UNIVERSITY OF CAMBRIDGE

Who needs science to design materials?

Gareth Conduit

Theory of Condensed Matter Group, Department of Physics

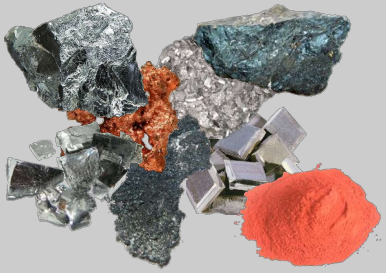
Neural network algorithm that can

Merge simulations, physical laws, and experimental data

Applications in materials discovery and drug design

Black box for materials design

Composition



Properties

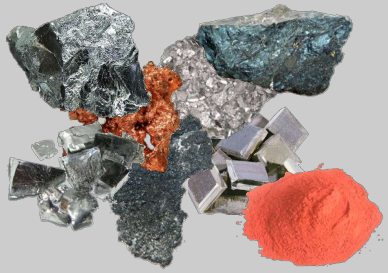
UTS

Hardness

Cost

Training the neural network

Composition



Properties

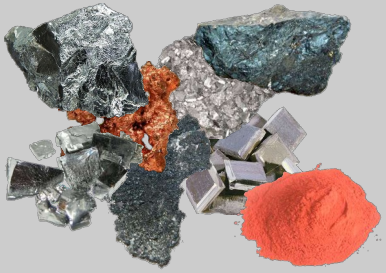
UTS

Hardness

Cost

Neural network for materials design

Composition



Properties

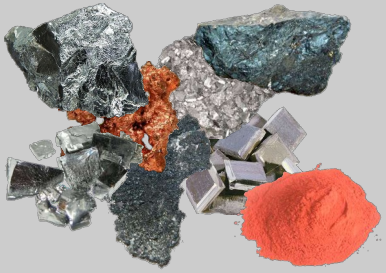
UTS

Hardness

Cost

Neural network to exploit all available correlations

Composition



Properties

UTS

Hardness

Cost

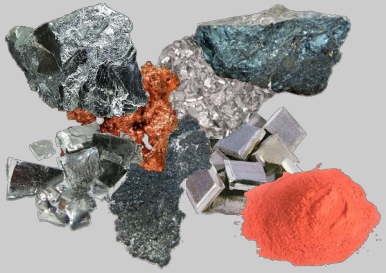
Simulations

Density Functional

Molecular dynamics

Finite element

Composition



Properties

UTS

Hardness

Cost

Simulations

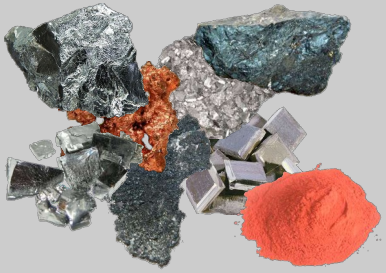
Density Functional

Molecular dynamics

Finite element

Neural network is top down

Composition



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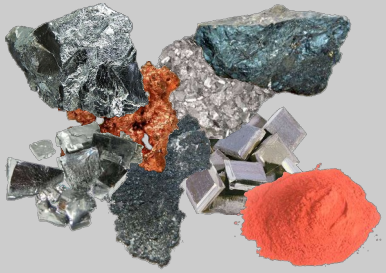
Finite element

Composition



Properties

UTS

Hardness

Cost

Simulations

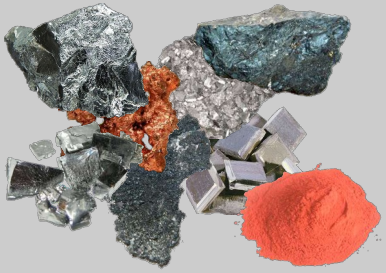
Density Functional

Molecular dynamics

Finite element

Neural network is top down and bottom up

Composition



Properties

UTS

Hardness

Cost

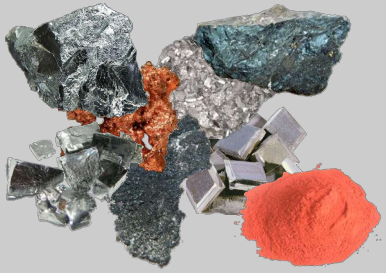
Simulations

Density Functional

Molecular dynamics

Finite element

Composition



Properties

UTS

Hardness

Cost

Simulations

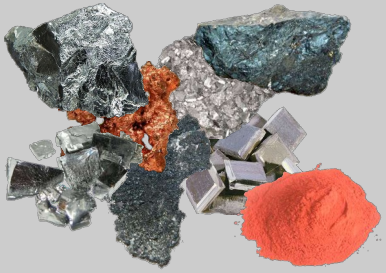
Density Functional

Molecular dynamics

Finite element

Neural network must handle fragmented data

Composition



Properties

UTS

Hardness

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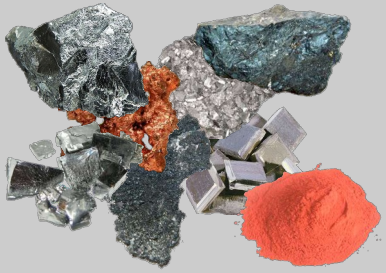
Molecular dynamics

Finite element

Composition



Properties

UTS

Hardness

Cost

Simulations

Density Functional

Molecular dynamics

Finite element

Fragmented training data set

Composition	UTS	Hardness
✔	✔	✔
✔	✘	✔
✘	✔	✔
✔	✔	✘

Neural network: train on complete data

Materials design

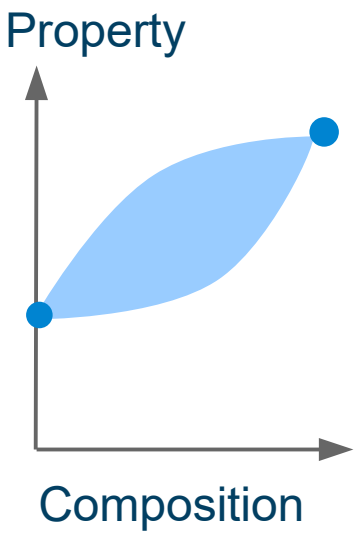
Materials design

Proposed neural network: train on fragmented data

Proposed neural network: predict on fragmented data

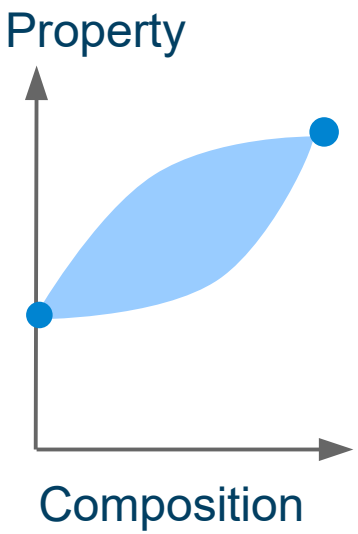
Neural network trained on experimental data

Experiment

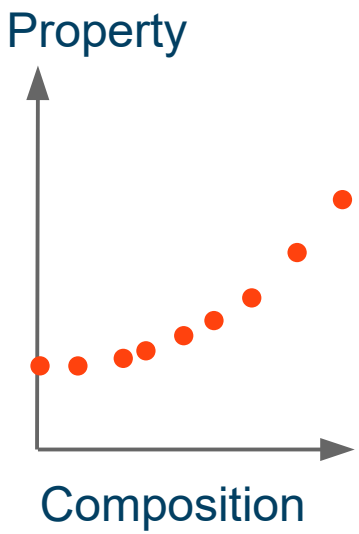


Further information is provided by a simulation

Experiment



Simulation

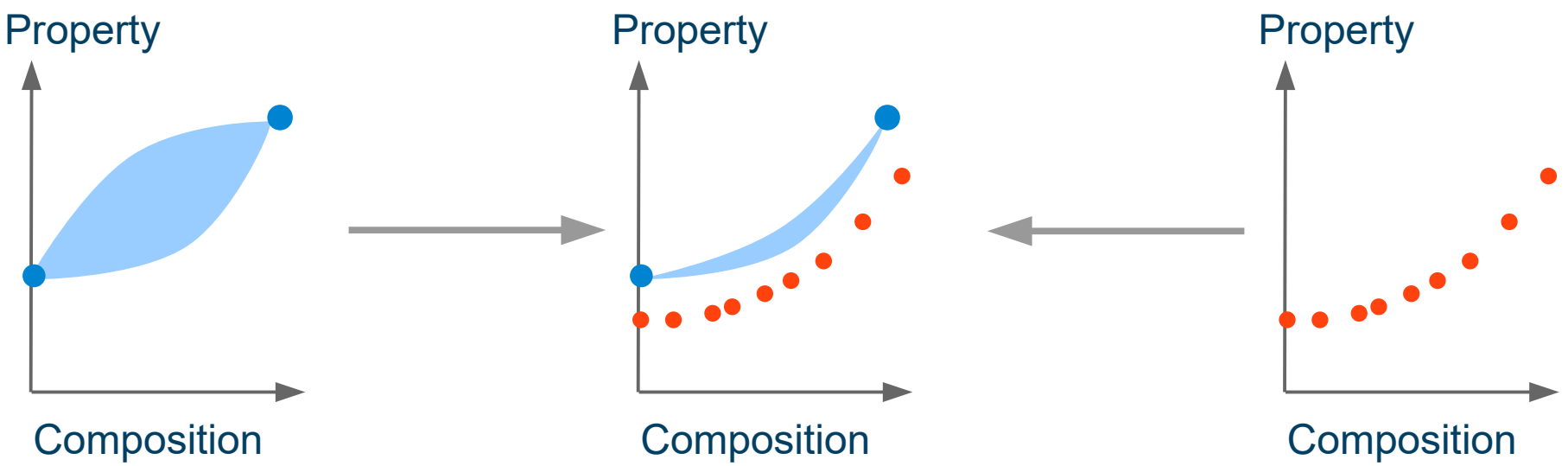


Neural network combines the two sources of data

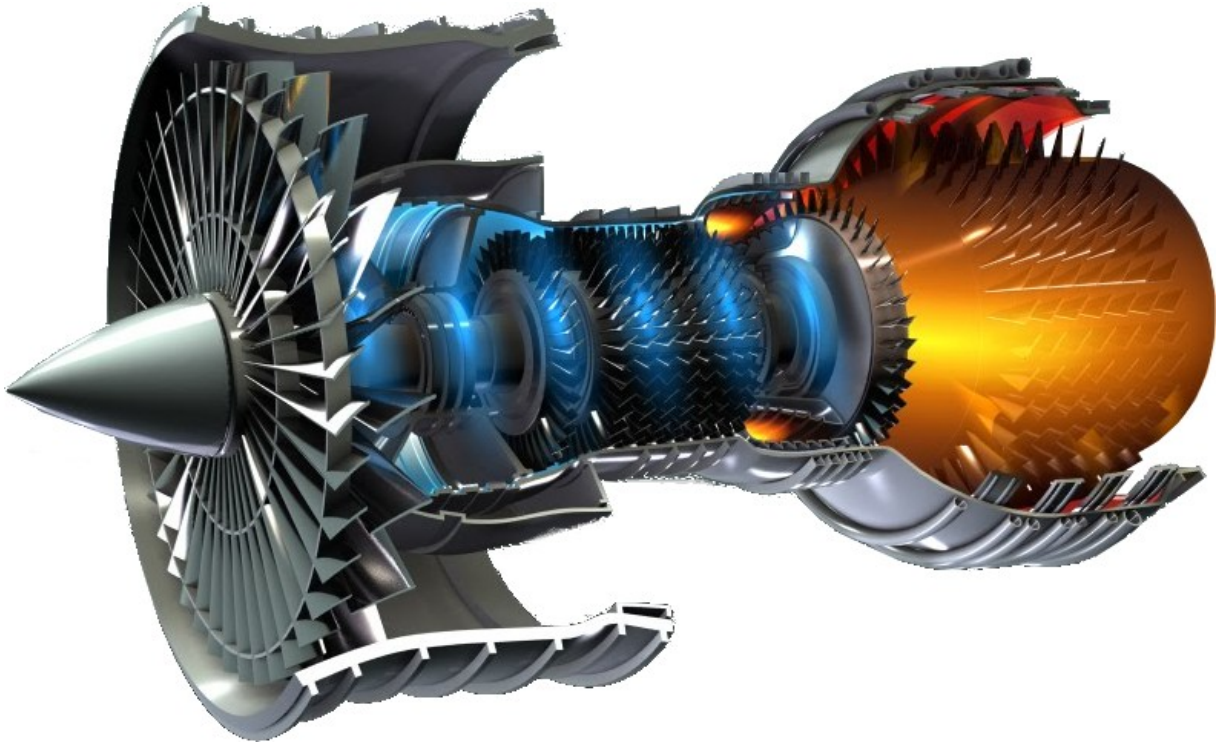
Experiment

Combined

Simulation



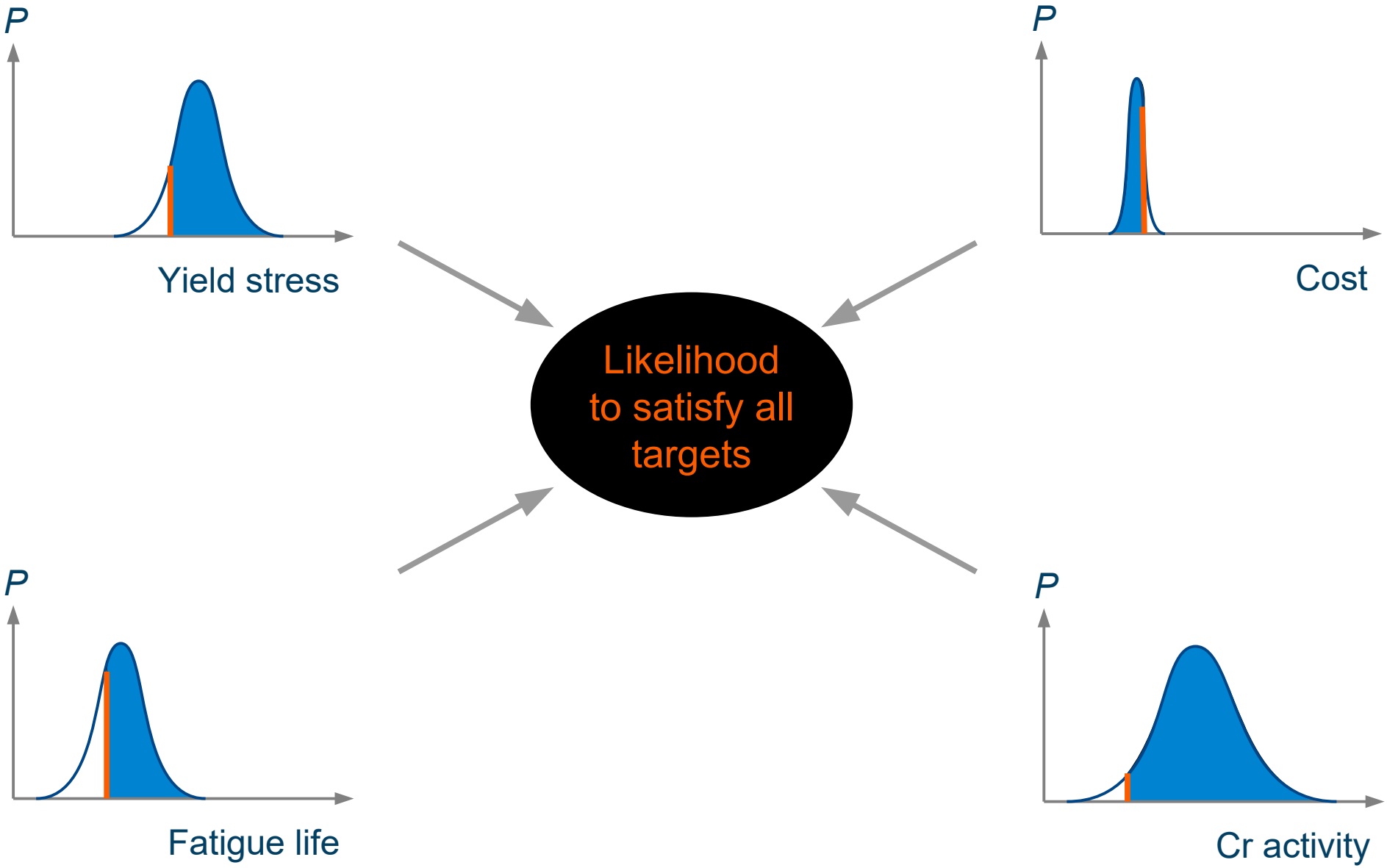
Schematic of an engine



Target properties

Cost	< 33.7 $\$kg^{-1}$
Density	< 8281 kgm^{-3}
γ’ content	< 50.4 vol%
Phase stability	> 99.0 vol%
Fatigue life	> $10^{3.9}$ cycles
Yield stress	> 752.2 MPa
Ultimate tensile strength	> 960.0 MPa
300hr stress rupture	> 674.5 MPa
Cr activity	> 0.14
γ’ solvus	> 983ºC
Tensile elongation	> 11.6%

Maximize the likelihood of success



Proposed alloy

Cr:15.8

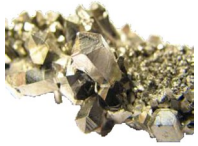
Co: 20.0

Mo: 0.5

W: 0.5

Ta: 4.9

Nb: 1.1



Al: 2.4

Ti: 3.0

Fe: 3.9

Mn: 0.2

Si: 0.2

C: 0.02

B: 0.06

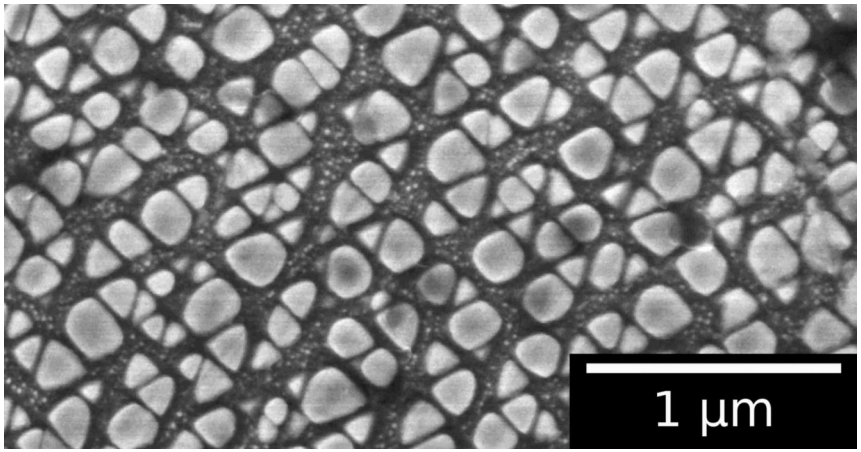
Zr: 0.18

Ni: 47.2

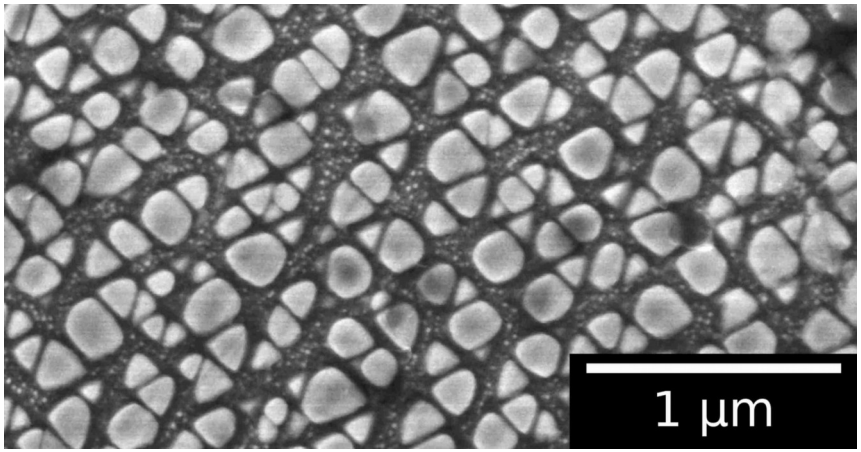
900ºC

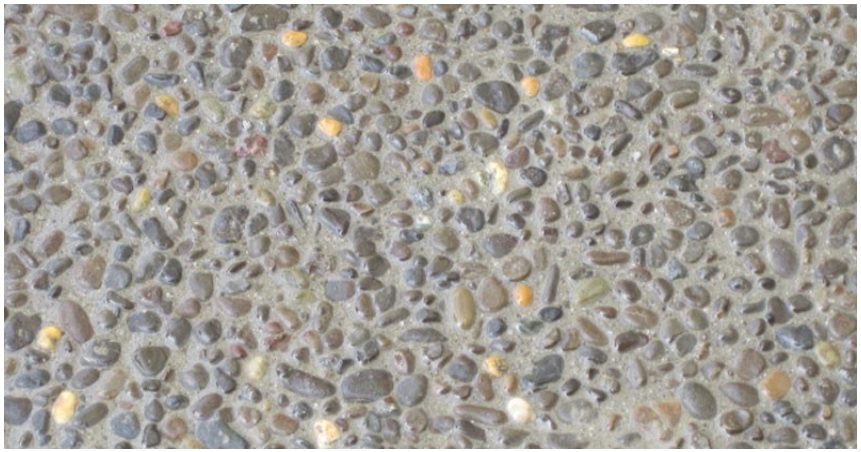
30 hours

Microstructure

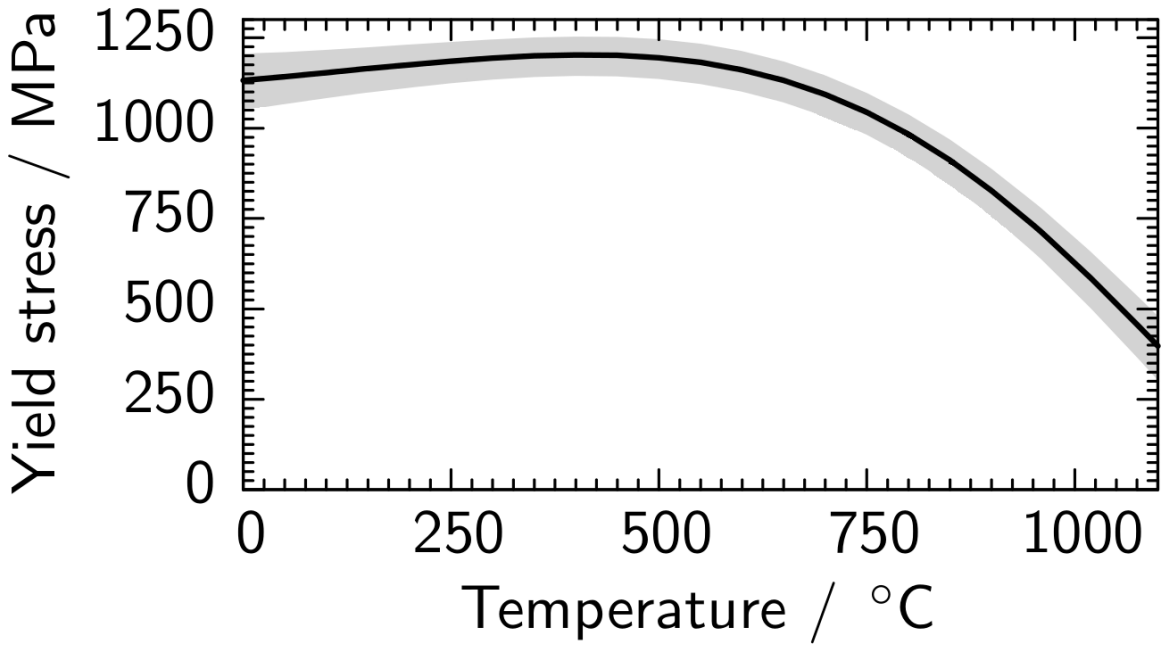


Precipitates strengthen the alloy



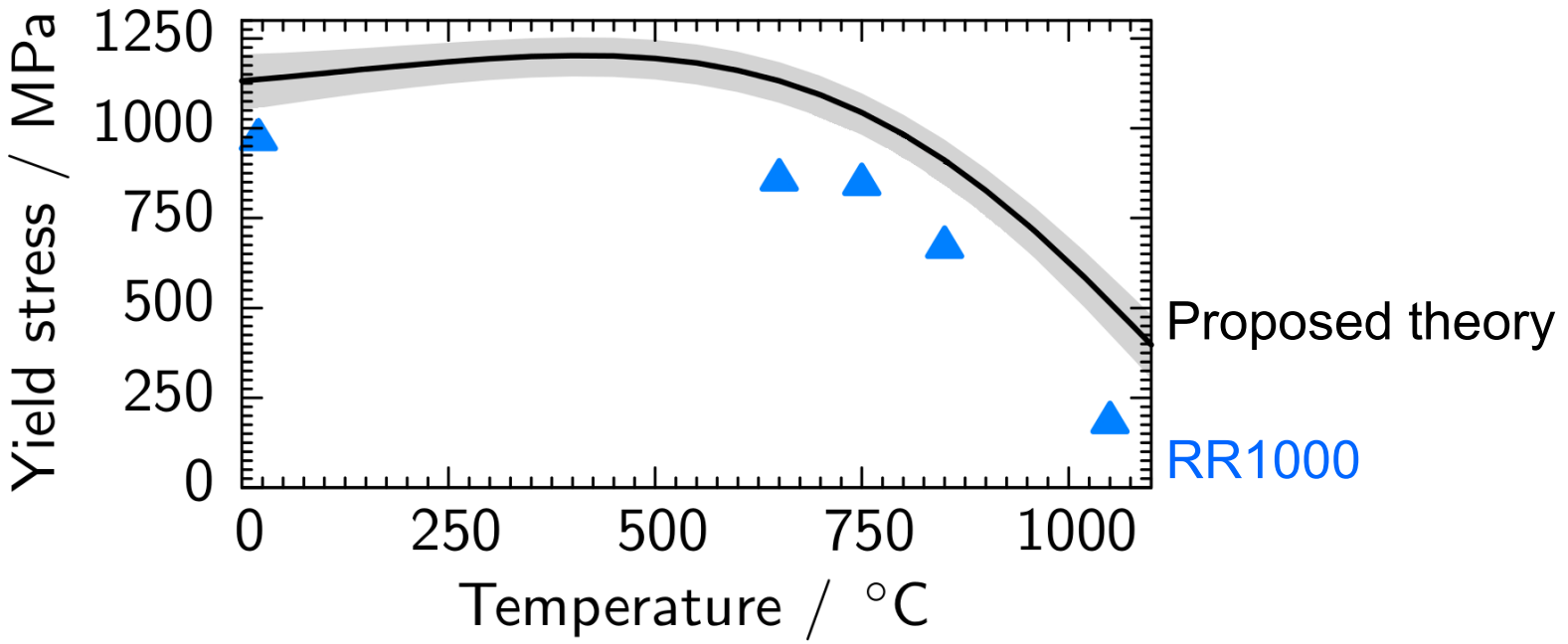


Predict the yield stress

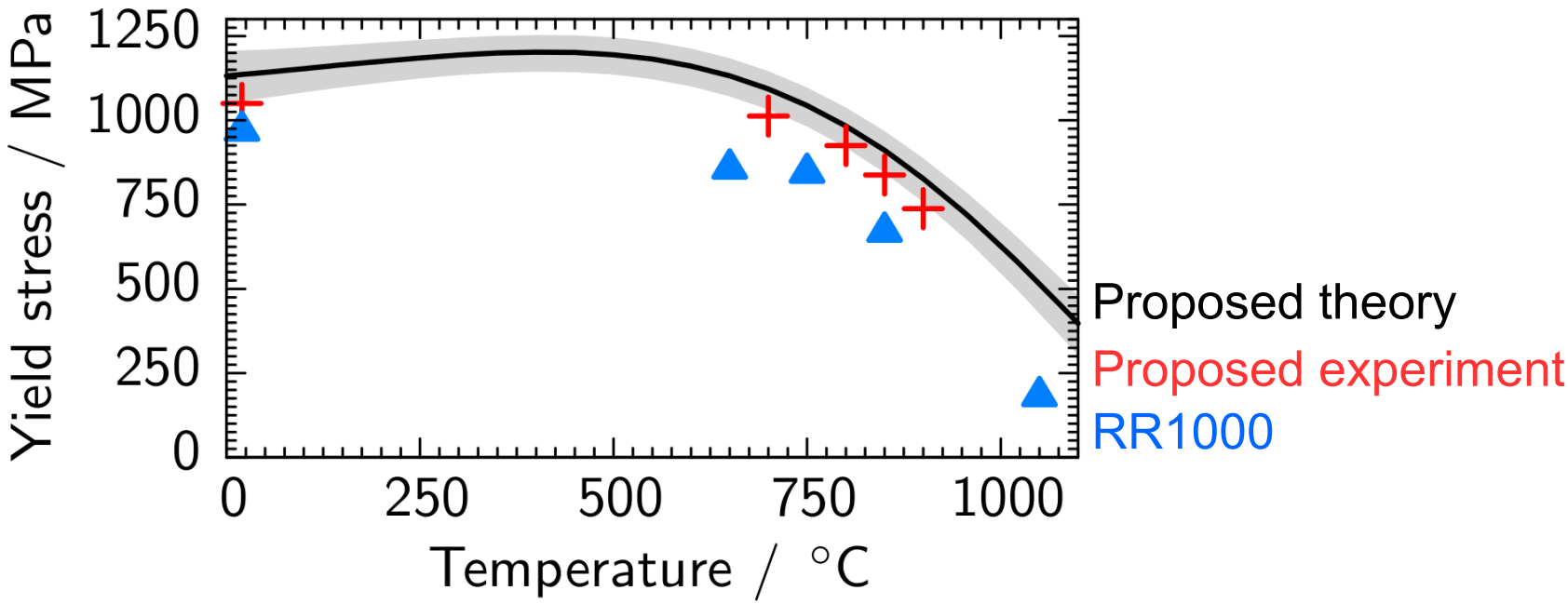


Proposed theory

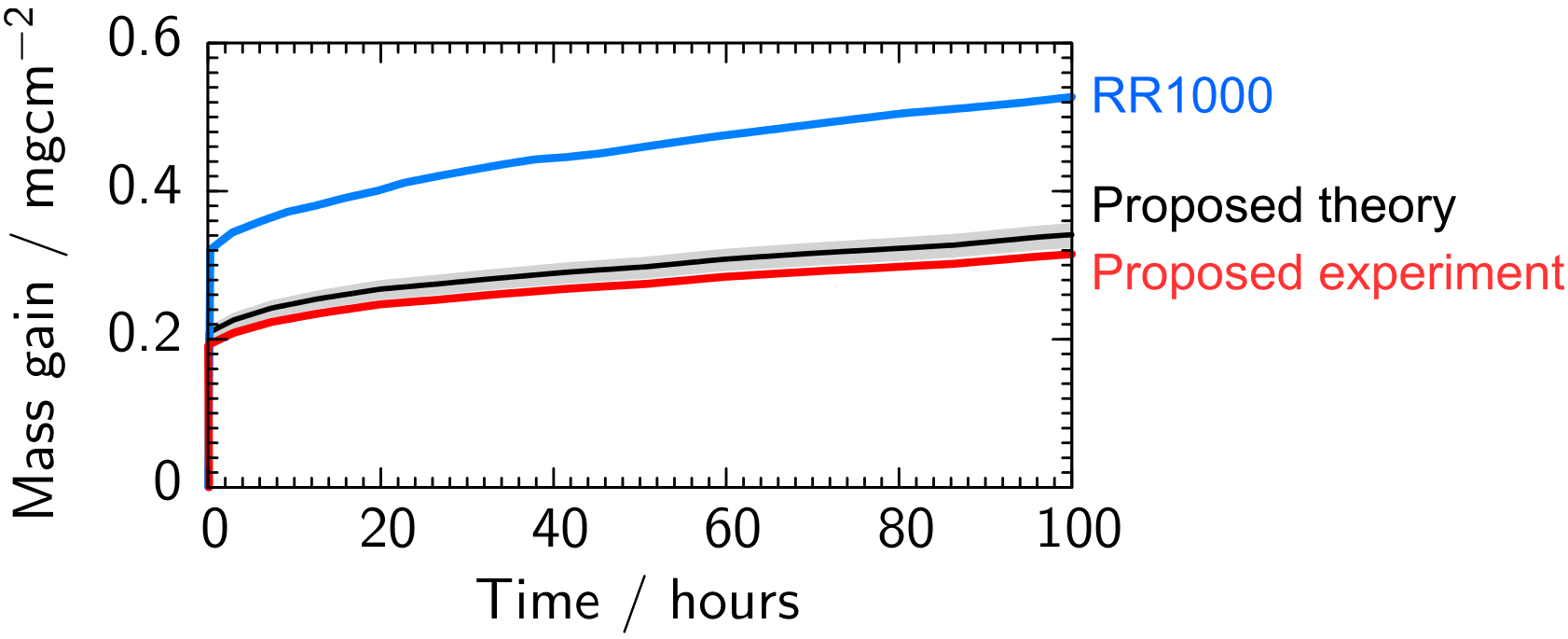
Test the yield stress



Test the yield stress

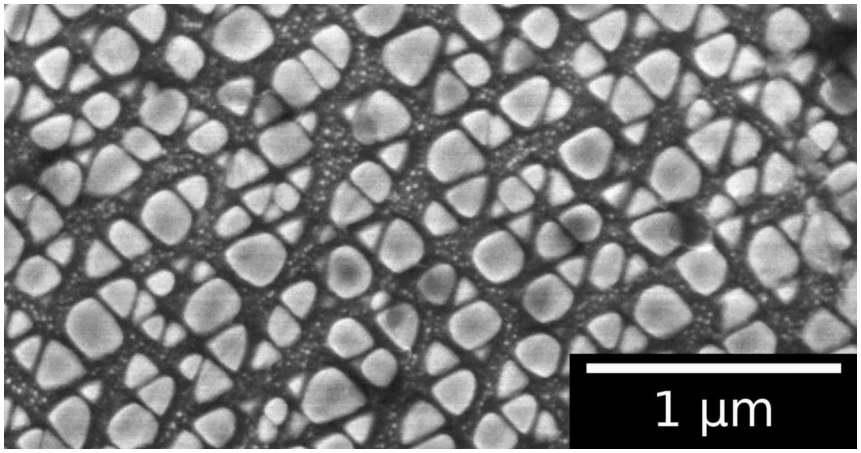


Test the oxidation resistance

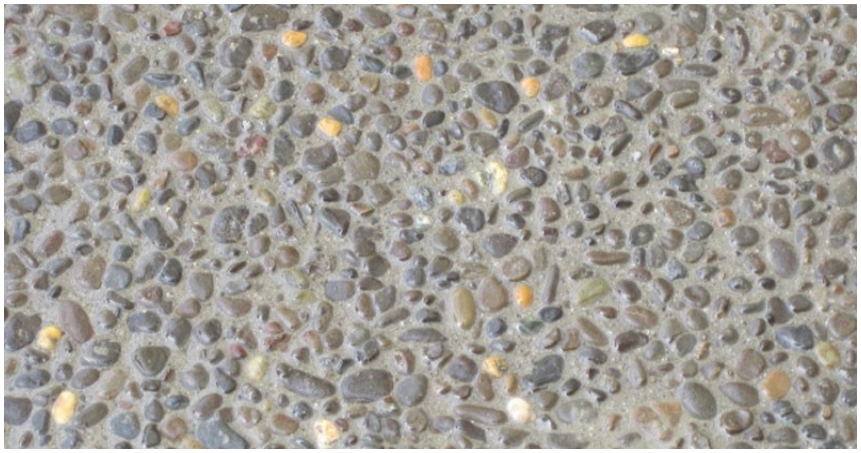


Microstructure strengthens the alloy

Precipitates

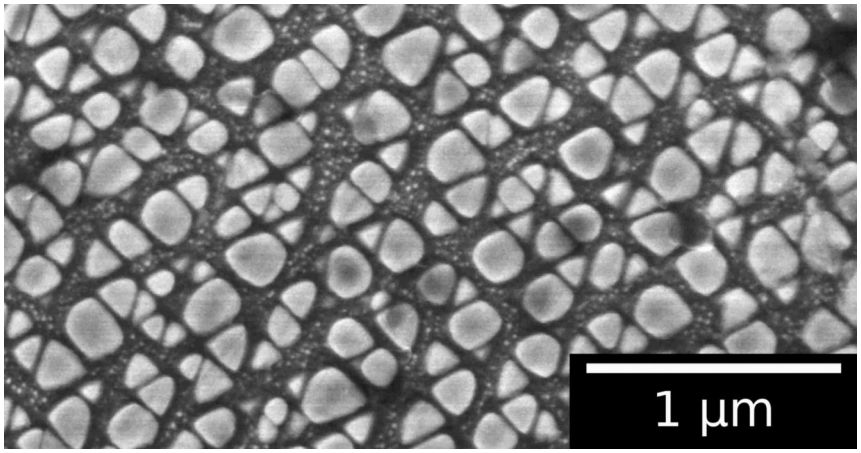


Aggregate

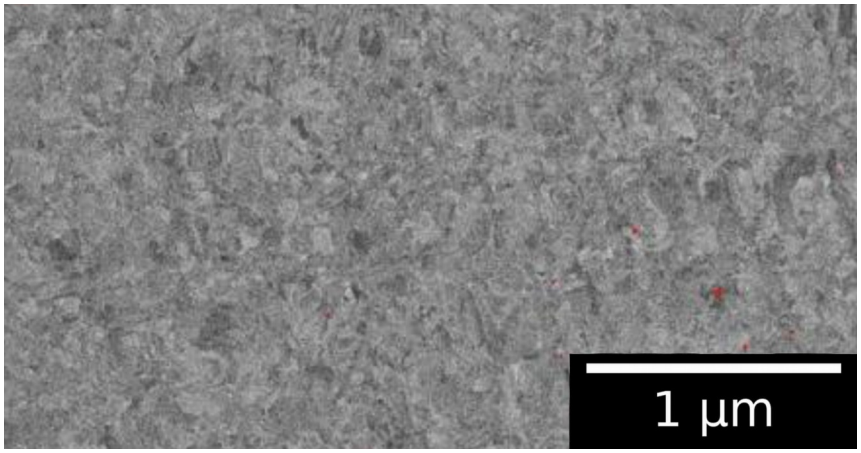


Microstructure defined by the heat treatment

Correct heat treatment

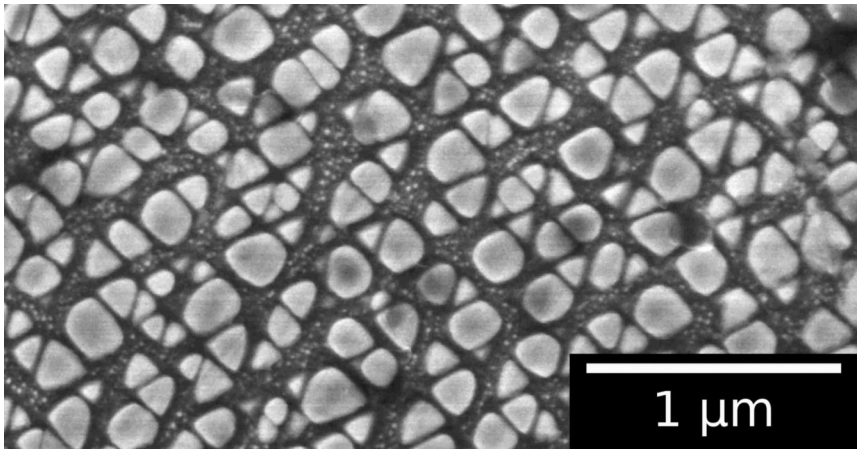


Incorrect heat treatment



Microstructure noise contains information about the heat treatment

Correct heat treatment



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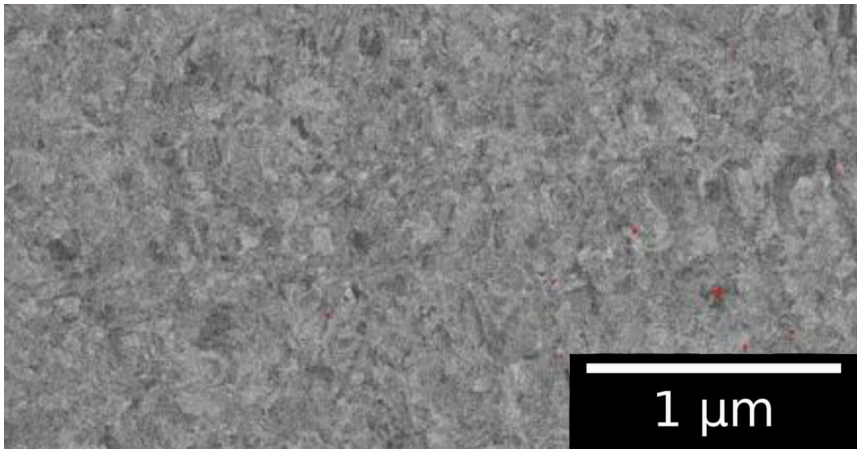

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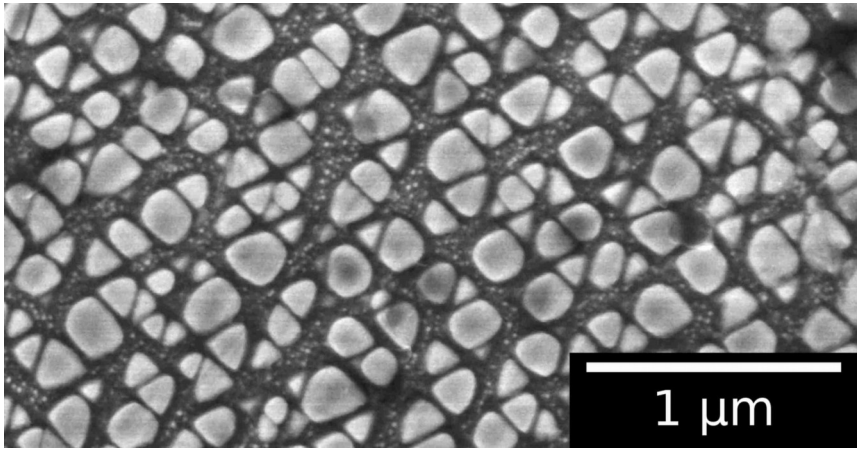
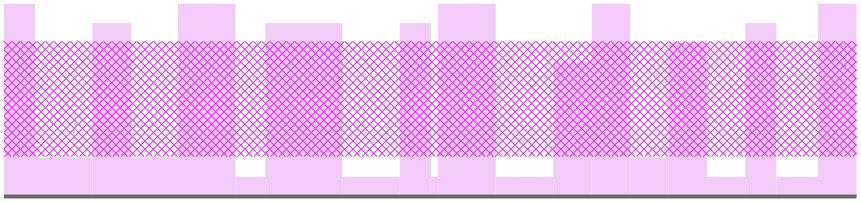
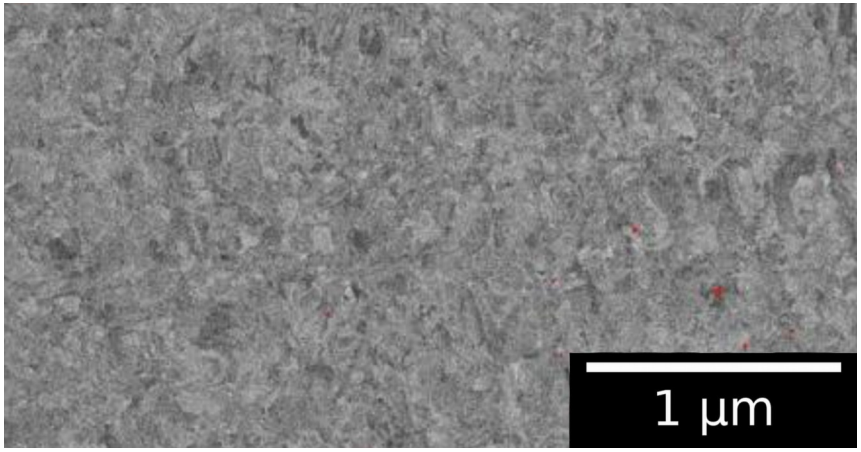
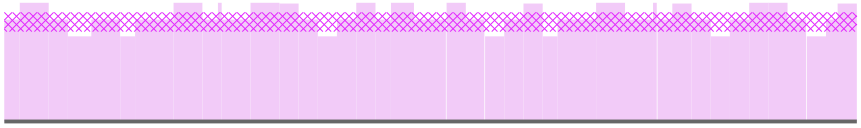
Correct heat treatment





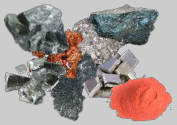
Incorrect heat treatment





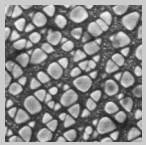
Standard neural network

Composition



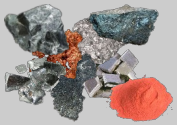
Heat treatment

Phase behavior



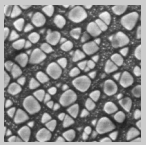
Properties

Composition



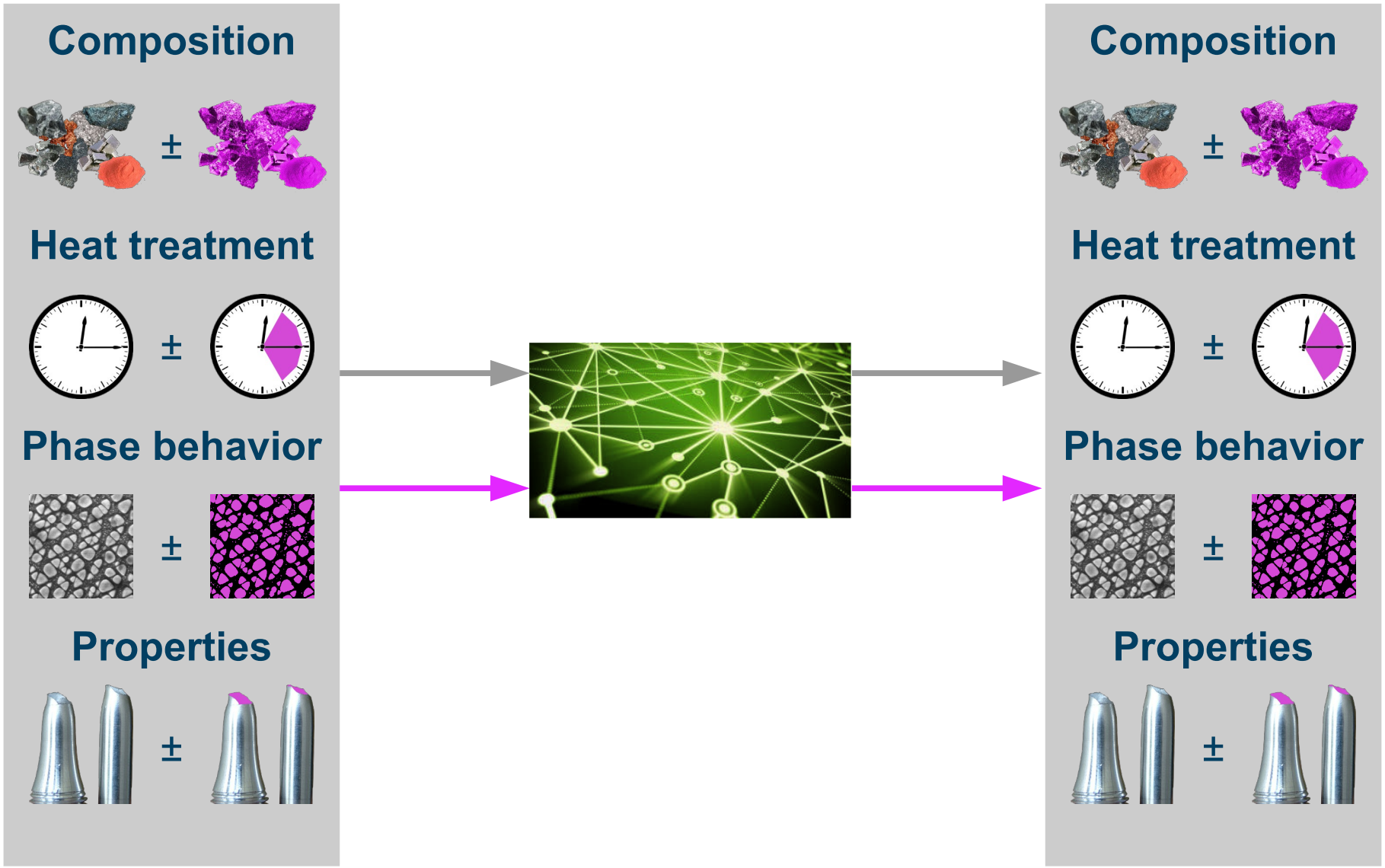
Heat treatment

Phase behavior



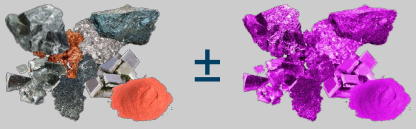
Properties

Neural network transmits noise as uncertainty

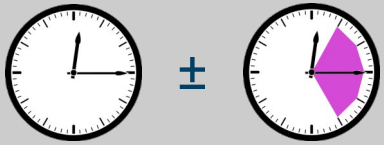


Incorporate noise into the neural network

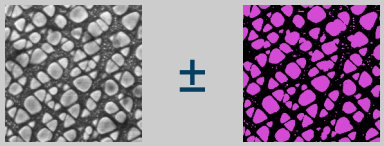
Composition



Heat treatment

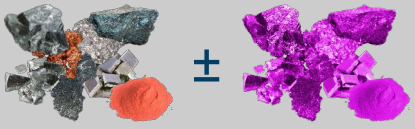


Phase behavior

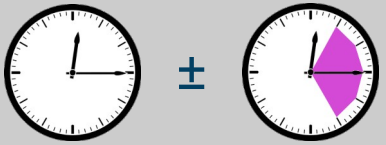


Properties

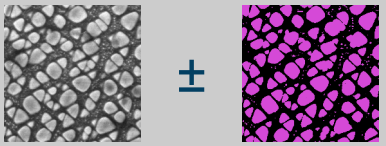
Composition



Heat treatment

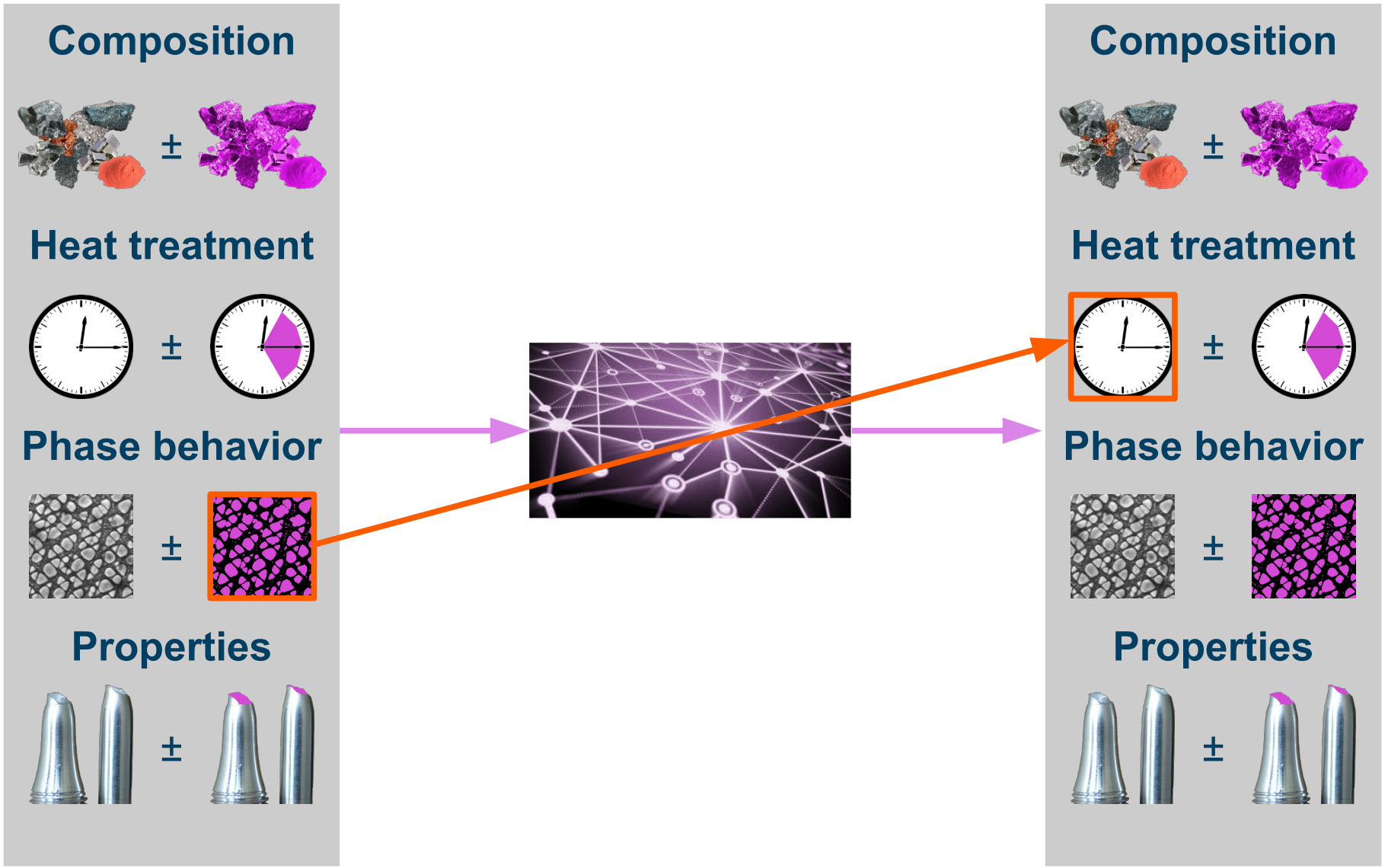


Phase behavior

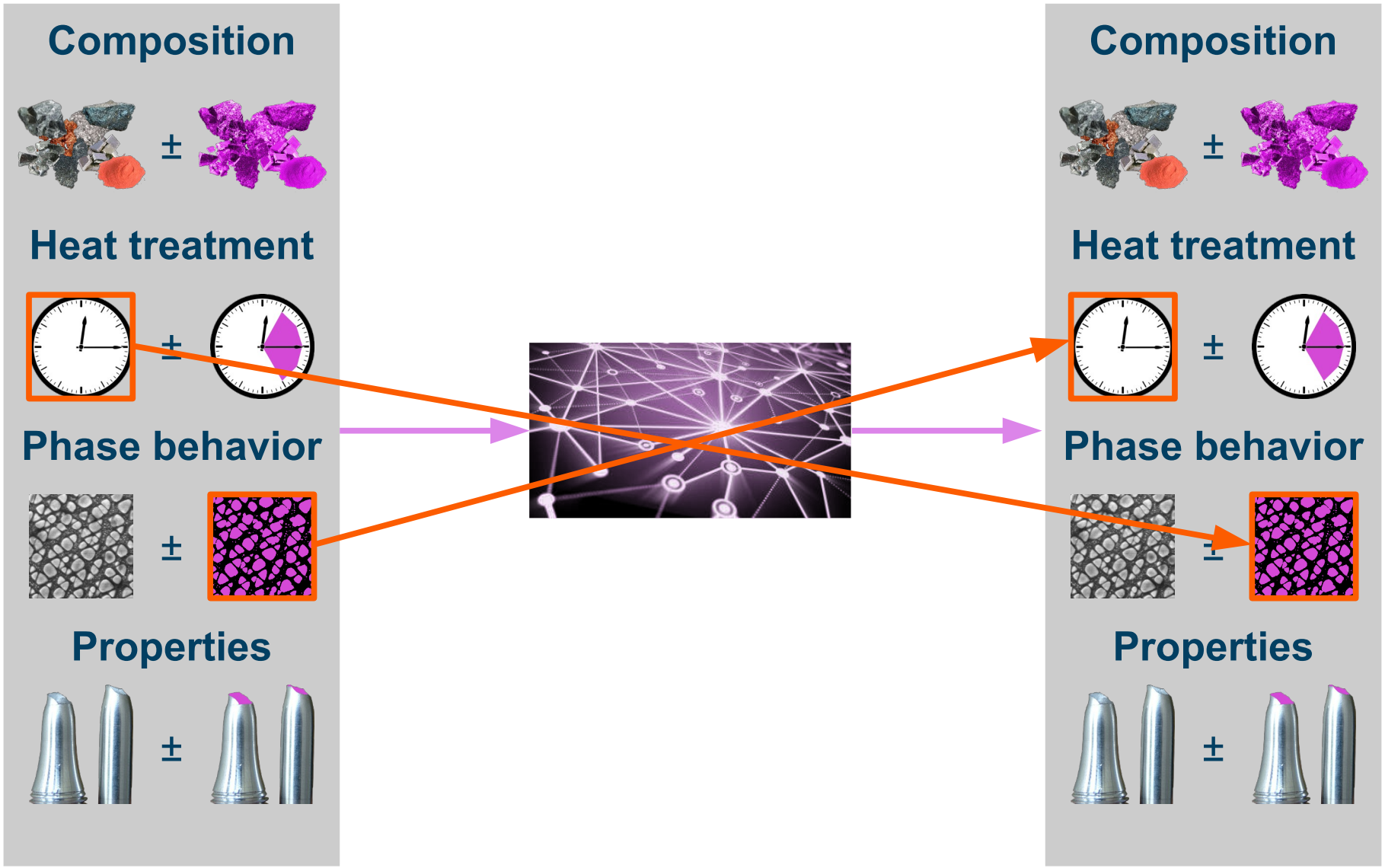


Properties

Exploit noise in the neural network

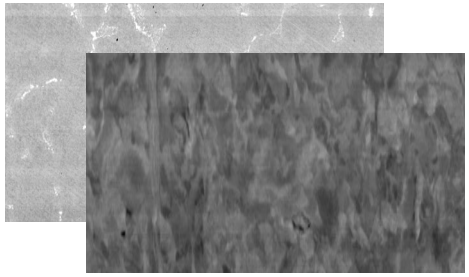


Exploit noise in the neural network

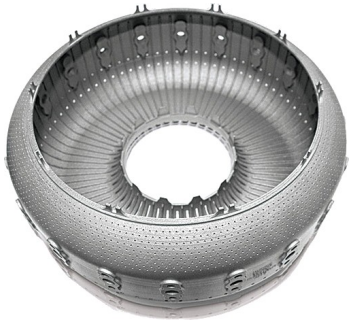


More materials designed: top down

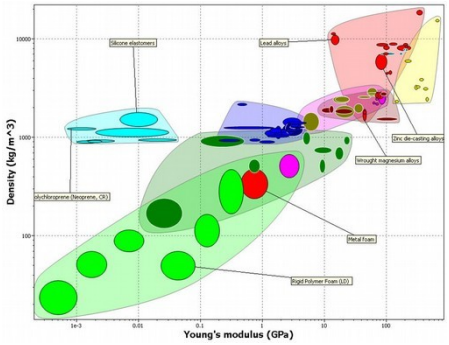
Molybdenum forging alloys



3D printed alloy designed from 7 data entries



Found 192 errors in materials databases



ROLLS ROYCE

ROLLS ROYCE Materials Solutions

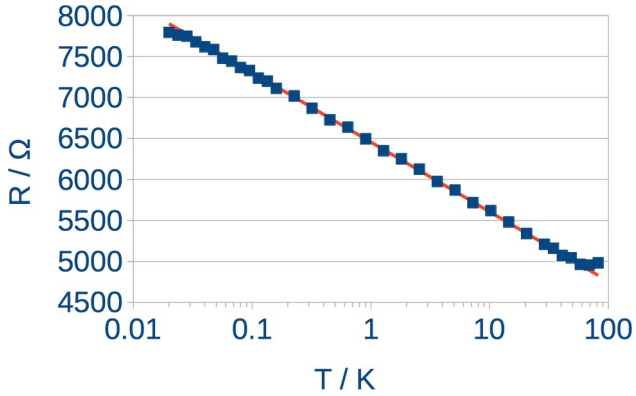
GRANTA MATERIAL INSPIRATION

Even more materials designed: top down and bottom up

Battery design with DFT and experimental data

Designing lubricants with DFT and experimental data

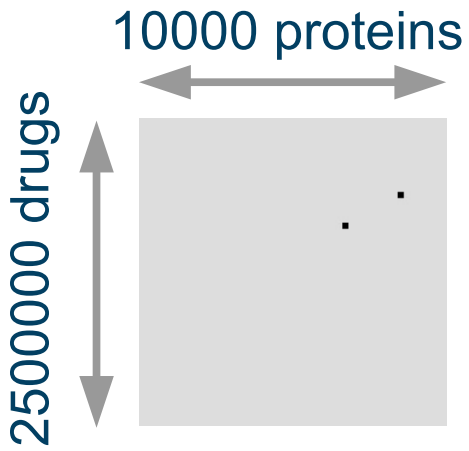
Thermometer with quantum and experimental data



Data available for drug discovery

10,000 proteins with 2,500,000 compounds

Original dataset 0.05% complete



e-therapeutics

Impute the database used for drug discovery

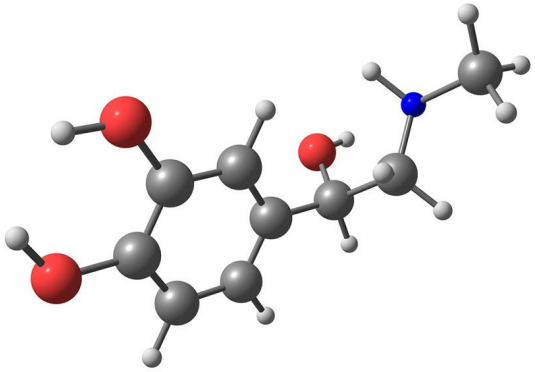
10,000 proteins with 2,500,000 compounds

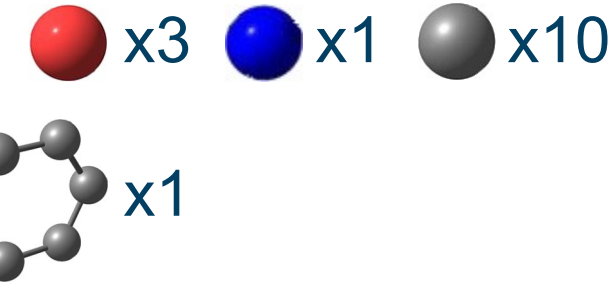
Original dataset 0.05% complete

Filled 32% of the entries

e-therapeutics

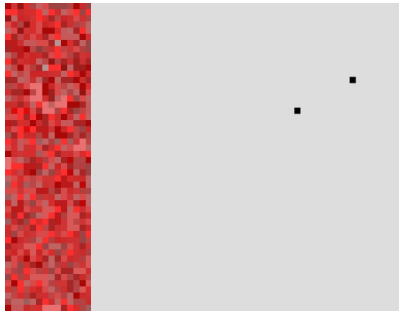
Drug discovery with additional descriptors





1101 Morse descriptor

200



e-therapeutics

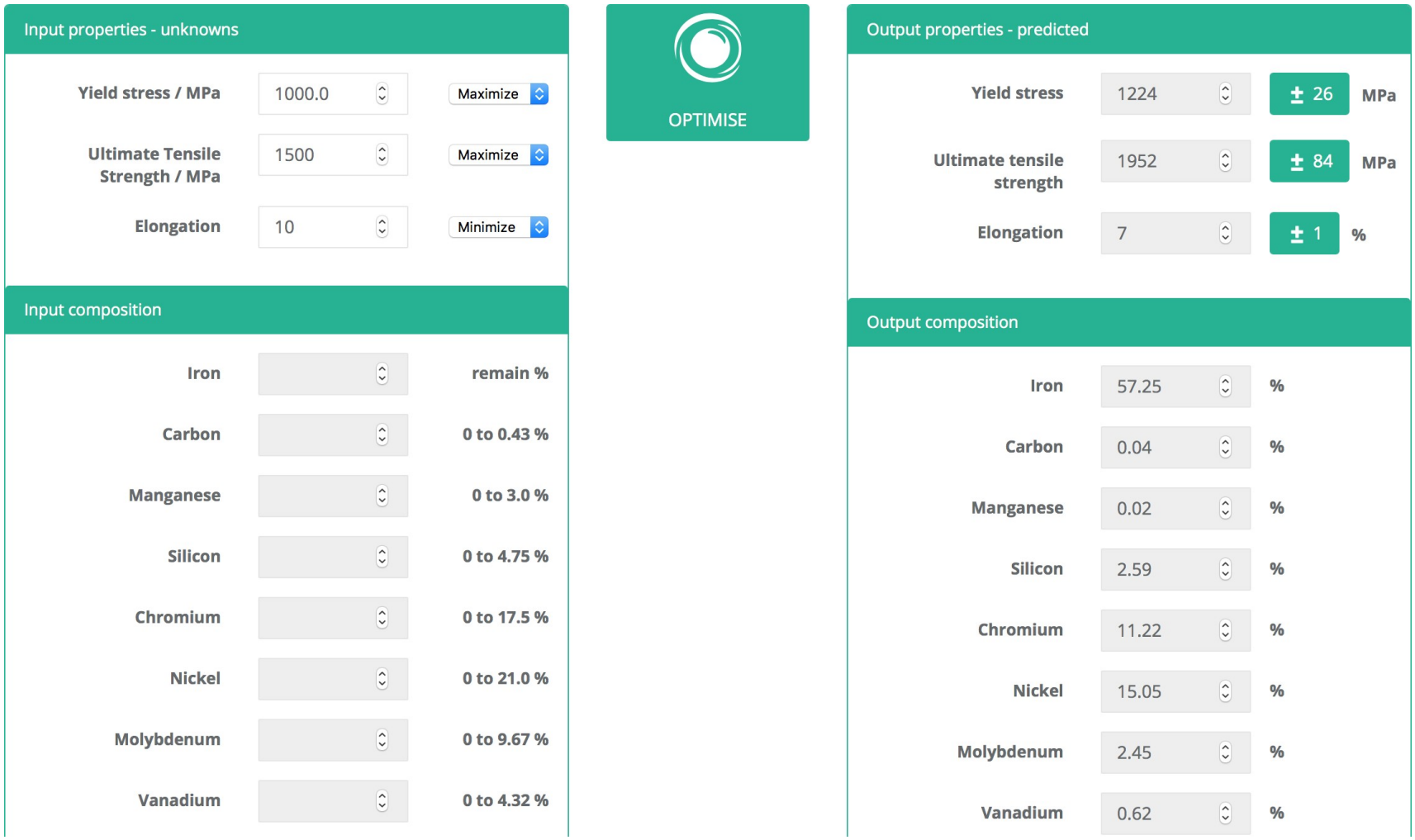
Improved drug discovery

Include drug structural information to fill to 46%

Saved >$1billion in experimental costs

e-therapeutics

Startup intellegens productizing the neural network



Summary: progress

Apply deep learning to high-value fragmented data

Exploit knowledge of noise in the data

Experimentally proven materials design with 7 companies, founded startup intellegens

Summary: opportunities

Apply deep learning to high-value fragmented data

Exploit knowledge of noise in the data

Experimentally proven materials design with 7 companies, founded startup intellegens

Merge experiments and simulations into holistic design tool

Summary: challenges

Apply deep learning to high-value fragmented data

Exploit knowledge of noise in the data

Experimentally proven materials design with 7 companies, founded startup intellegens

Merge experiments and simulations into holistic design tool

Scientists establish all possible sources of information