



Who needs science to design materials?

Gareth Conduit

Neural network algorithm to

Merge simulations, physical laws, and experimental data

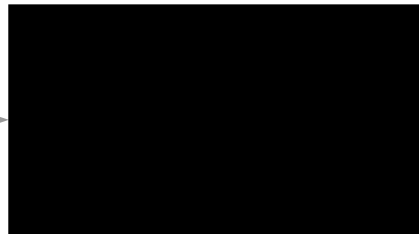
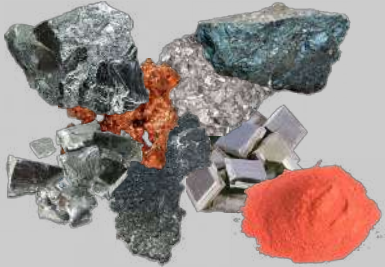
Reduce the need for expensive experimental development

Accelerate materials and drugs discovery

Generic with **proven** applications in materials discovery and drug design

Black box for materials design

Composition



Properties

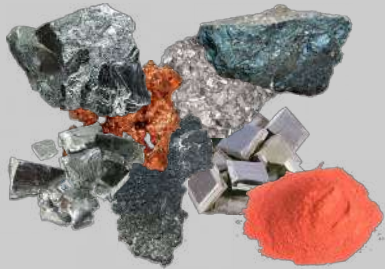
UTS

Hardness

Cost

Training the neural network

Composition



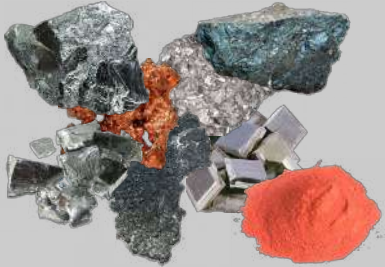
Properties

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203332721994995
976579342243418
394046703960393
597692868112392
376413439487341
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UTS
Hardness
Cost

Neural network for materials design

Composition



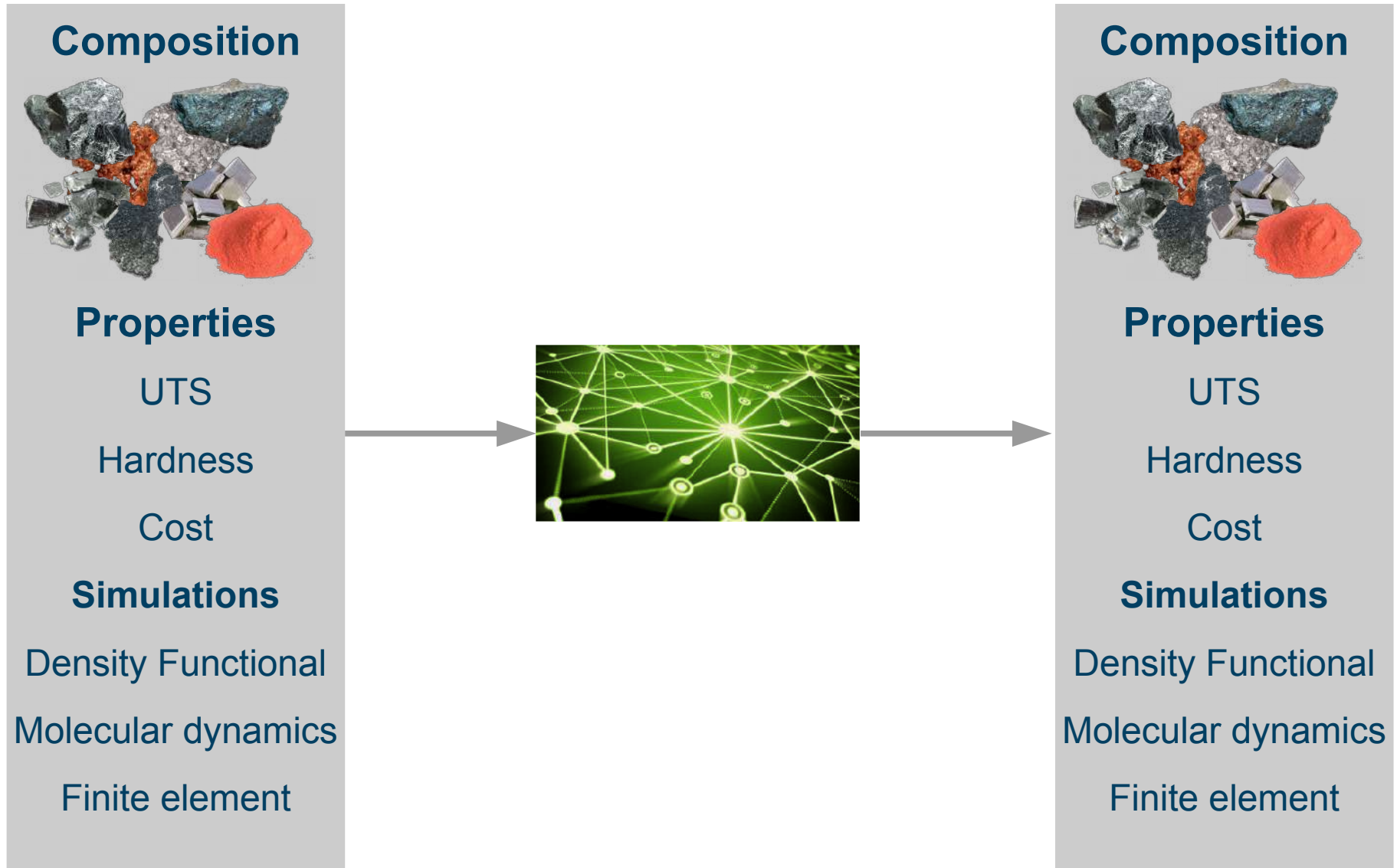
Properties

UTS

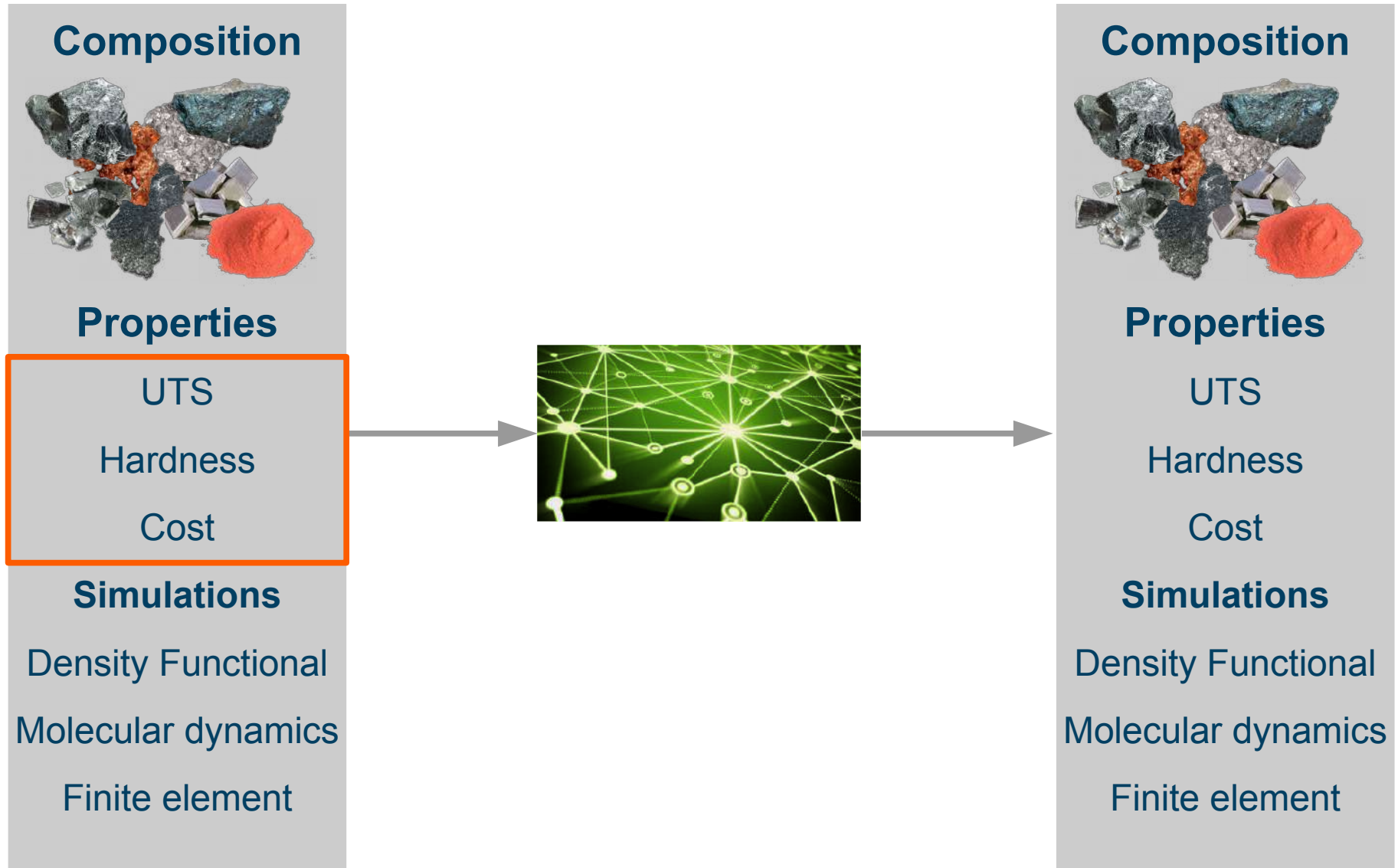
Hardness

Cost

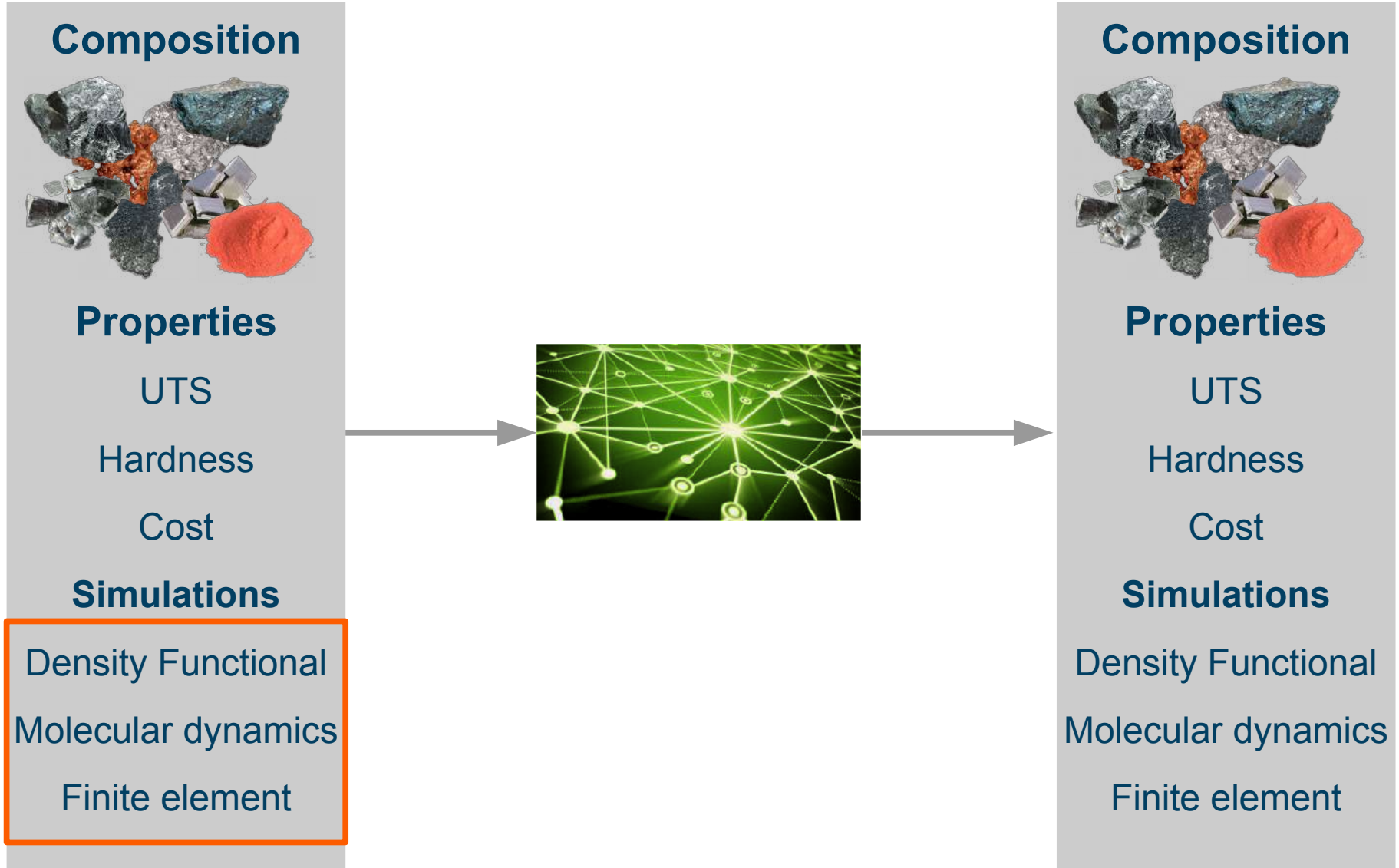
Neural network to exploit all available correlations



Neural network is top down



Neural network is top down and bottom up



Fragmented training data set

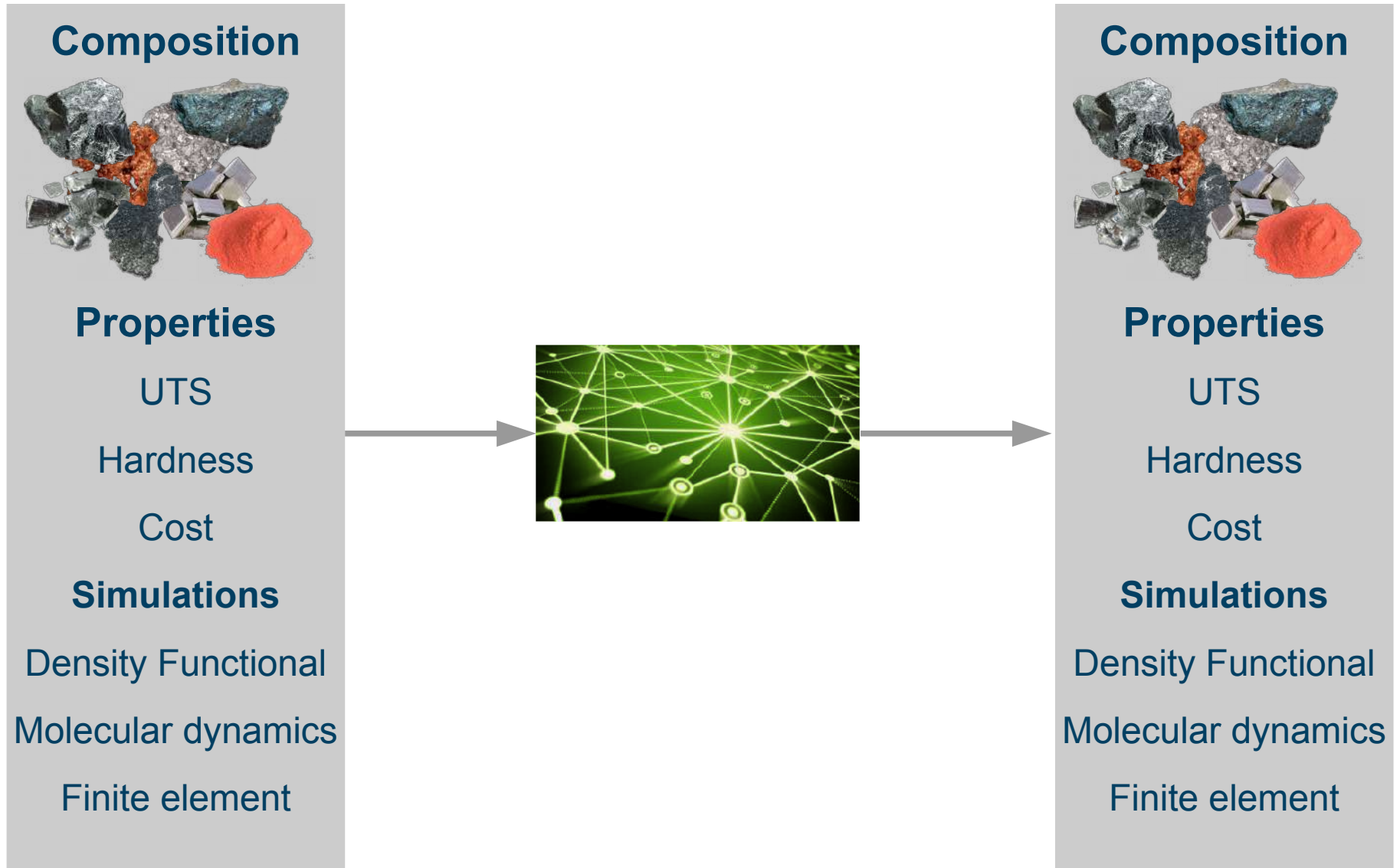
Composition

UTS

Hardness

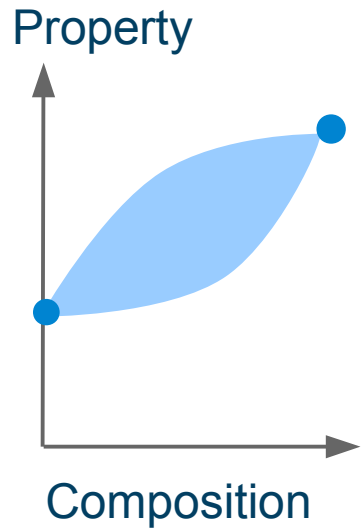


Neural network must handle fragmented data



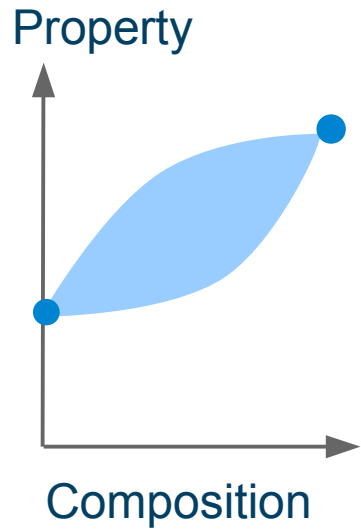
Neural network trained on experimental data

Experiment

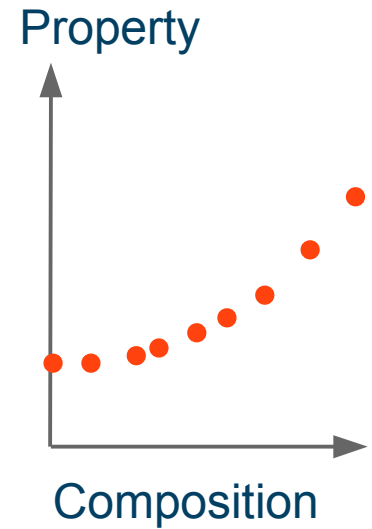


Further information is provided by a simulation

Experiment

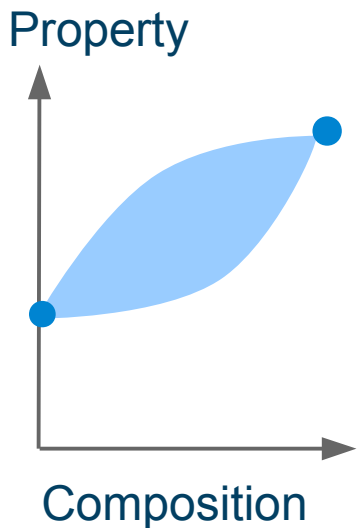


Simulation

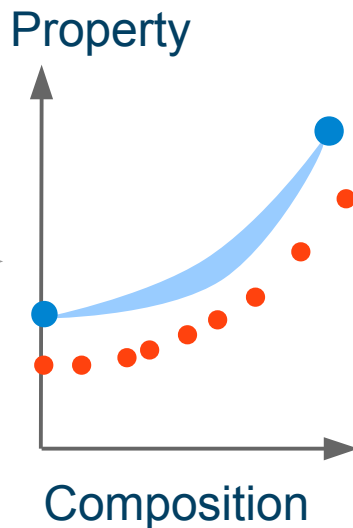


Neural network combines the two sources of data

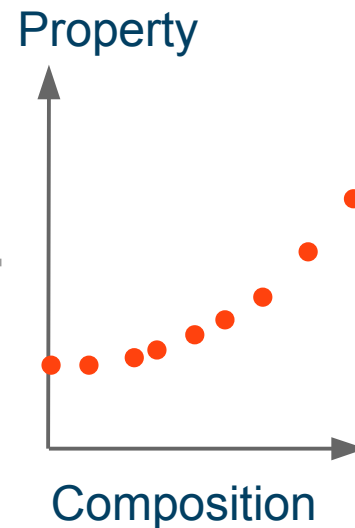
Experiment



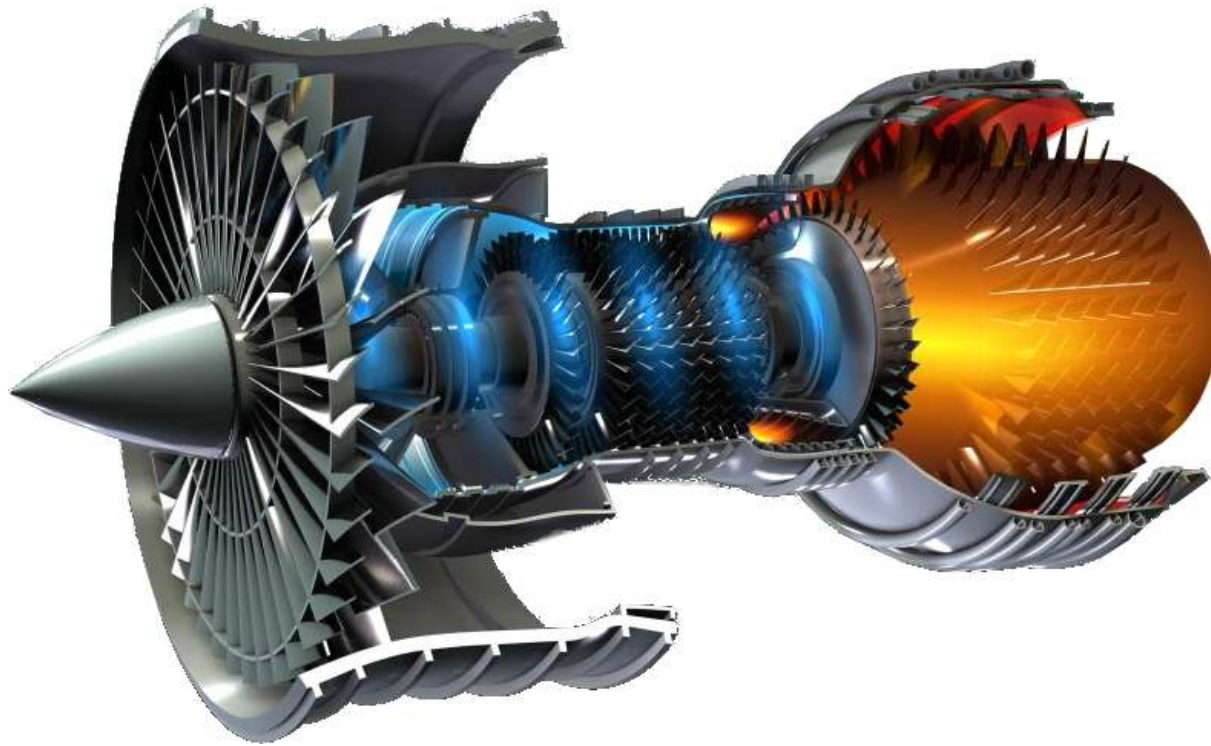
Combined



Simulation



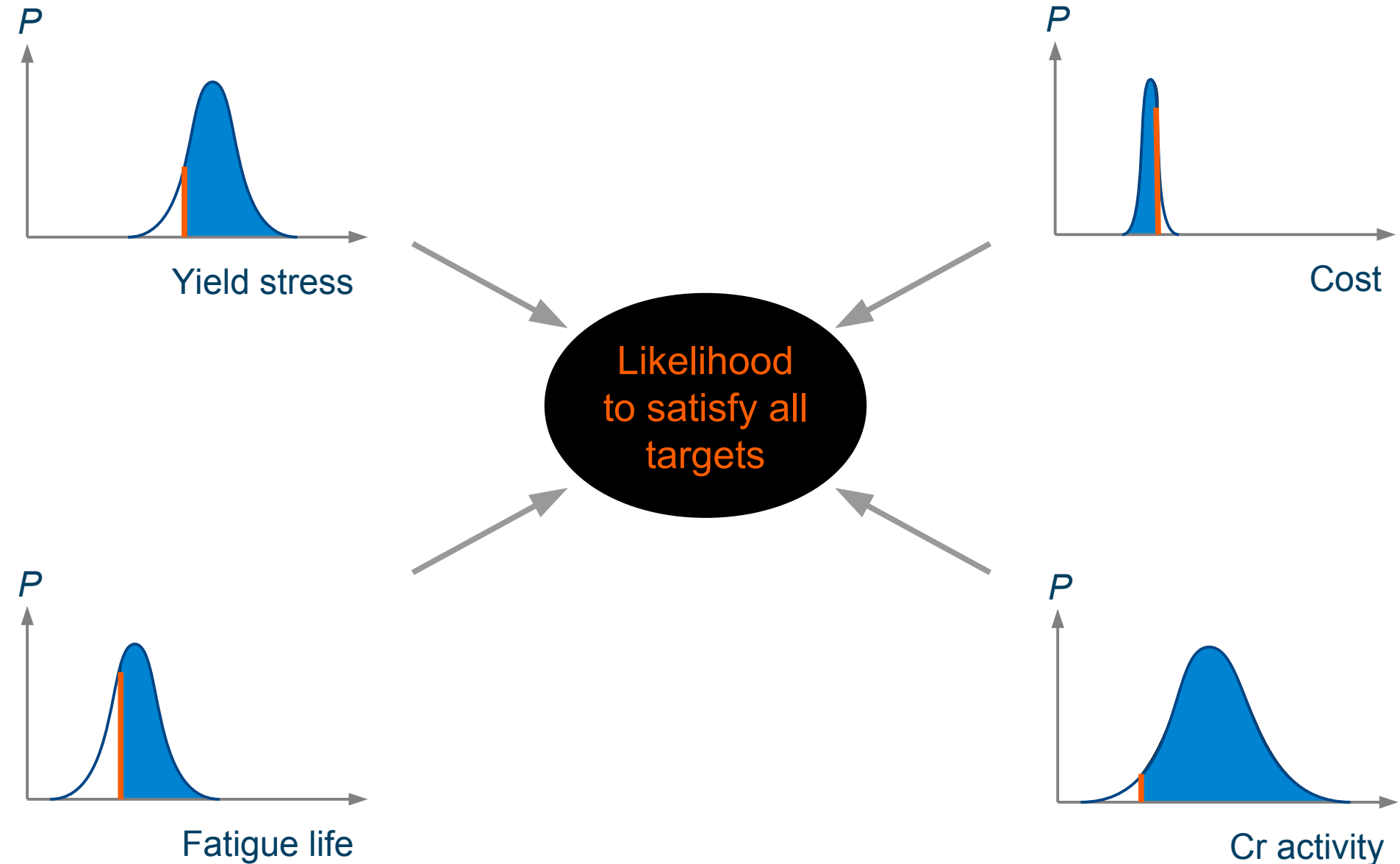
Schematic of an engine



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	> 983°C
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



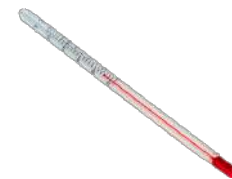
Zr: 0.18



Ni: 47.2



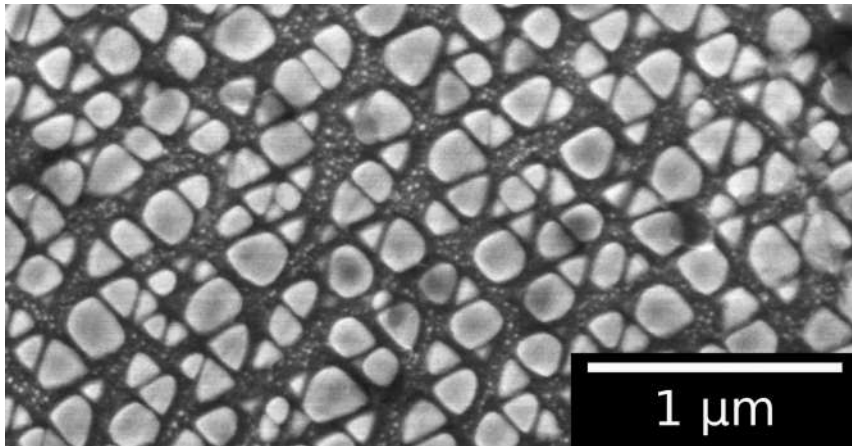
900°C



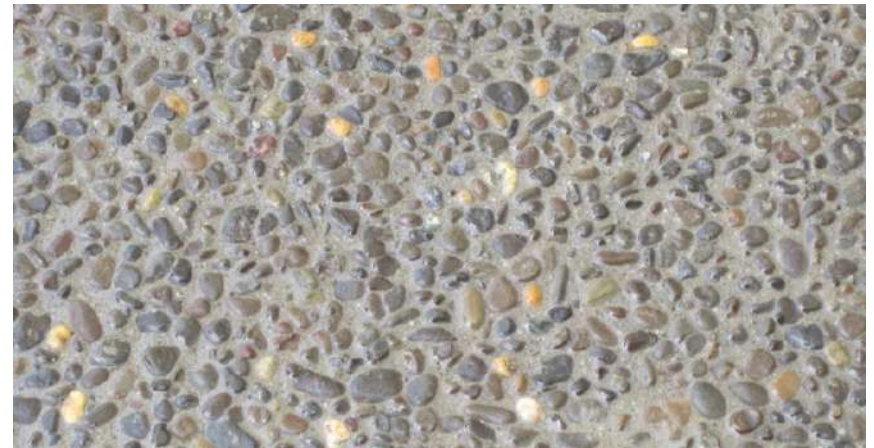
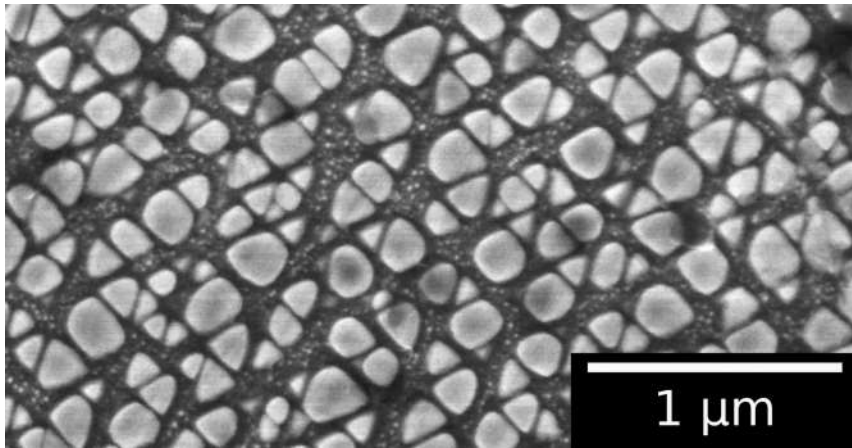
30 hours



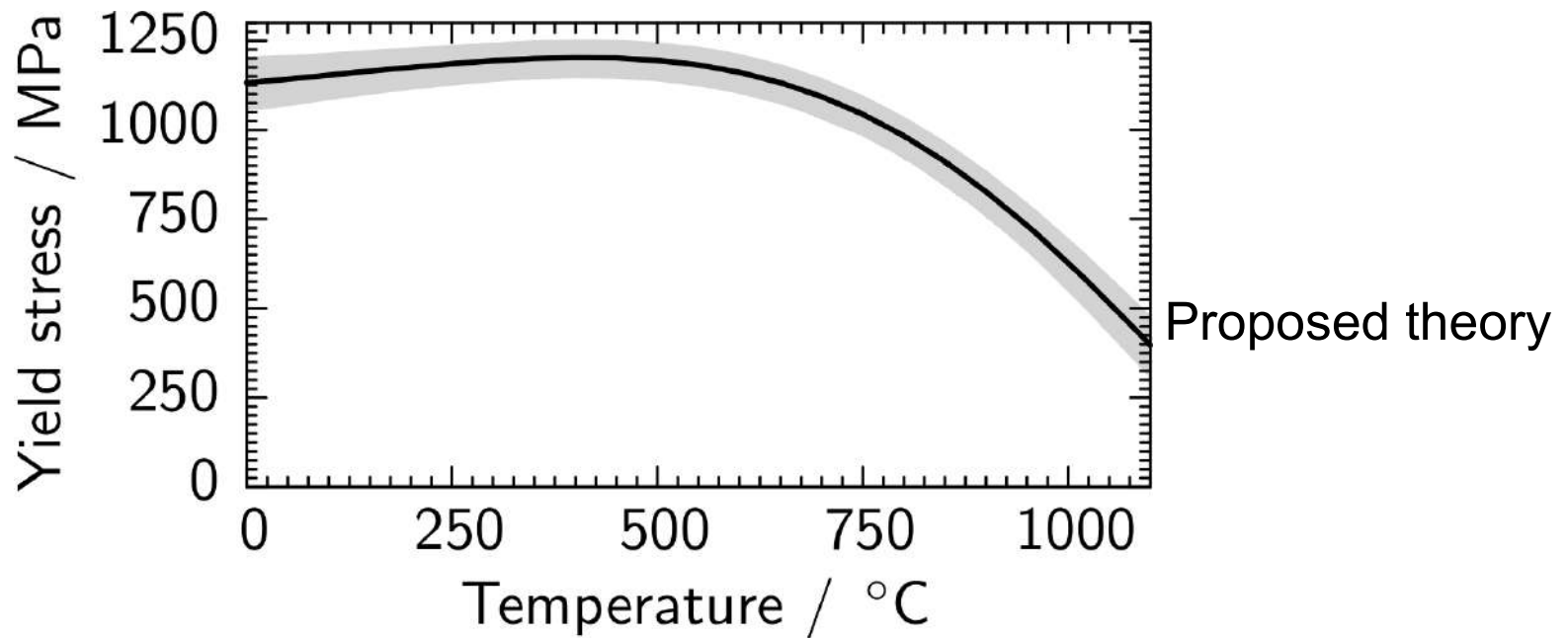
Microstructure



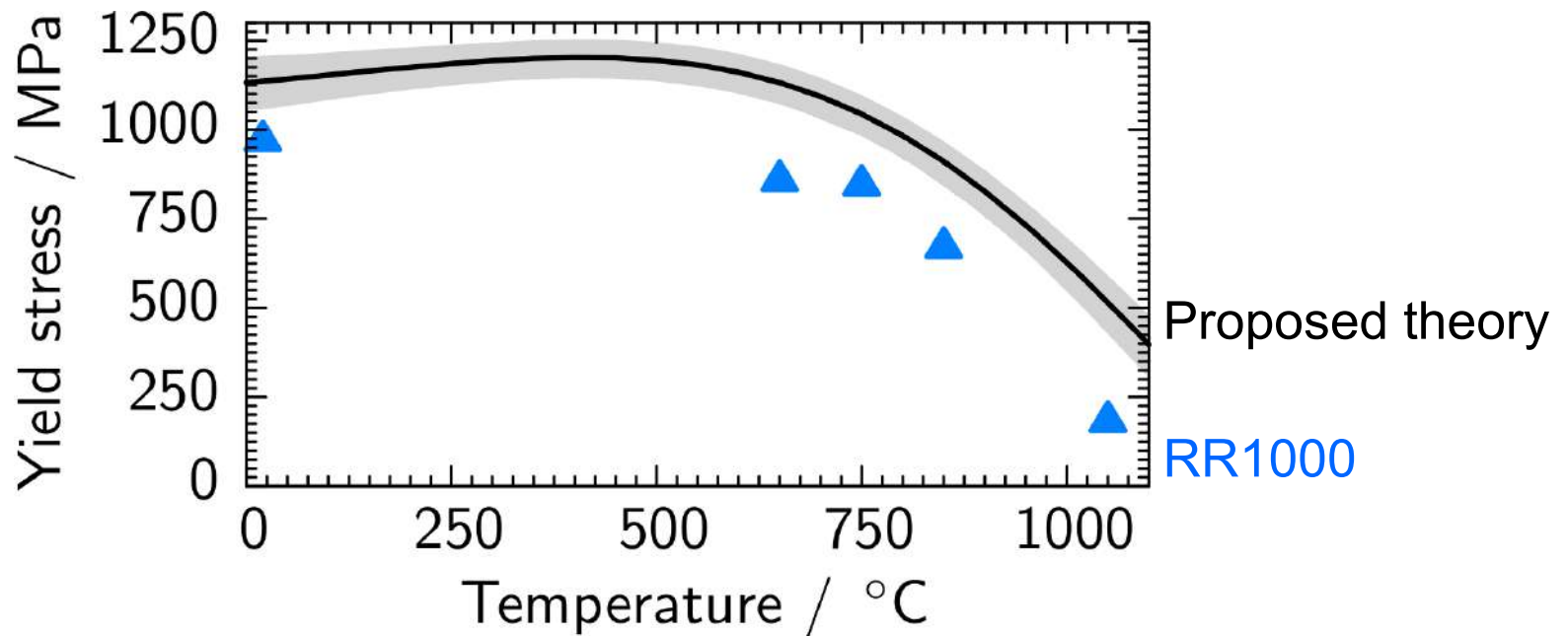
Precipitates strengthen the alloy



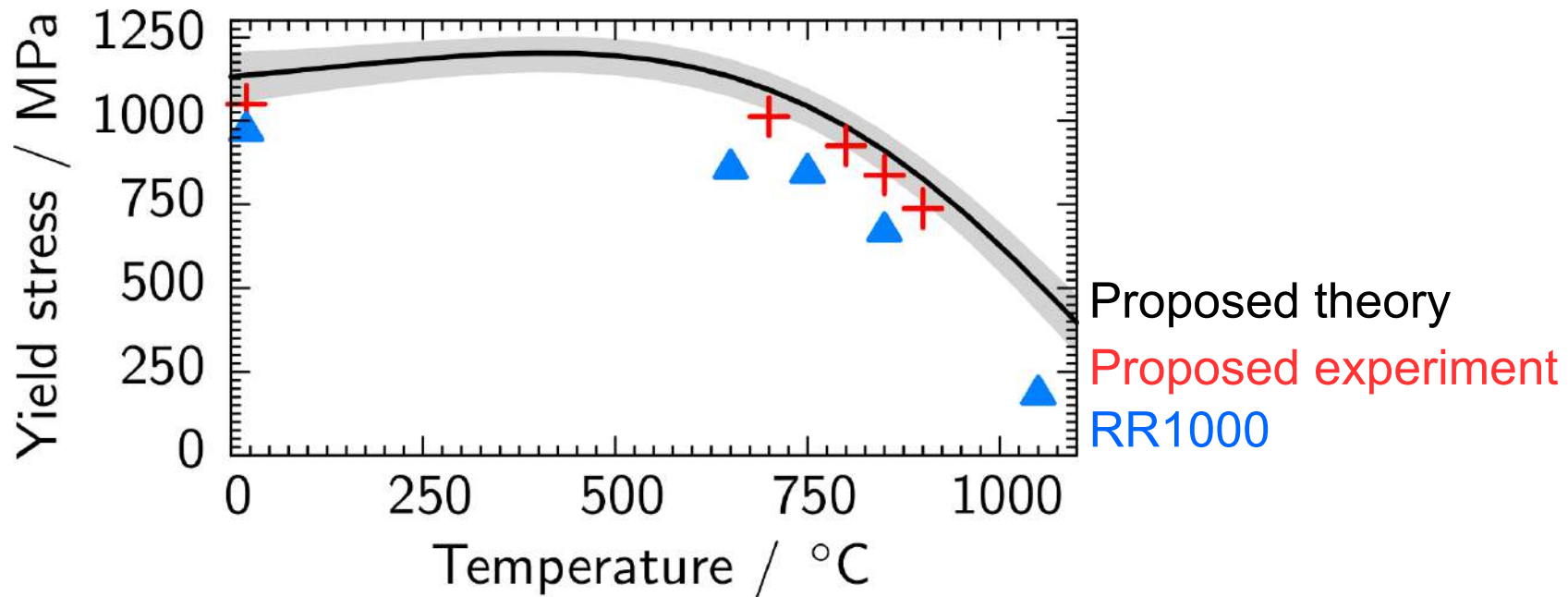
Predict the yield stress



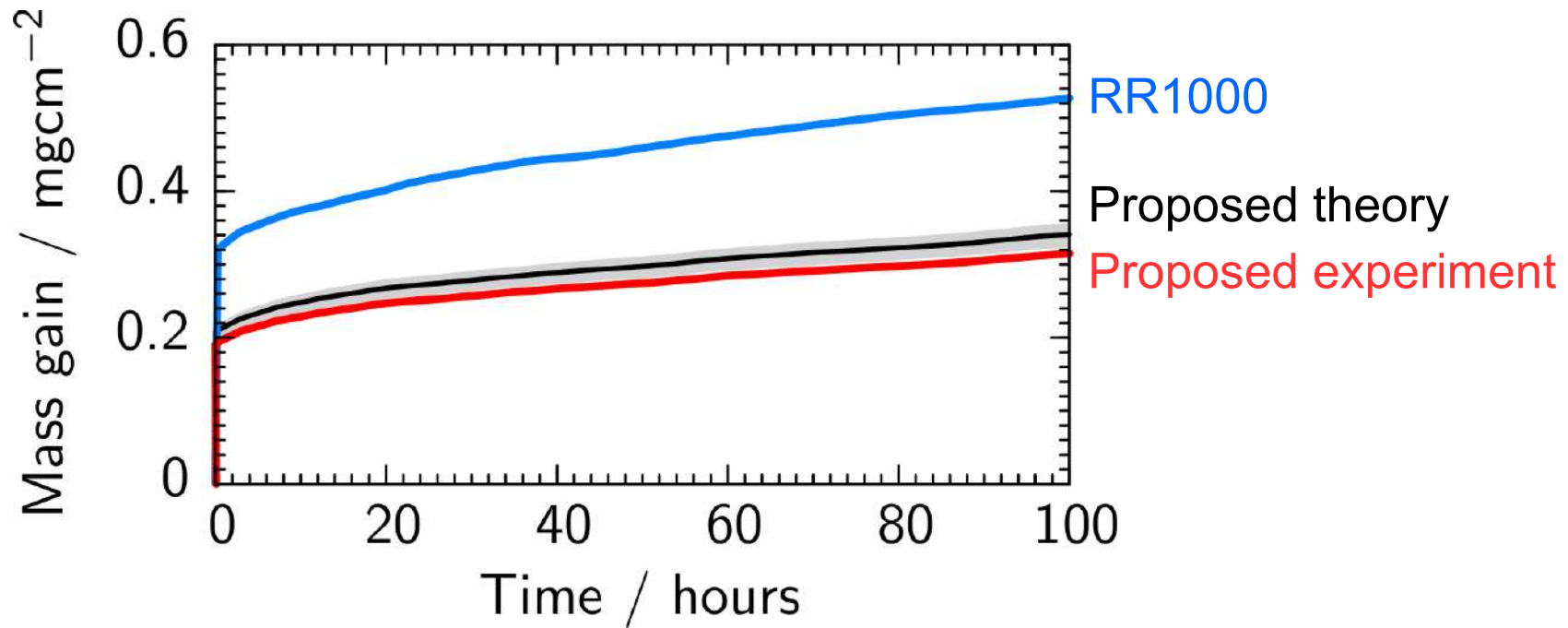
Test the yield stress



Test the yield stress

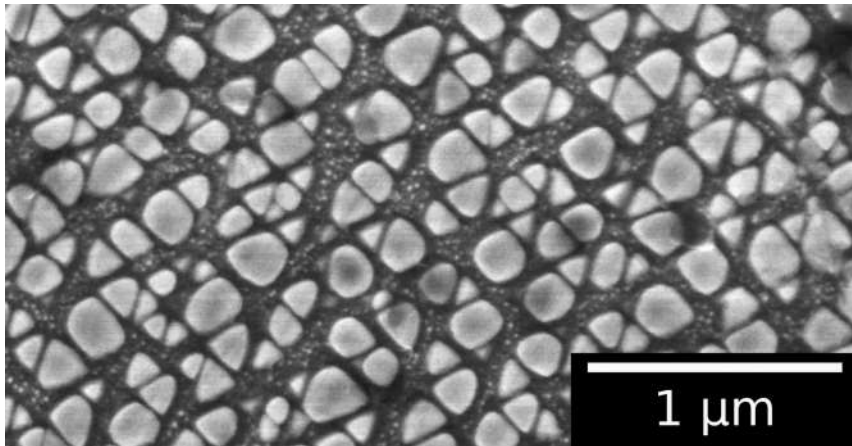


Test the oxidation resistance

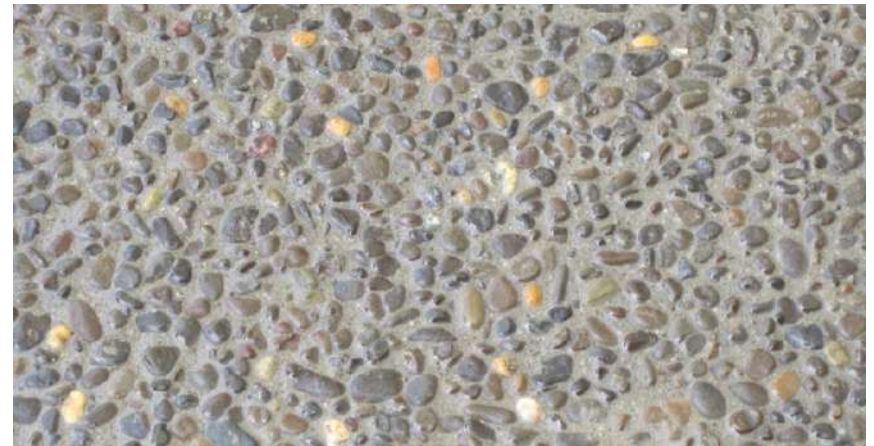


Microstructure strengthens the alloy

Precipitates

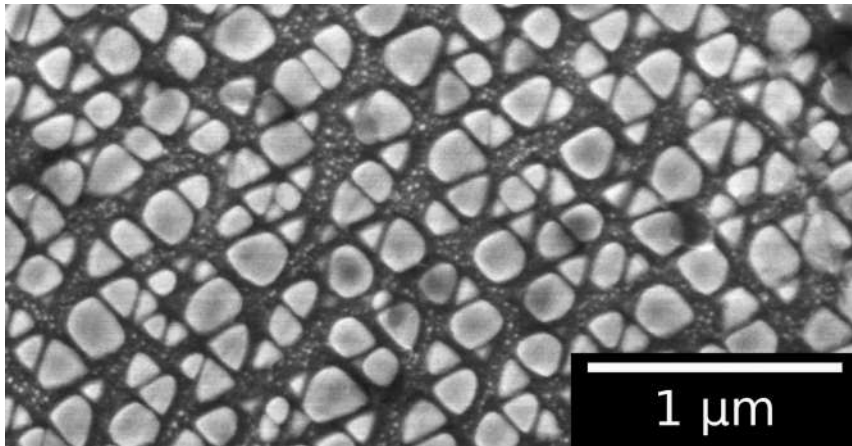


Aggregate

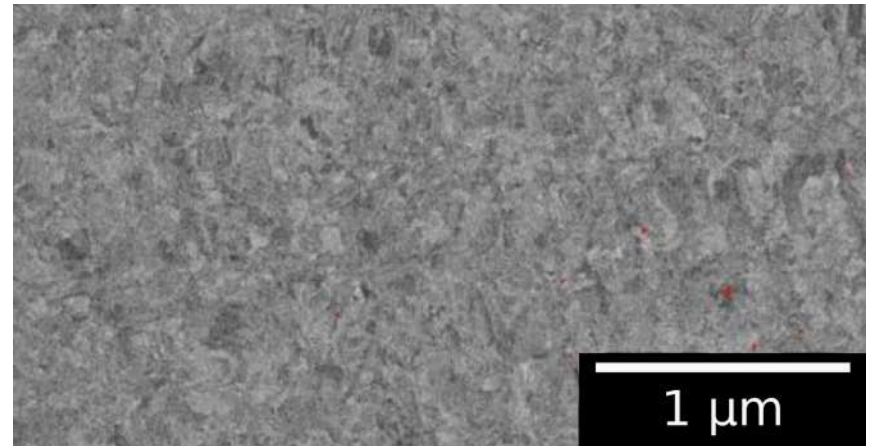


Microstructure defined by the heat treatment

Correct heat treatment

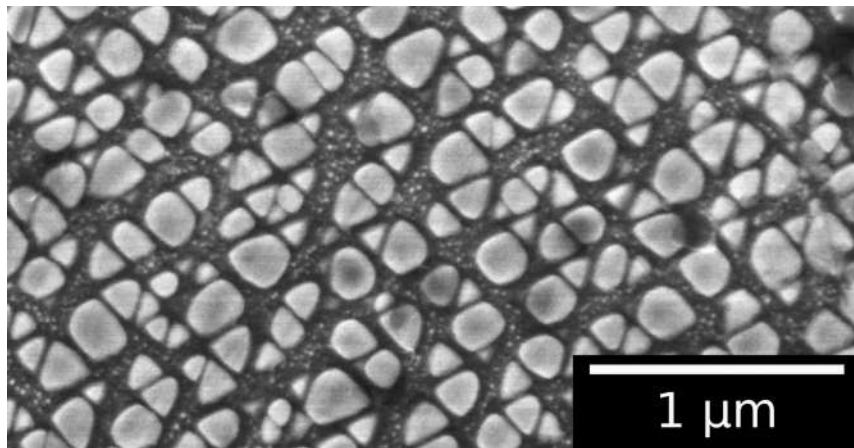


Incorrect heat treatment

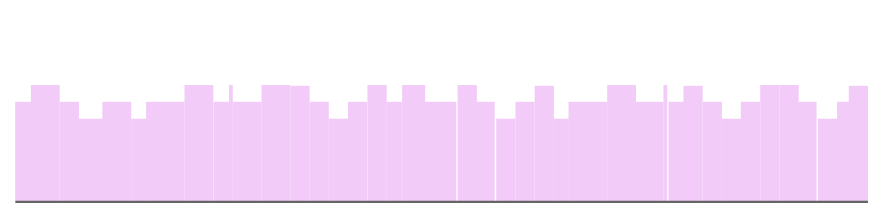
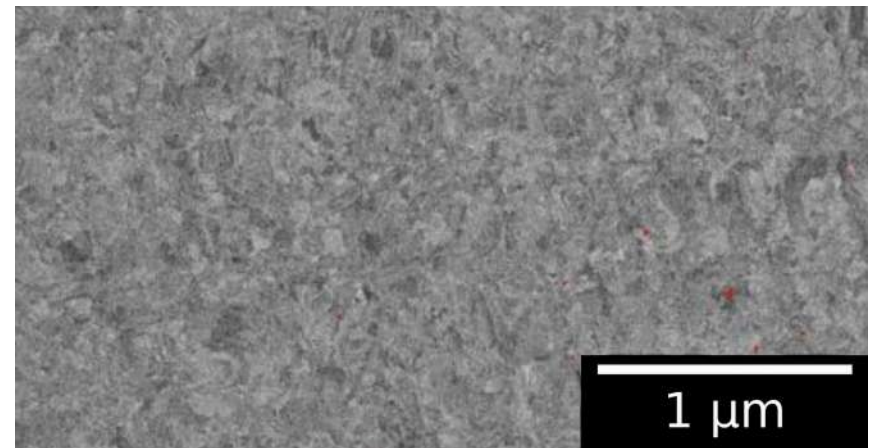


Microstructure distribution links to the heat treatment

Correct heat treatment

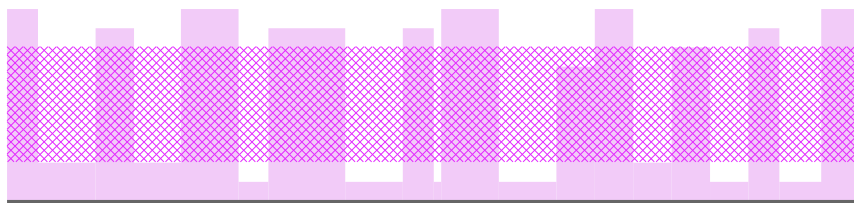
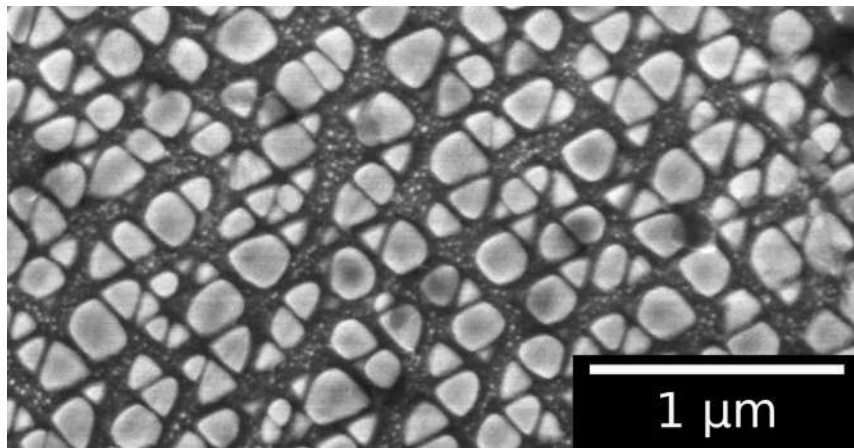


Incorrect heat treatment

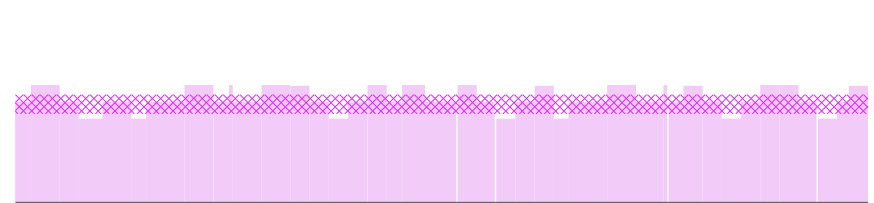
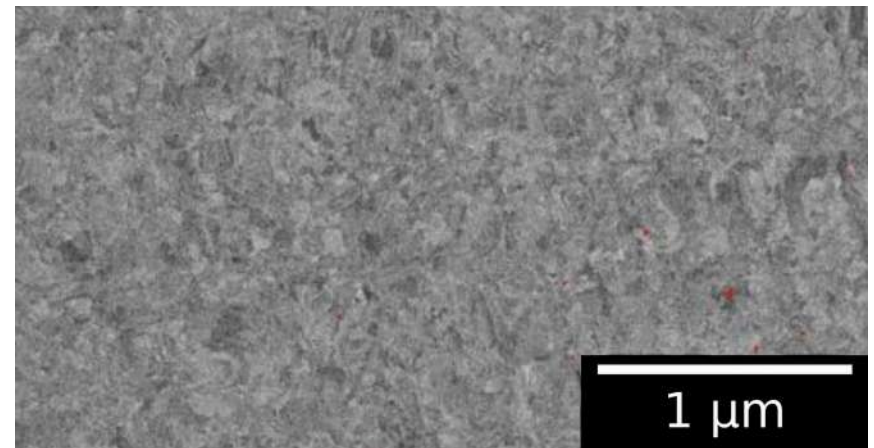


Microstructure distribution links to the heat treatment

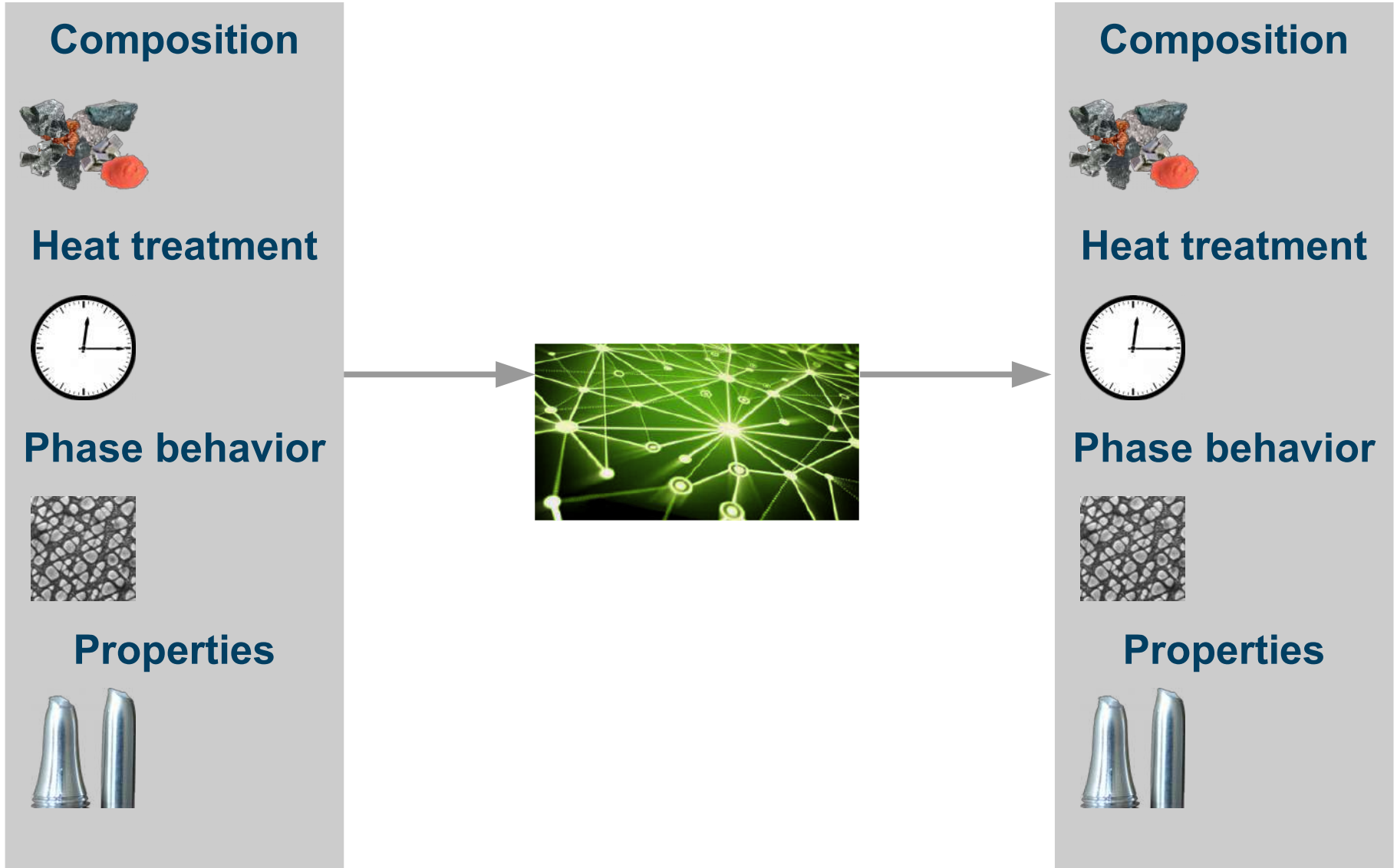
Correct heat treatment



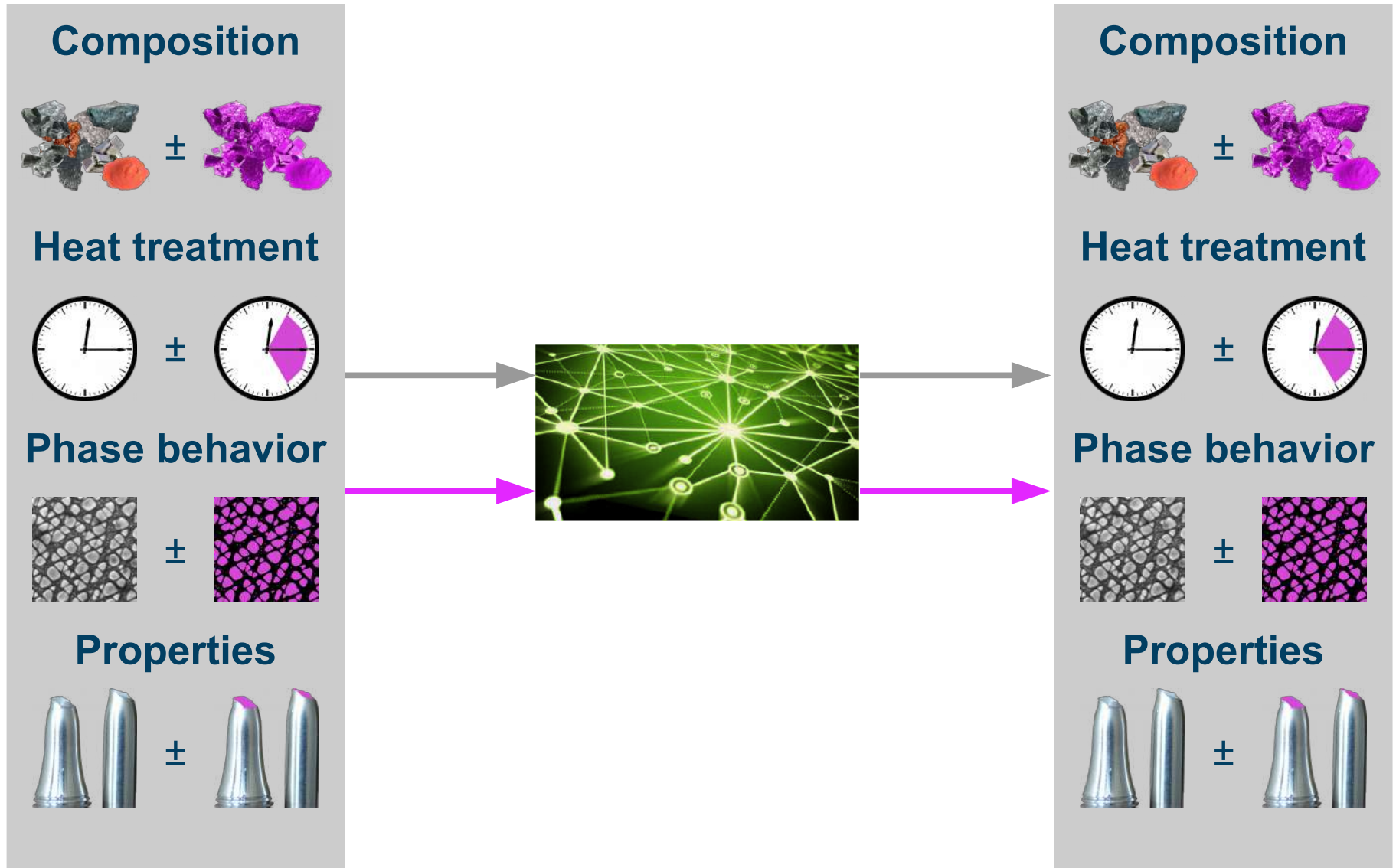
Incorrect heat treatment



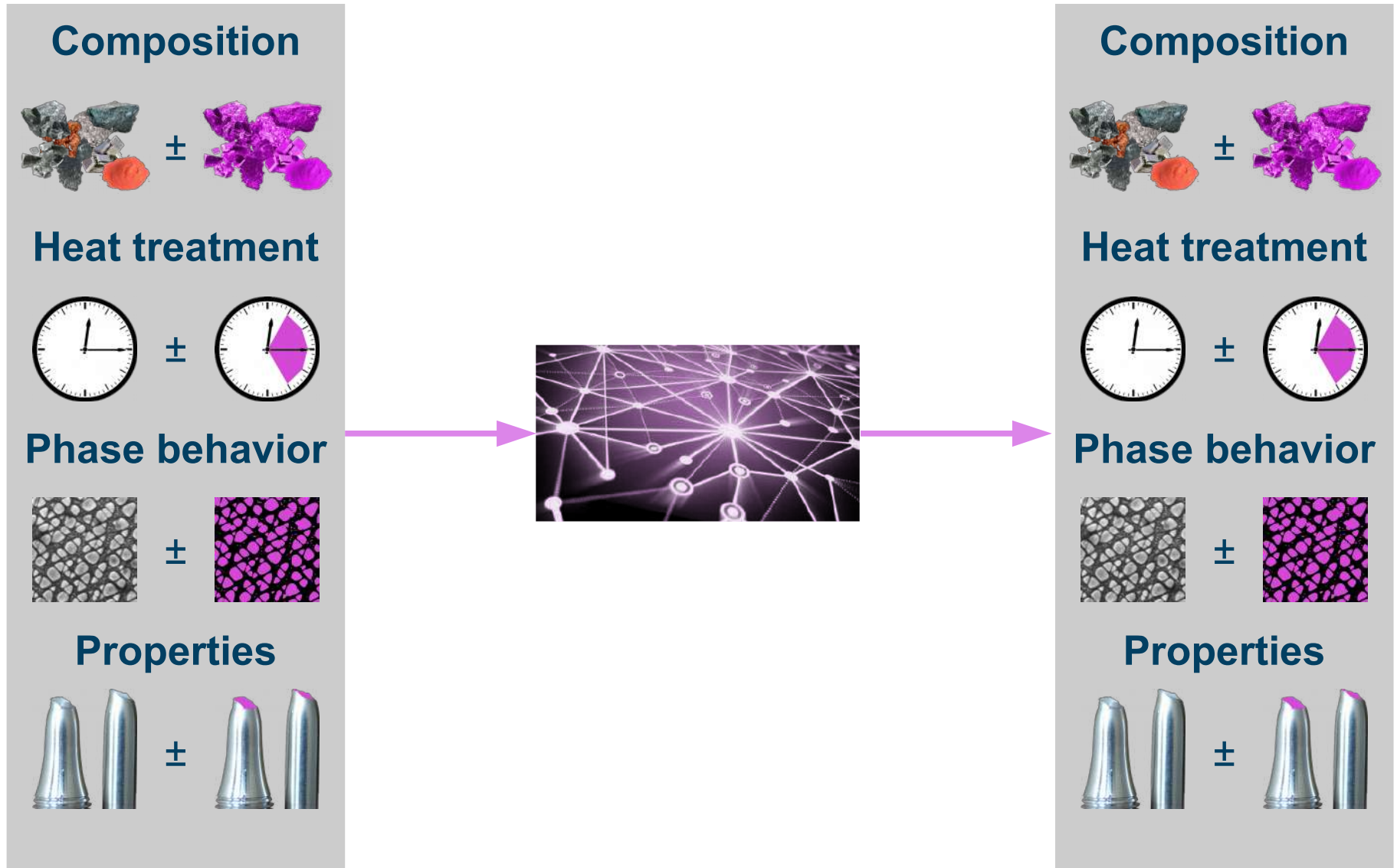
Standard neural network



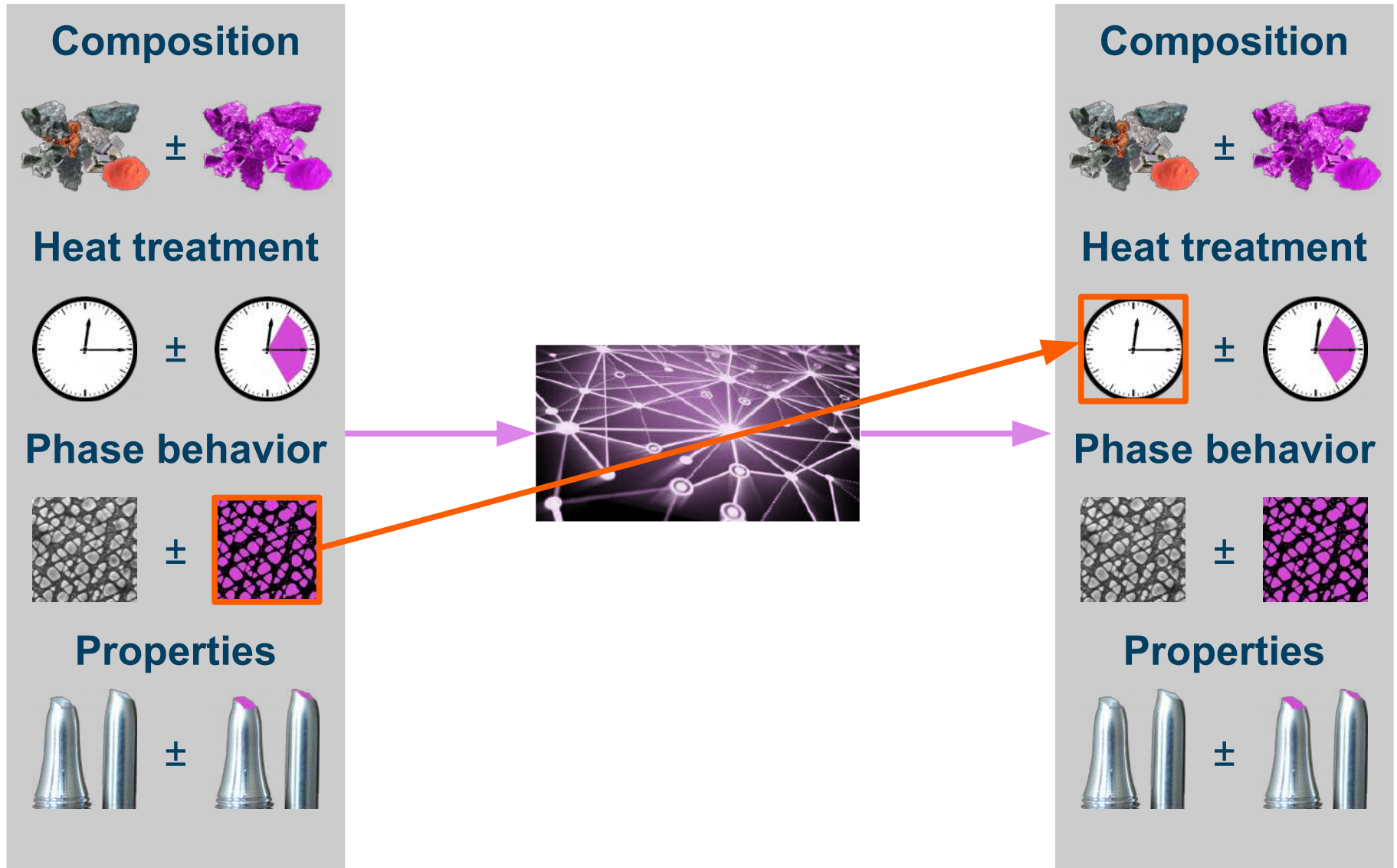
Neural network transmits noise as uncertainty



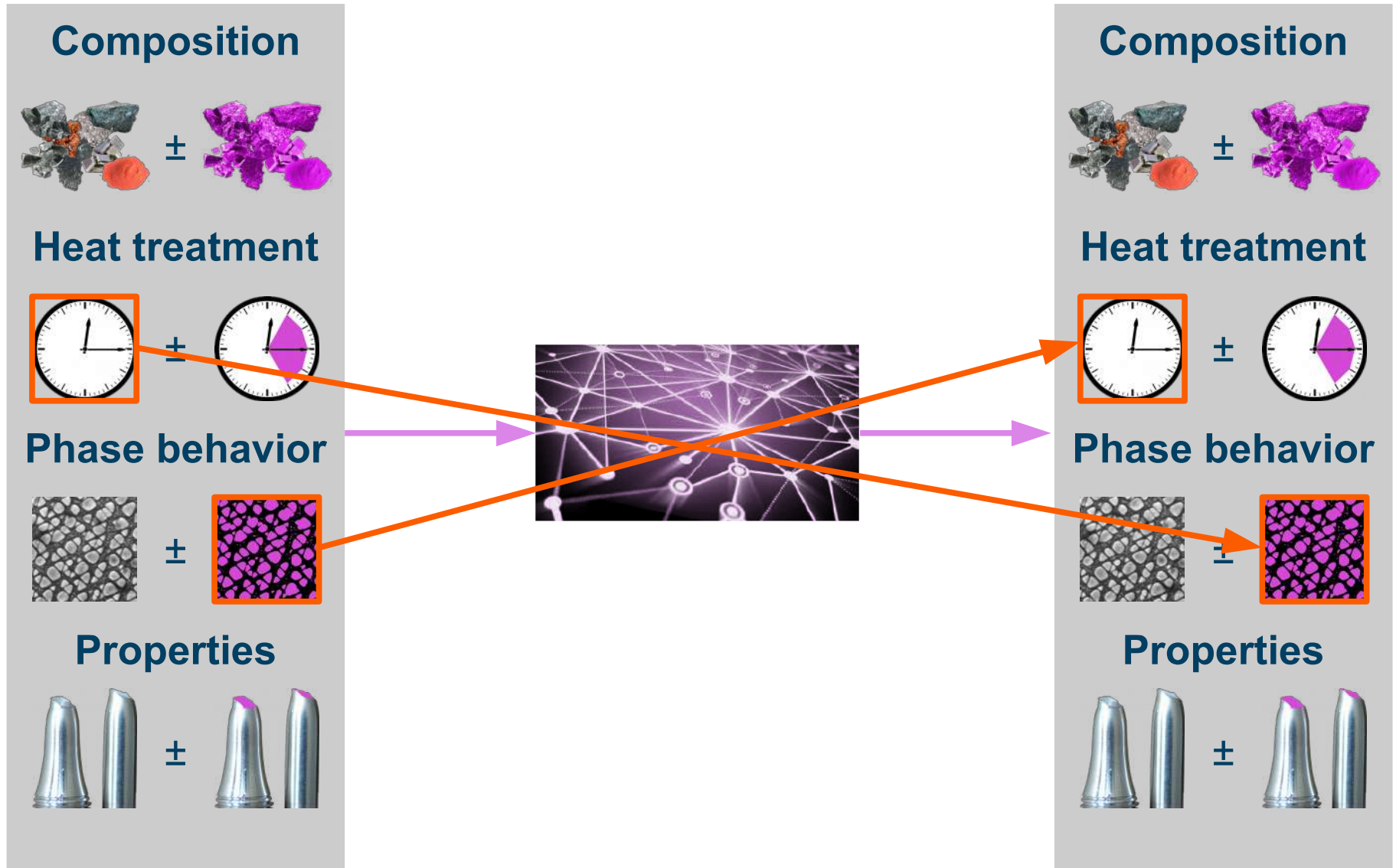
Incorporate noise into the neural network



Exploit noise in the neural network



Exploit noise in the neural network



Point cloud: noise in the data

Near

Far



Point cloud: benefits of including noise

Recover presence of people to **90%** accuracy

Also applies to **trees** and **railings**



Even more materials designed

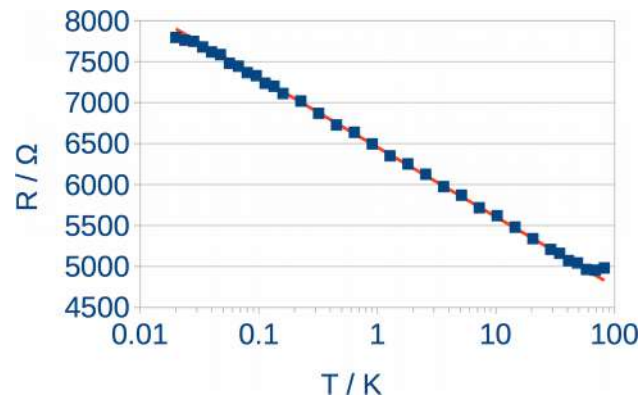
Battery design
with DFT and
experimental data



Designing lubricants
with DFT and
experimental data



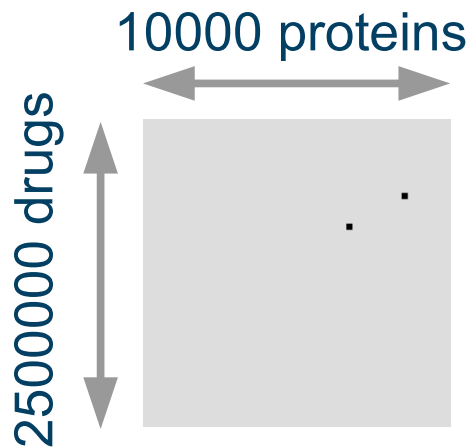
Thermometer with
quantum and
experimental data



Data available for drug discovery

10,000 proteins with 2,500,000 compounds

Original dataset 0.05% complete



Impute the database used for drug discovery

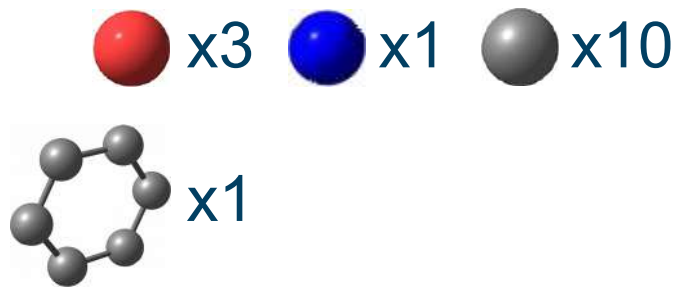
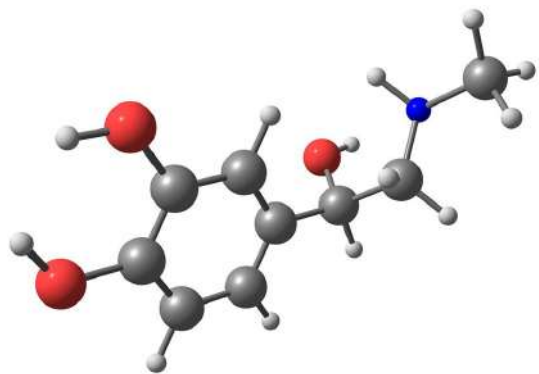
10,000 proteins with 2,500,000 compounds

Original dataset 0.05% complete

Filled 32% of the entries

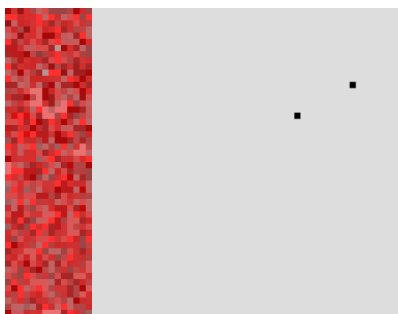


Drug discovery with additional descriptors



1101 Morse descriptor

200



Improved drug discovery

Include drug structural information to fill to 46%

Saved >\$1billion in experimental costs



Startup intellegens productizing the neural network

Input properties - unknowns

Yield stress / MPa	1000.0	Maximize
Ultimate Tensile Strength / MPa	1500	Maximize
Elongation	10	Minimize

Input composition

Iron		remain %
Carbon		0 to 0.43 %
Manganese		0 to 3.0 %
Silicon		0 to 4.75 %
Chromium		0 to 17.5 %
Nickel		0 to 21.0 %
Molybdenum		0 to 9.67 %
Vanadium		0 to 4.32 %



Output properties - predicted

Yield stress	1224	± 26 MPa
Ultimate tensile strength	1952	± 84 MPa
Elongation	7	± 1 %

Output composition

Iron	57.25	%
Carbon	0.04	%
Manganese	0.02	%
Silicon	2.59	%
Chromium	11.22	%
Nickel	15.05	%
Molybdenum	2.45	%
Vanadium	0.62	%

Summary: progress

Apply deep learning to high-value **fragmented** data

Exploit knowledge of **probability distribution** of the data

Experimentally **proven** materials and drugs design with 7 companies, founded startup **intellegens**

Summary: opportunities

Apply deep learning to high-value **fragmented** data

Exploit knowledge of **probability distribution** of the data

Experimentally **proven** materials and drugs design with 7 companies, founded startup **intellegens**

Merge experiments and simulations into **holistic** design tool

Summary: future prospects

Apply deep learning to high-value **fragmented** data

Exploit knowledge of **probability distribution** of the data

Experimentally **proven** materials and drugs design with 7 companies, founded startup **intellegens**

Merge experiments and simulations into **holistic** design tool

Scientists establish all possible **SOURCES** of information