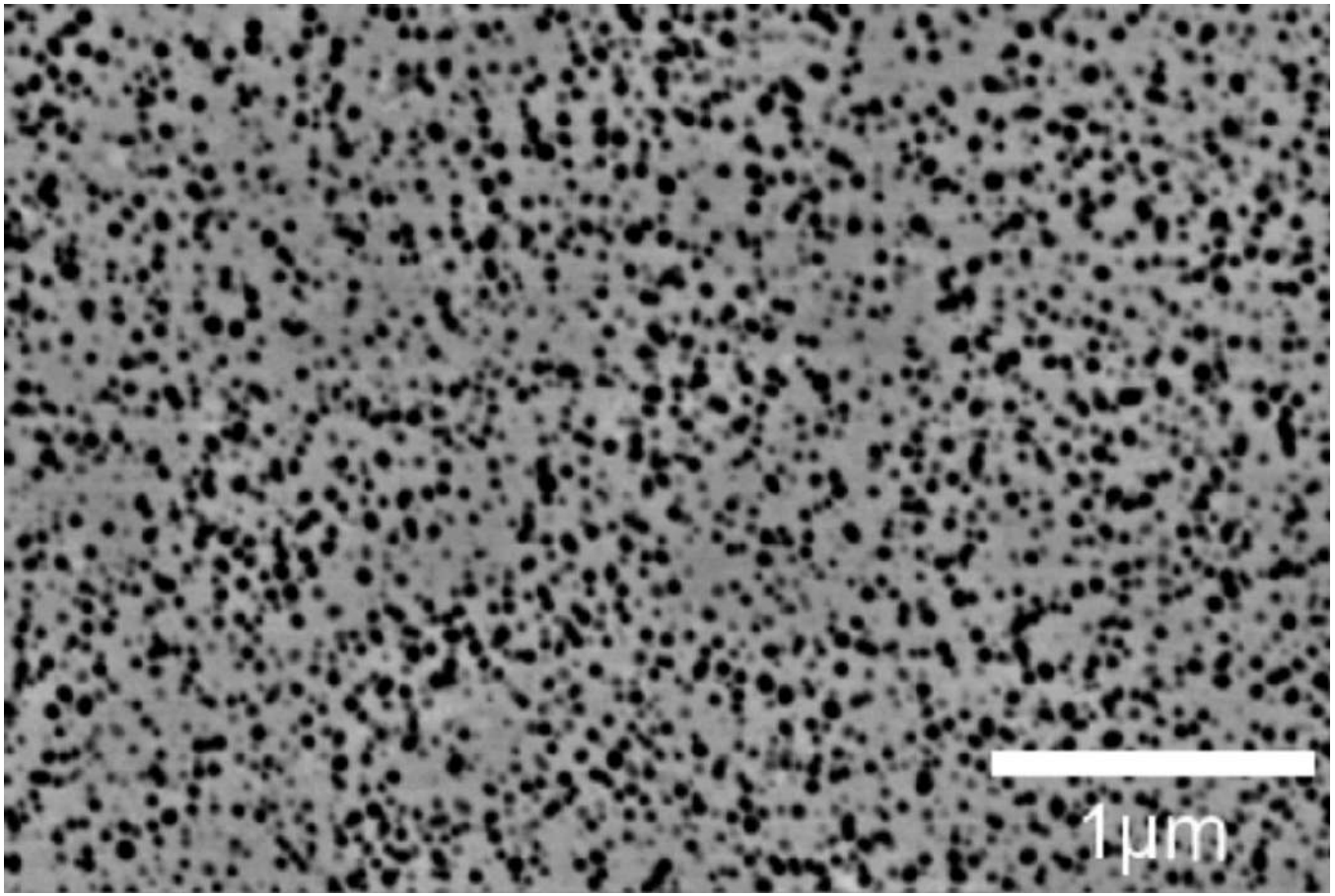
C: 0.04%

B: 0.01%

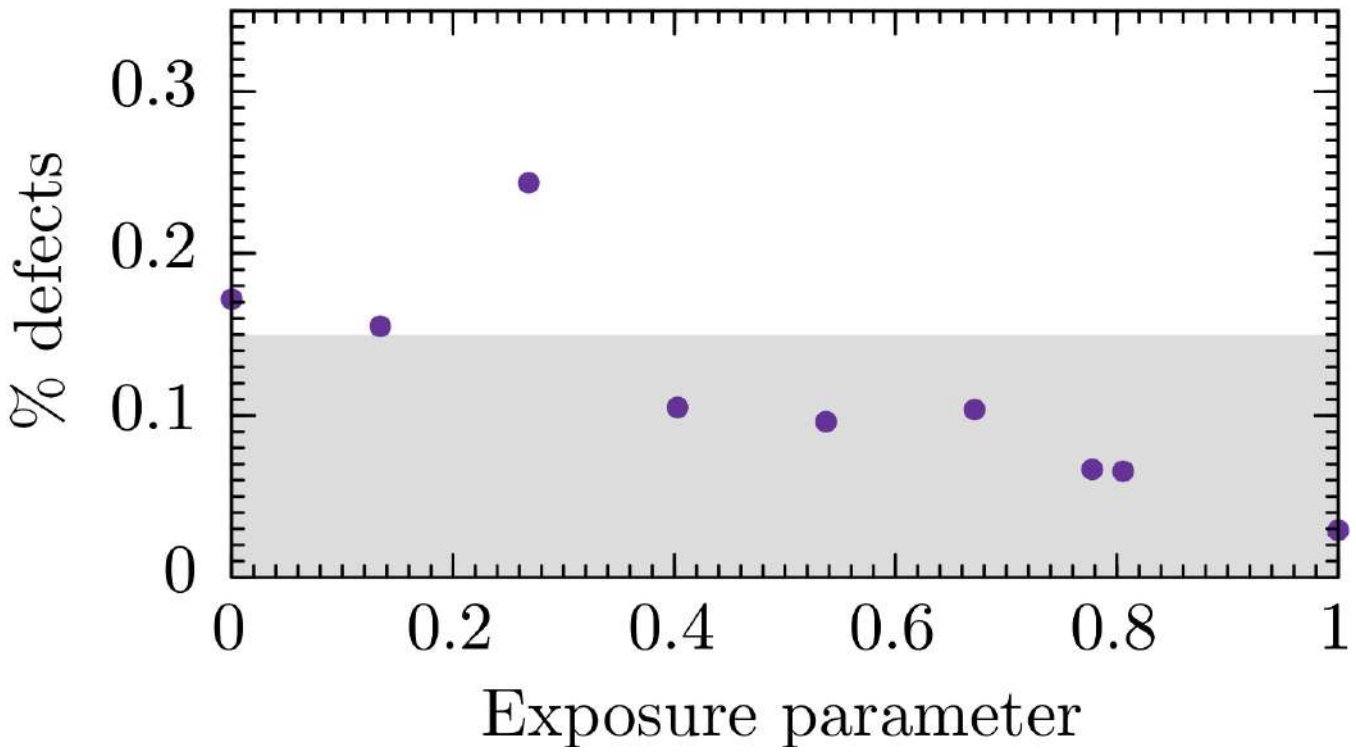
Ni

Expose 0.8

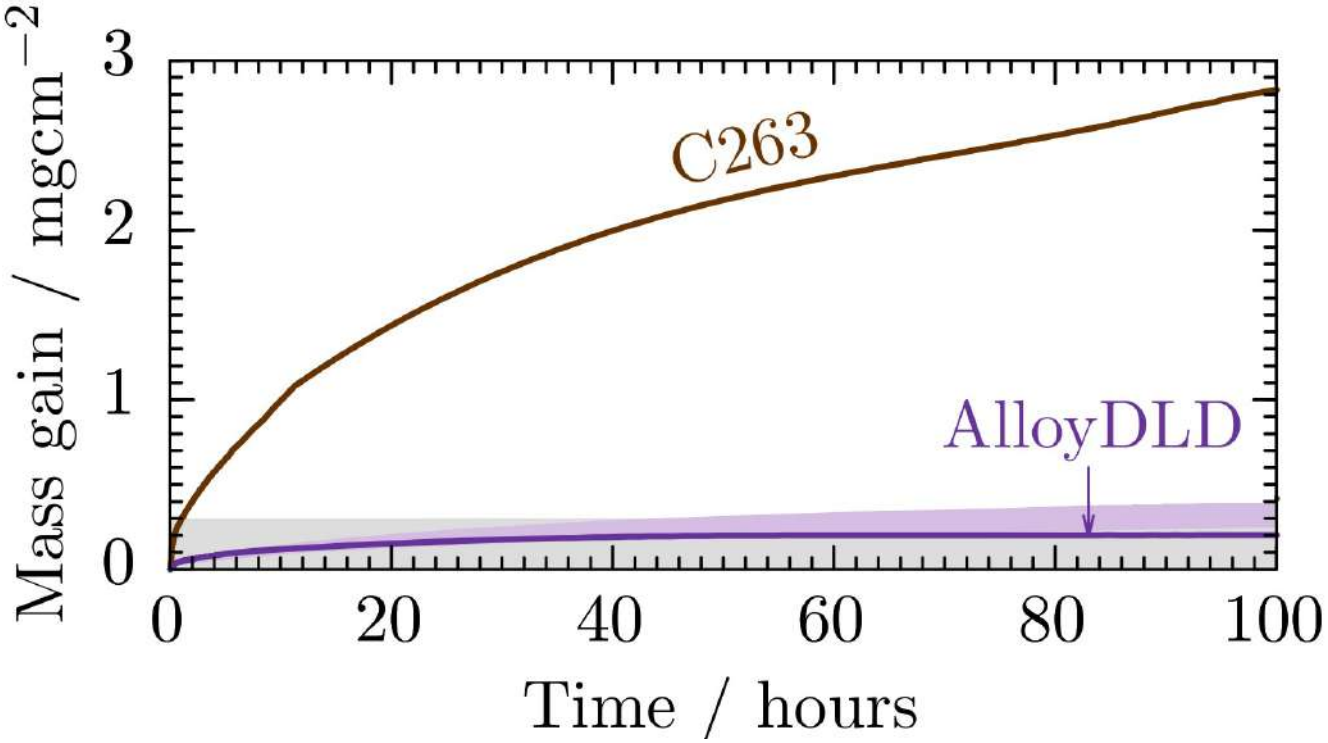
Microstructure



Testing the processability: horizontal printing



Testing the oxidation resistance



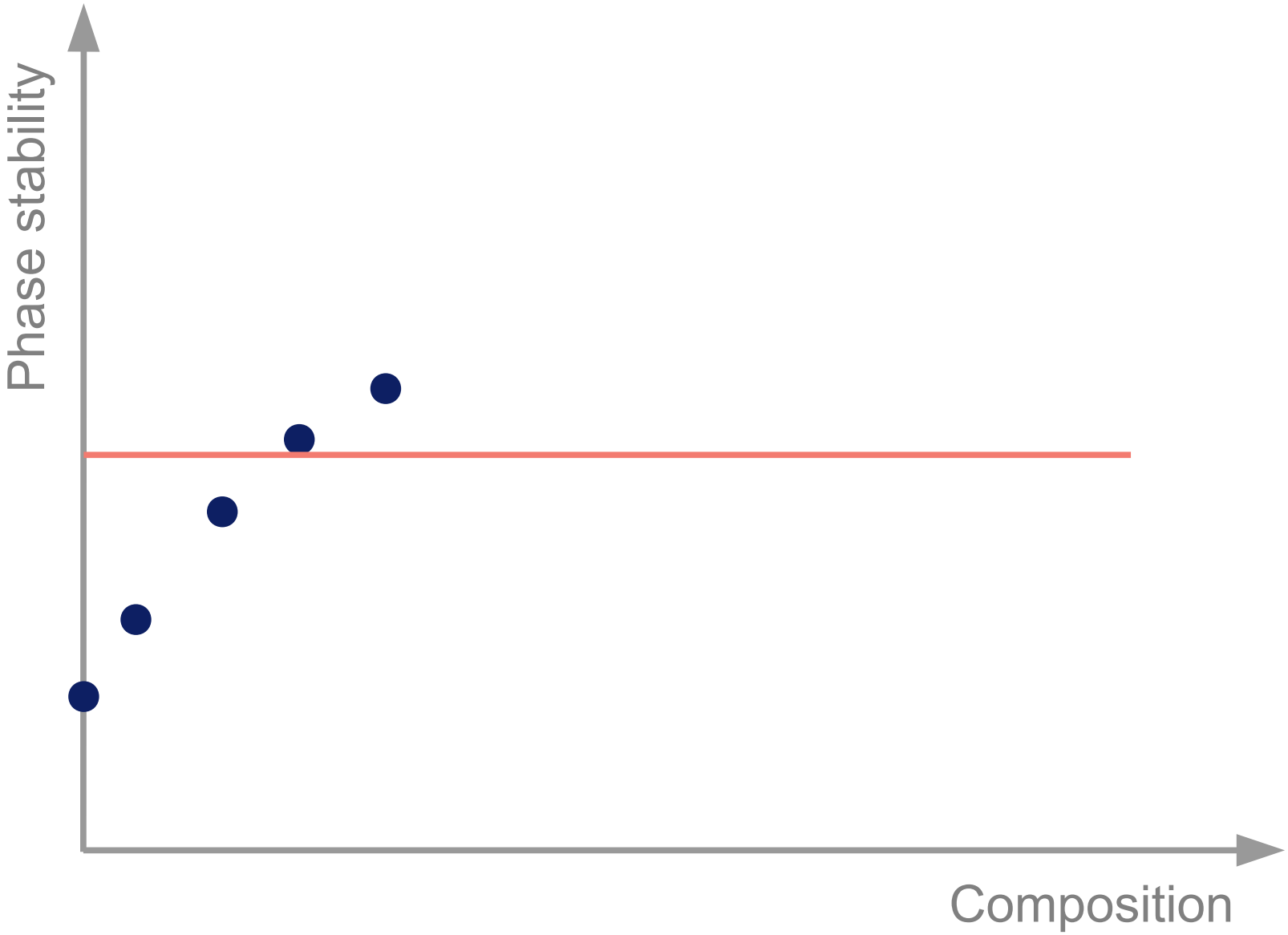
Printing components for an engine

Materials Solutions

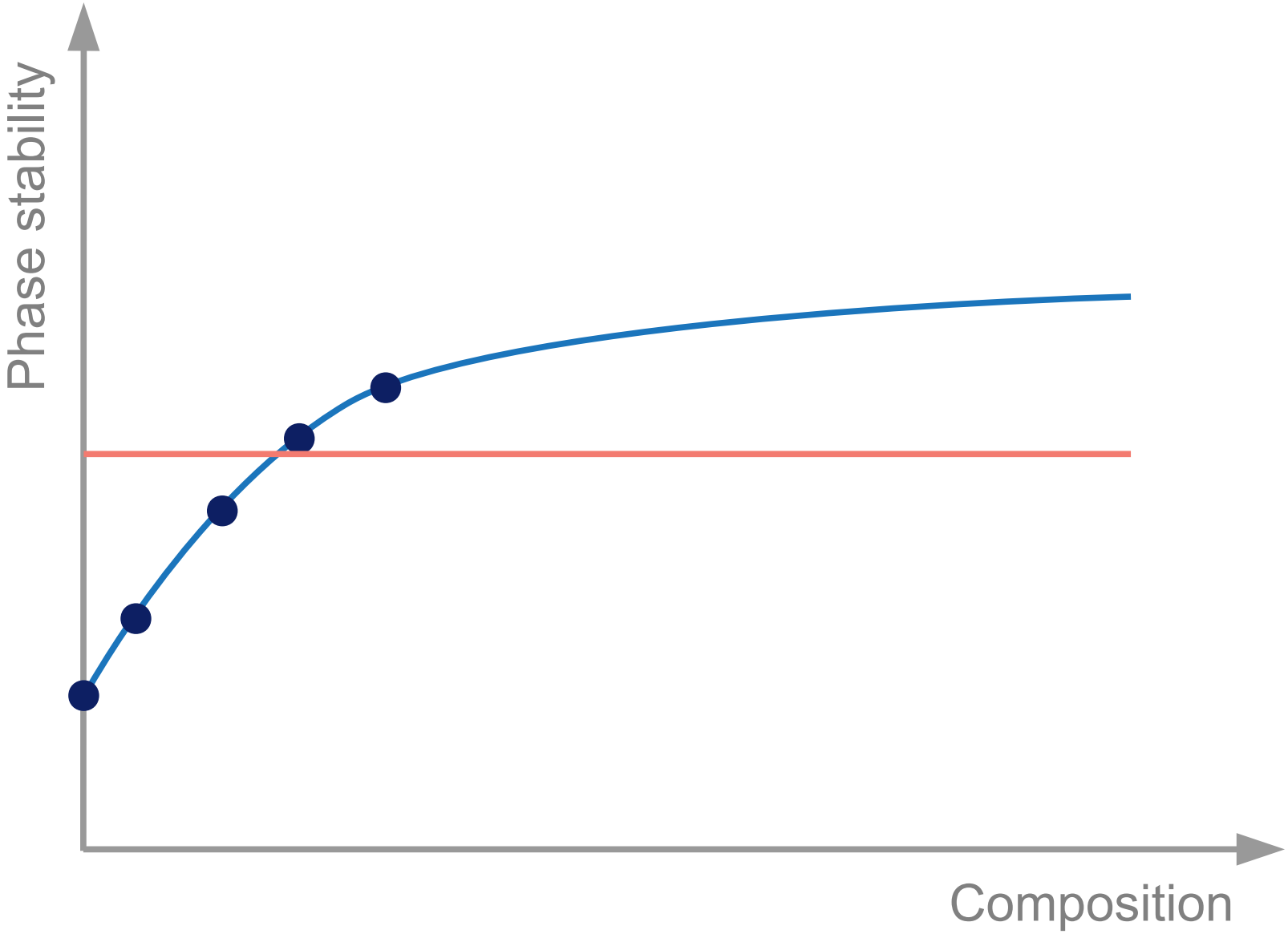
ROLLS ROYCE

Flowchart to train neural network

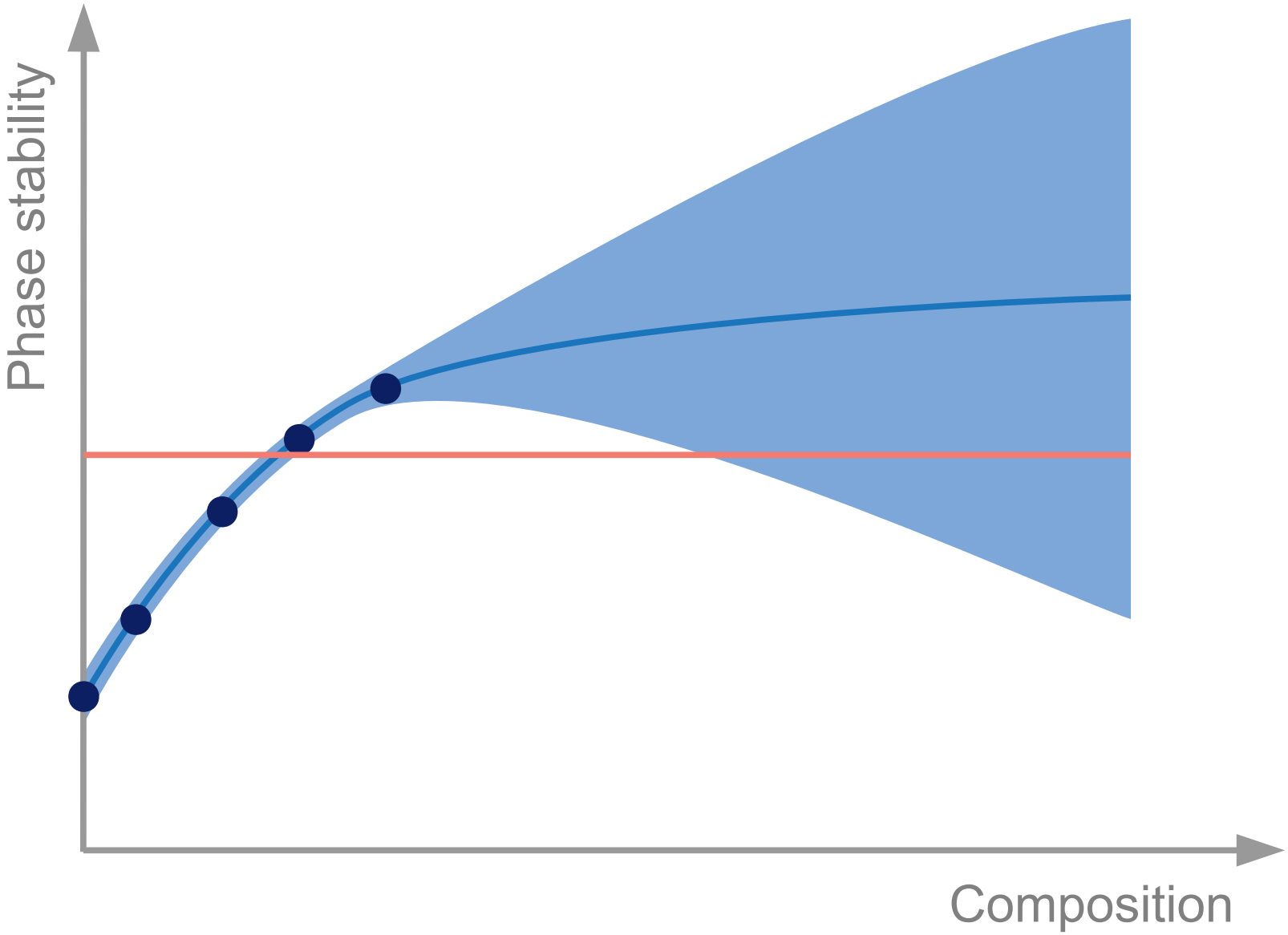
Prediction of phase behavior



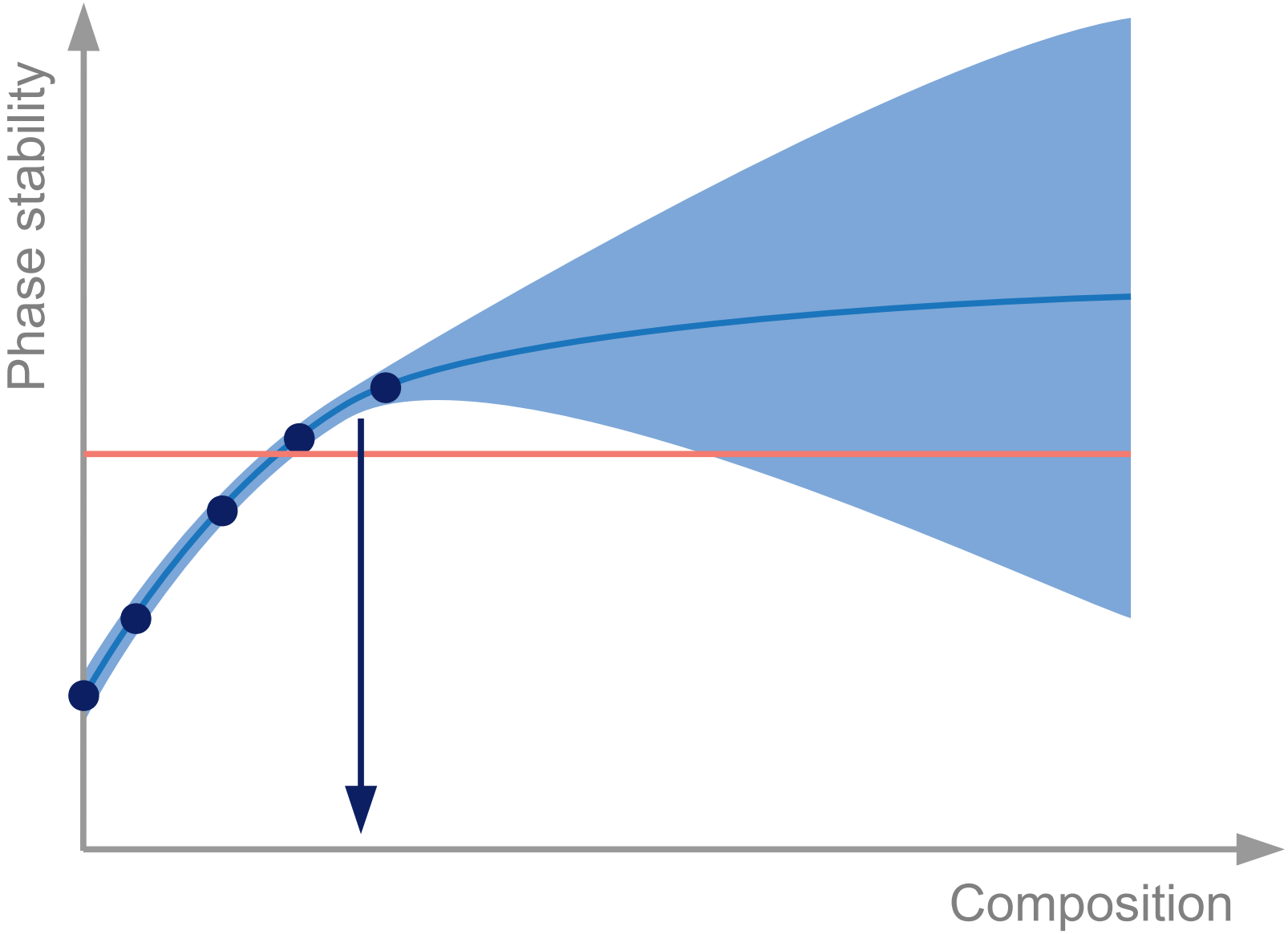
Prediction of phase behavior



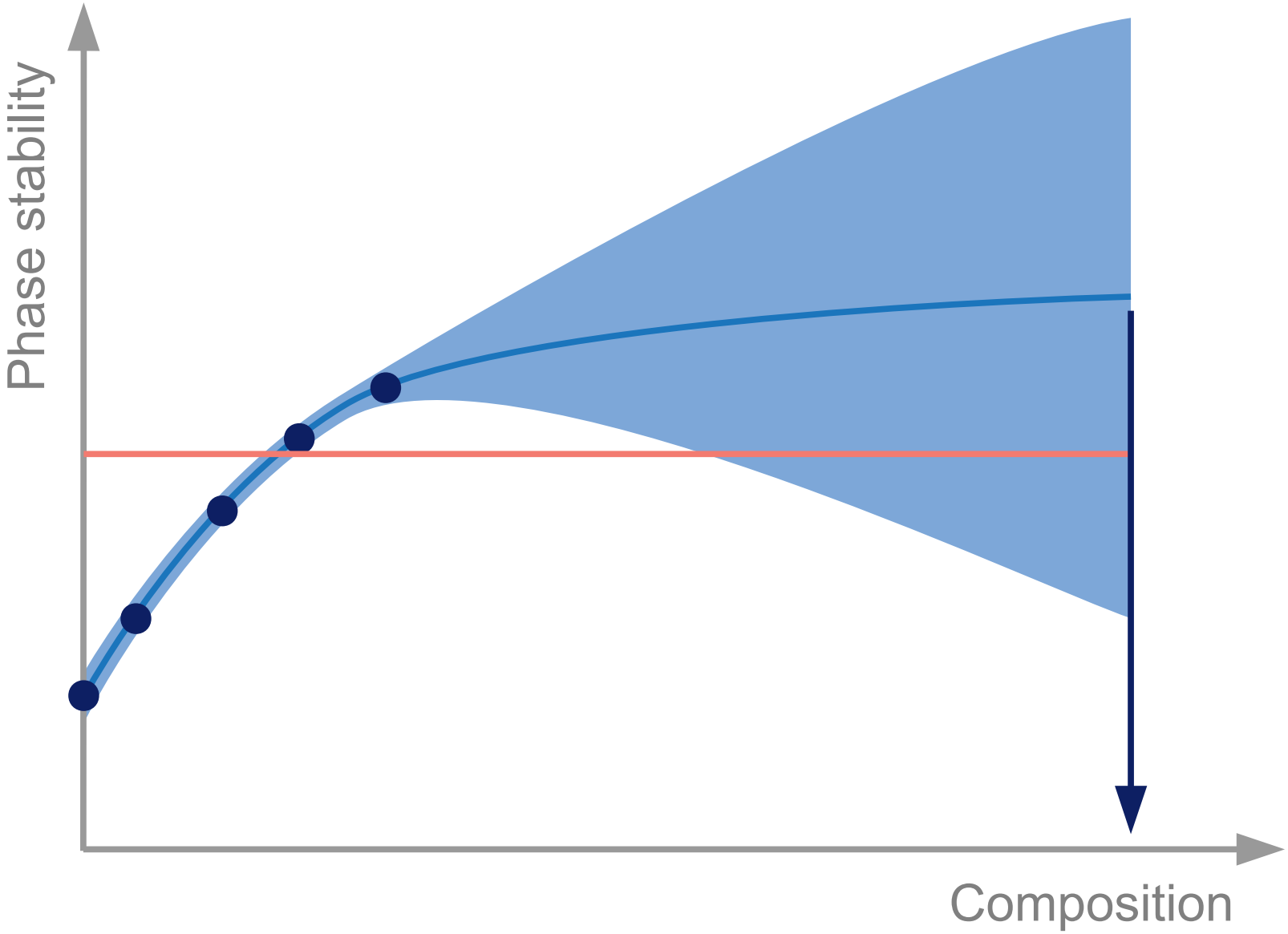
Uncertainty in neural network prediction



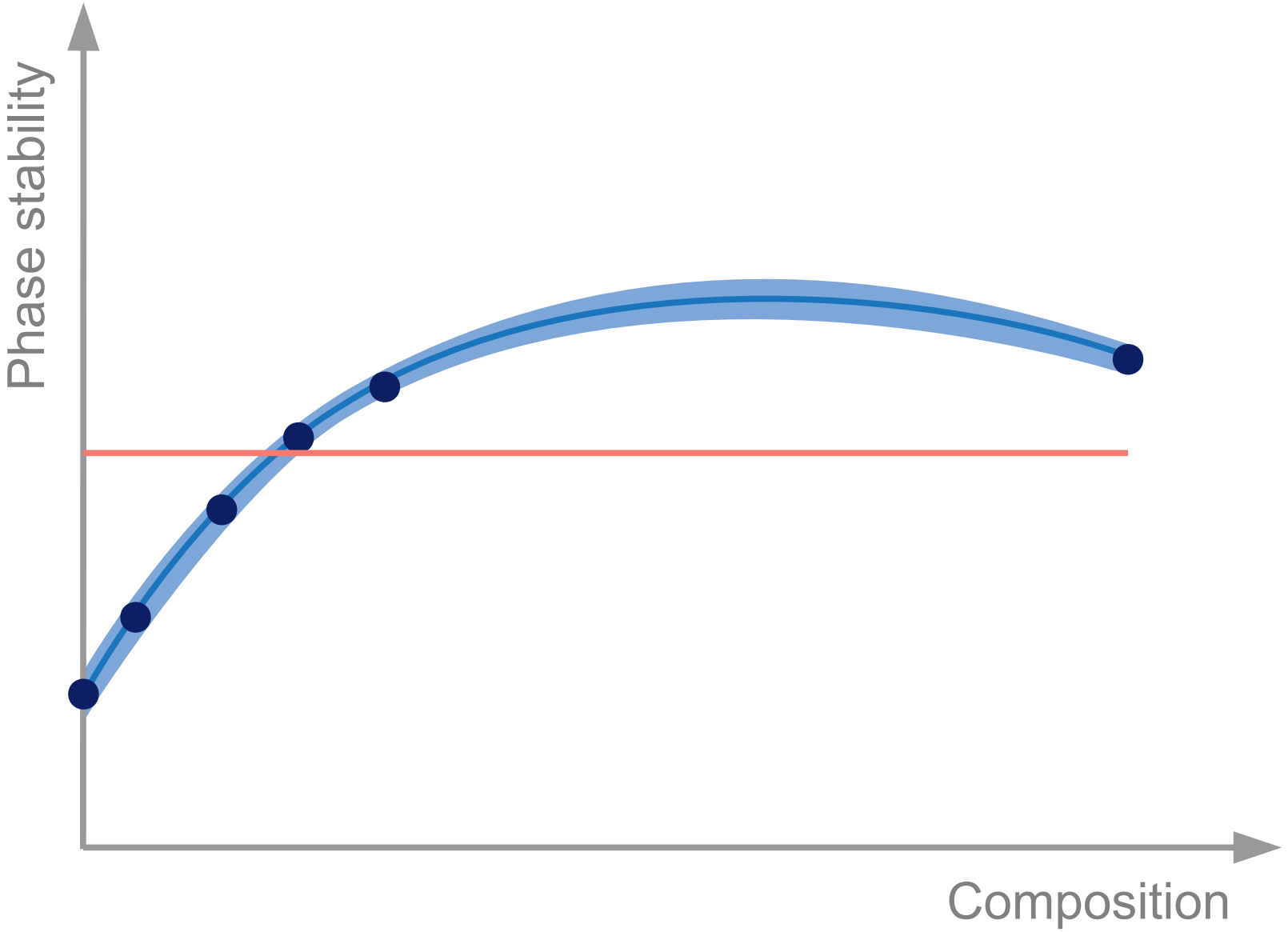
Material most likely to work



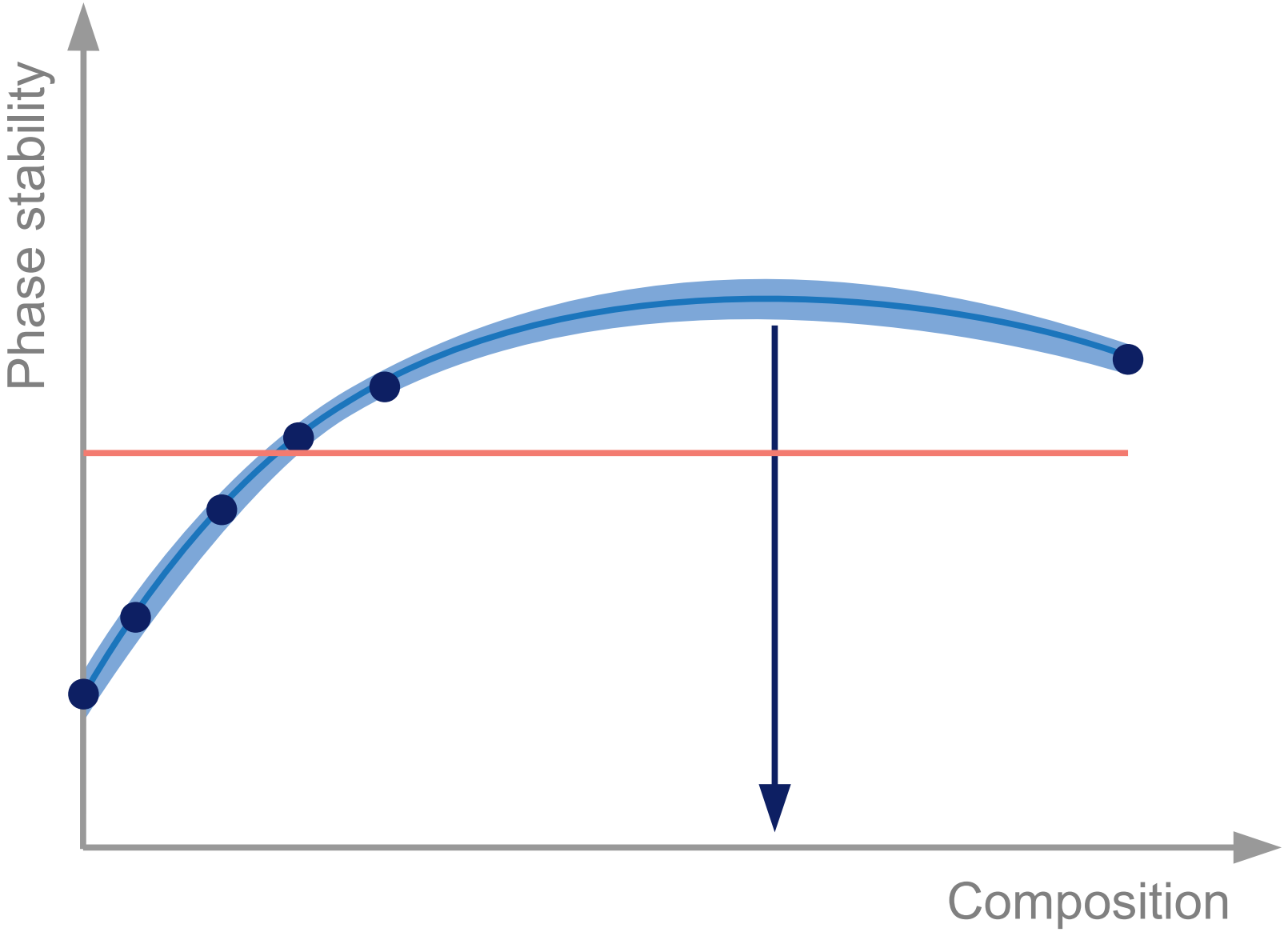
Most useful experiment



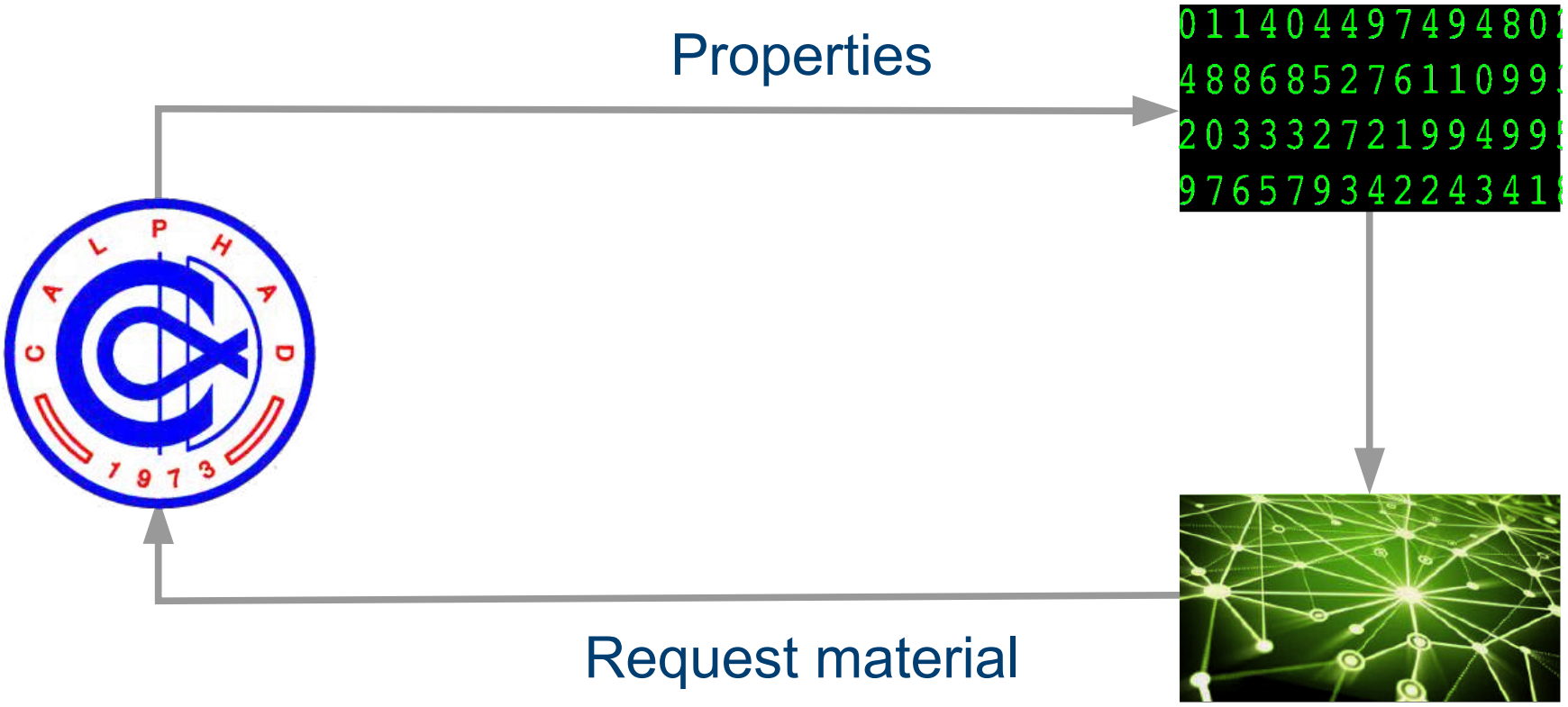
Improved neural network model



New material most likely to work

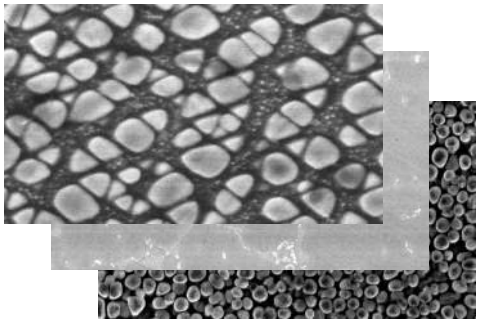


Flowchart with reinforcement learning



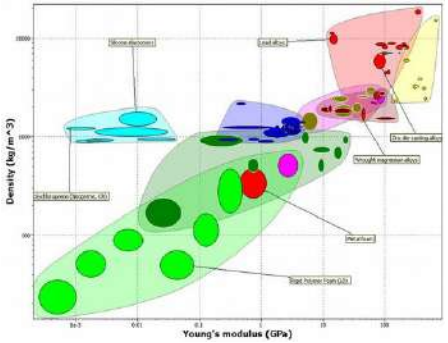
Materials designed

Nickel and molybdenum



Experiment and DFT for batteries

Identified and corrected errors in materials database

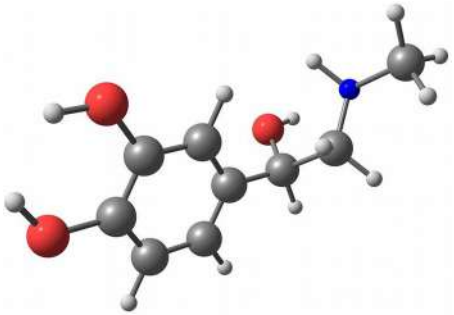


Beyond materials

Lubricants with molecular dynamics and experiments

bp

Assay activity



e-therapeutics

Drug design

optibrium

Summary

Merge different experimental quantities and computer simulations into a holistic design tool

Designed and experimentally verified alloy for direct laser deposition

Further experimentally proven materials, founded start-up intellegens.ai