UNIVERSITY OF CAMBRIDGE

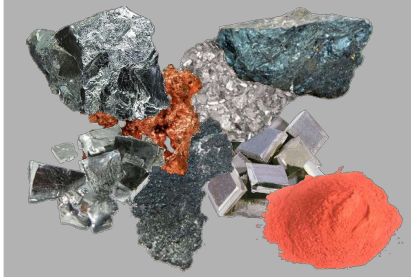
Materials discovery with artificial intelligence

Gareth Conduit

TCM Group, Department of Physics

Neural networks for materials design

Composition



Artificial intelligence

Properties

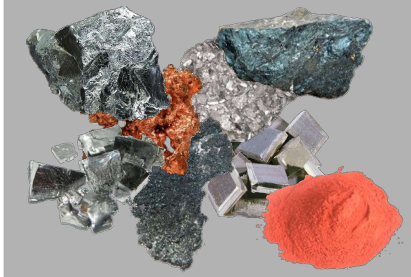
Cost

UTS

Hardness

Neural networks for materials design

Composition



Artificial intelligence

Properties

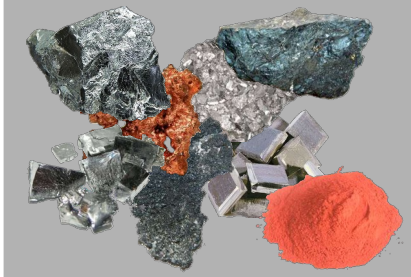
Cost

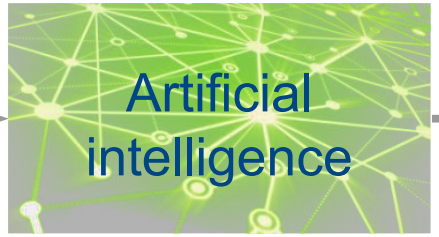
UTS

Hardness

Neural networks for materials design

Composition





Properties

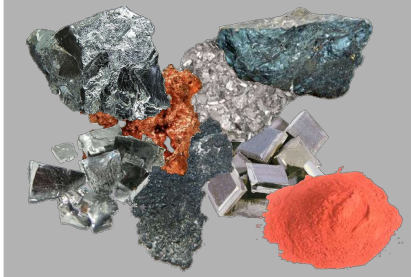
Cost

UTS

Hardness

Neural networks for materials design

Composition



Properties

Cost

UTS

Hardness

Simulations

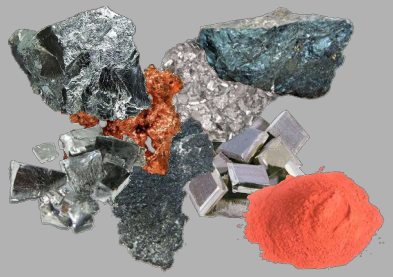
Density Functional

Molecular dynamics

Finite element

Artificial intelligence

Composition



Properties

Cost

UTS

Hardness

Simulations

Density Functional

Molecular dynamics

Finite element

Two important capabilities

Handle fragmented input data

Input 1	Input 2	Output
✓	✓	✓
✗	✓	✓
✓	✗	✓

Two important capabilities

Handle fragmented input data

Input 1	Input 2	Output
✓	✓	✓
✗	✓	✓
✓	✗	✓

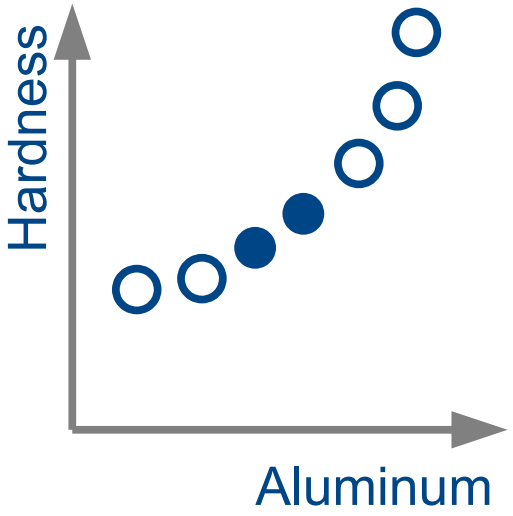
Combine uncertainties of the predictions to predict net likelihood

90% yield stress

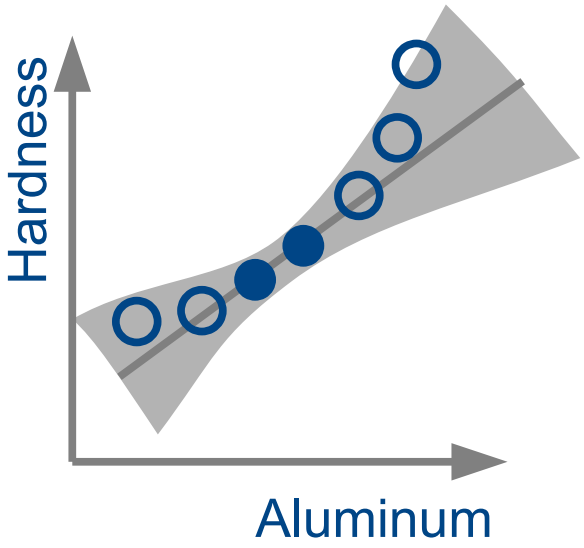
90% oxidation resistance

Overall 81%

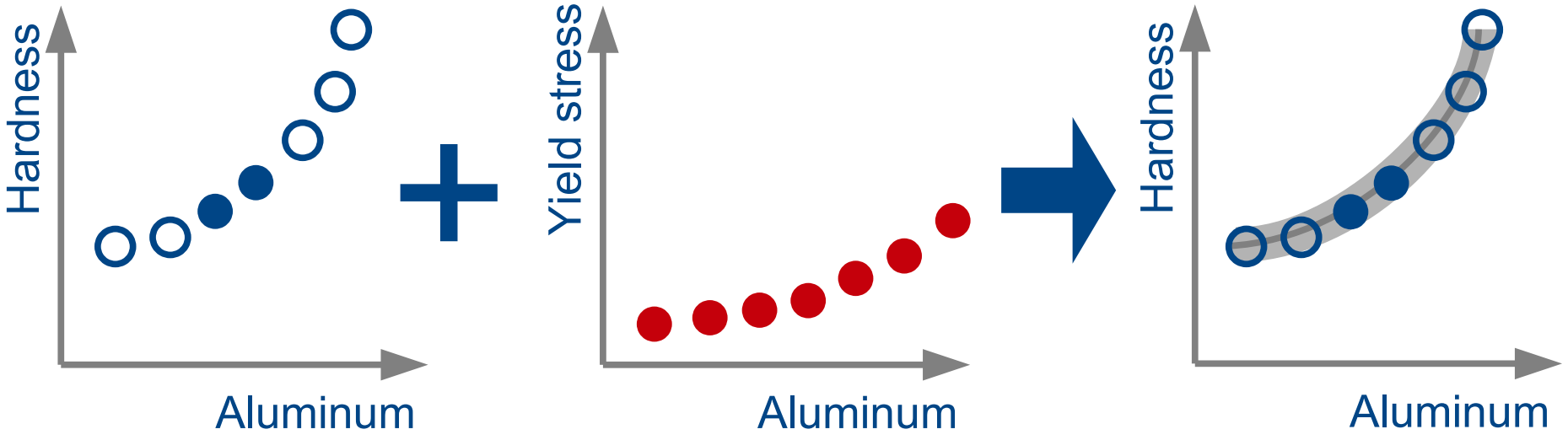
Correlations between properties



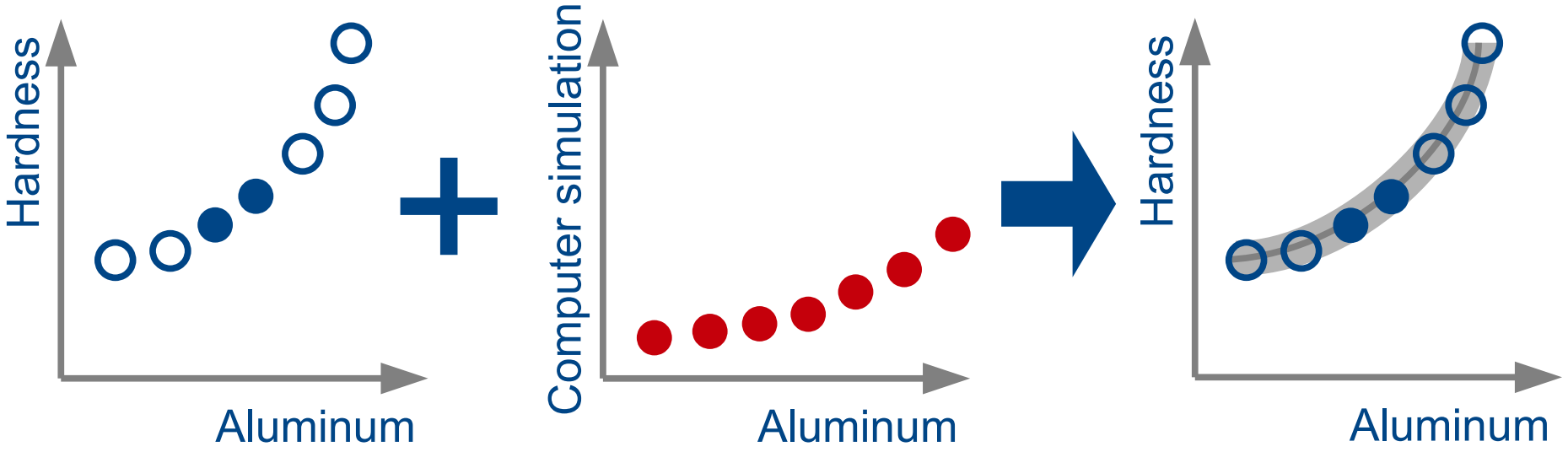
Correlations between properties



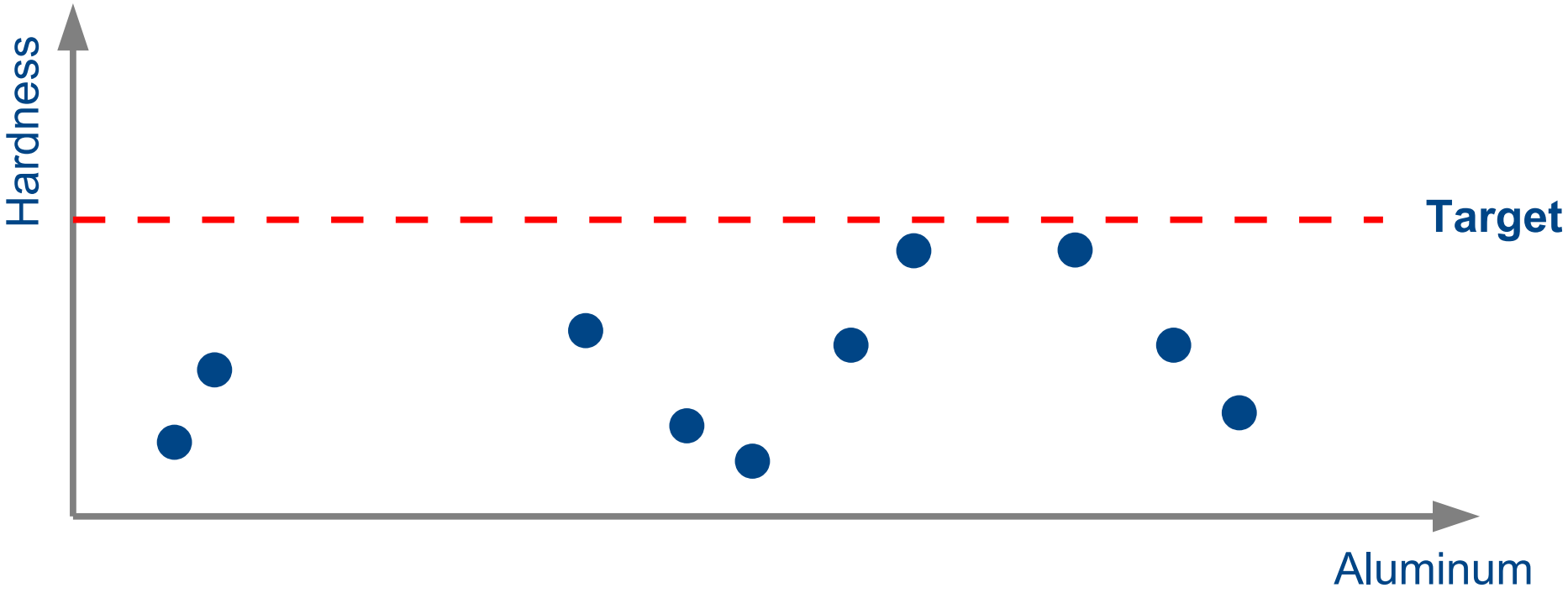
Correlations between properties



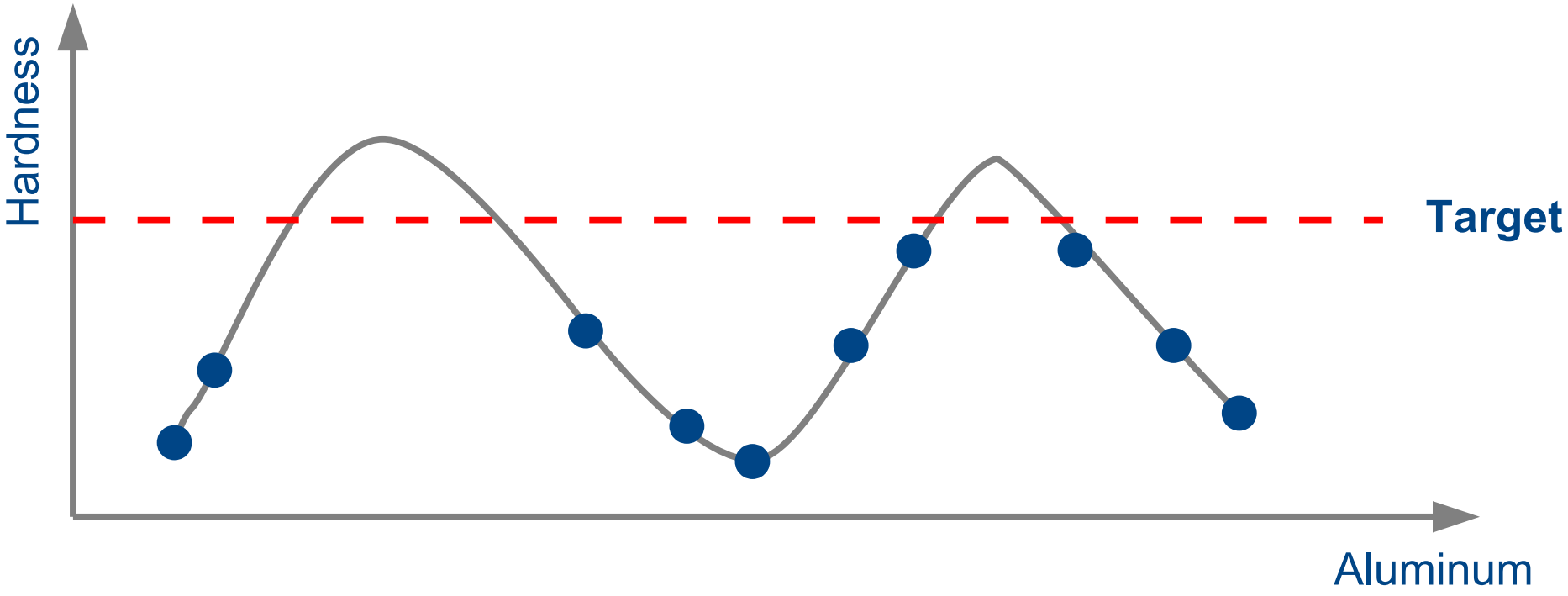
Correlations between properties



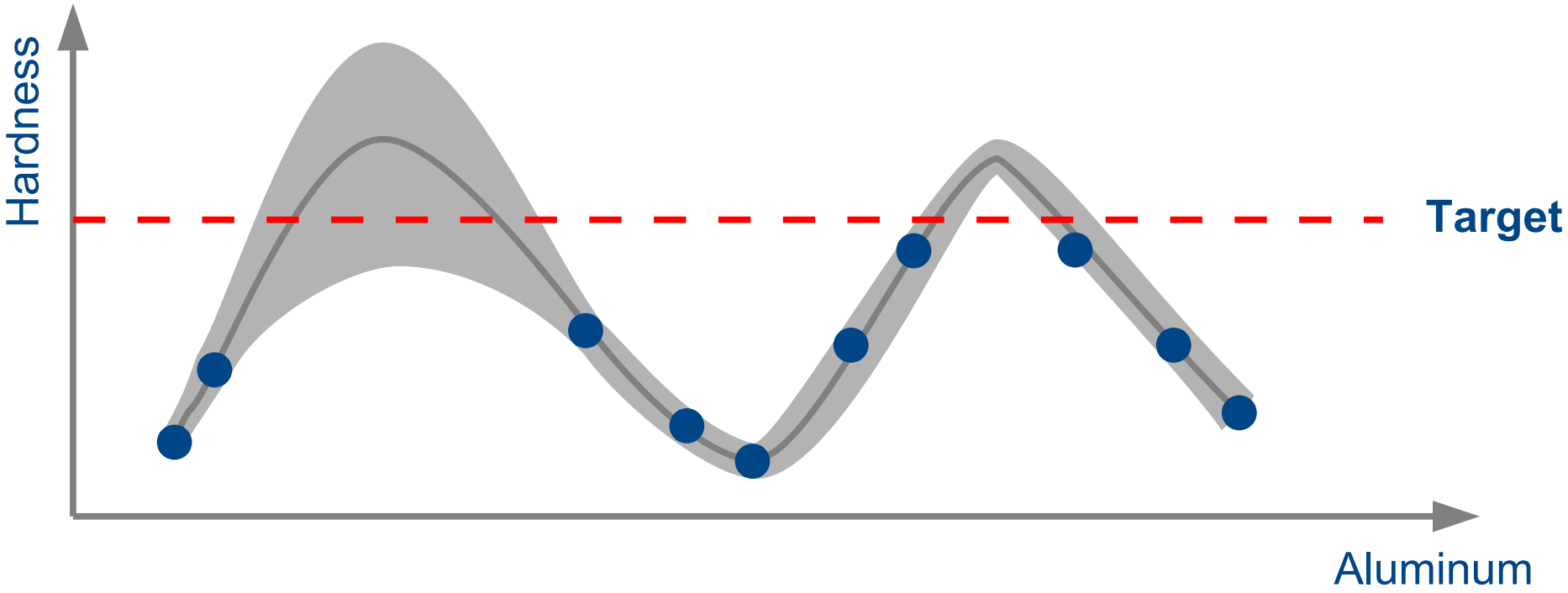
Prediction of uncertainty



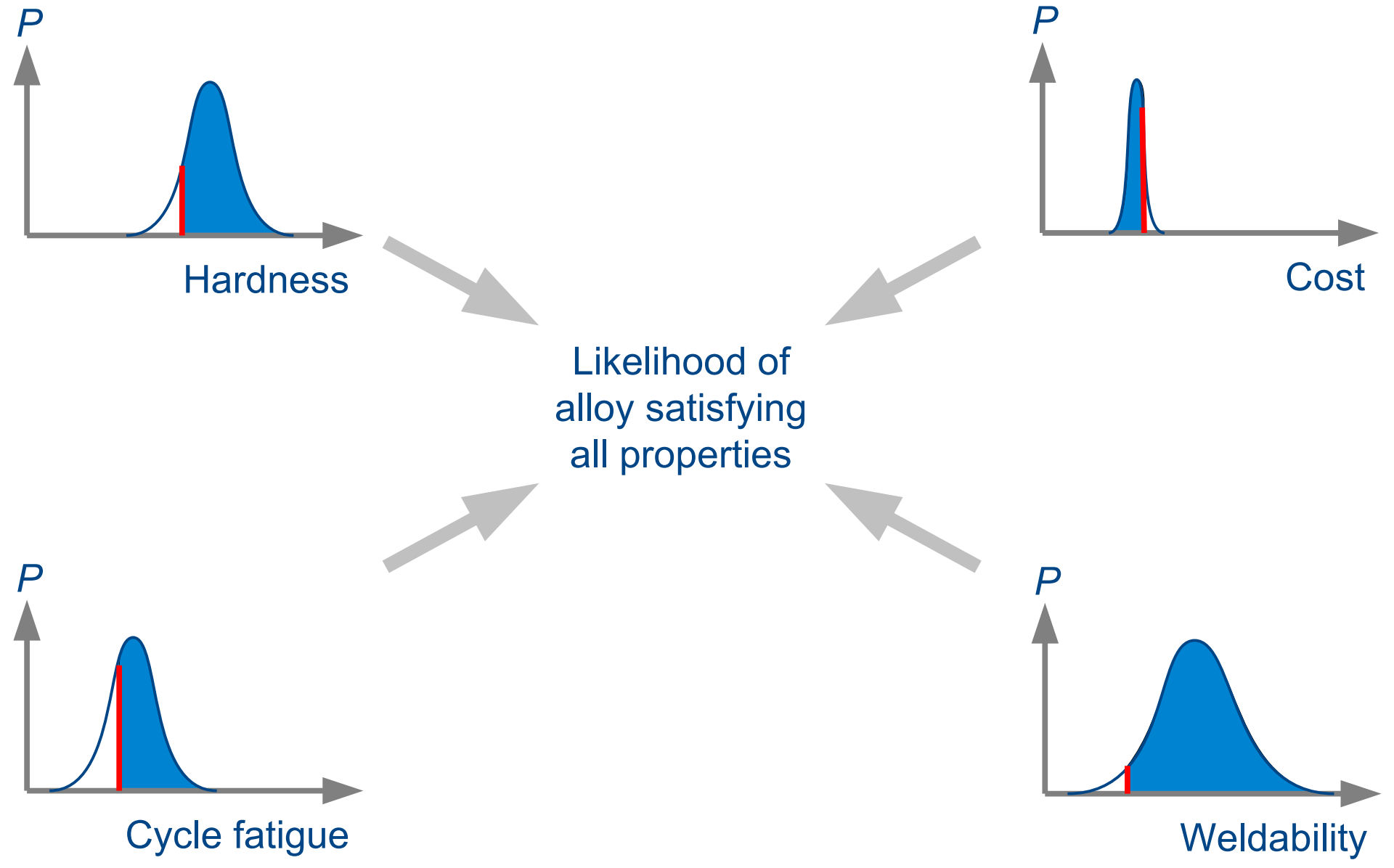
Prediction of uncertainty



Prediction of uncertainty



Combining likelihood



Industrial applications of neural network tool

DFT and experimental

SAMSUNG

DFT and experimental

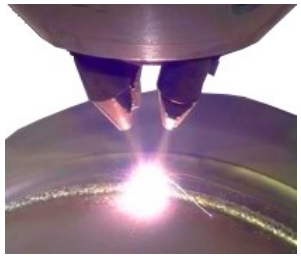
bp

Quantum mechanics and experimental

Lake Shore CRYOTRONICS

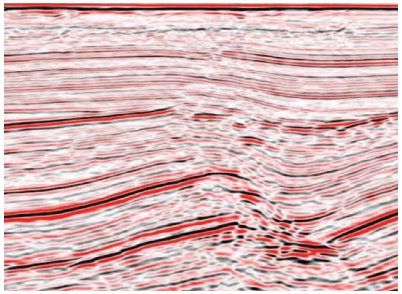
Industrial applications of neural network tool

DFT, common experimental, and rare experimental



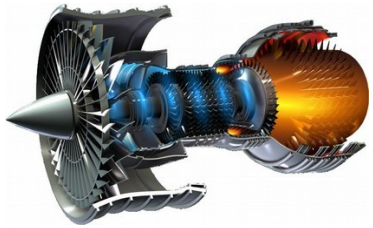
Fluid mechanics

Oil discovery

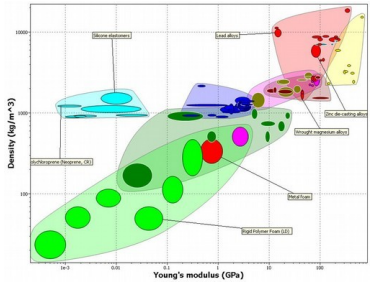


Industrial applications of neural network tool

Experimental

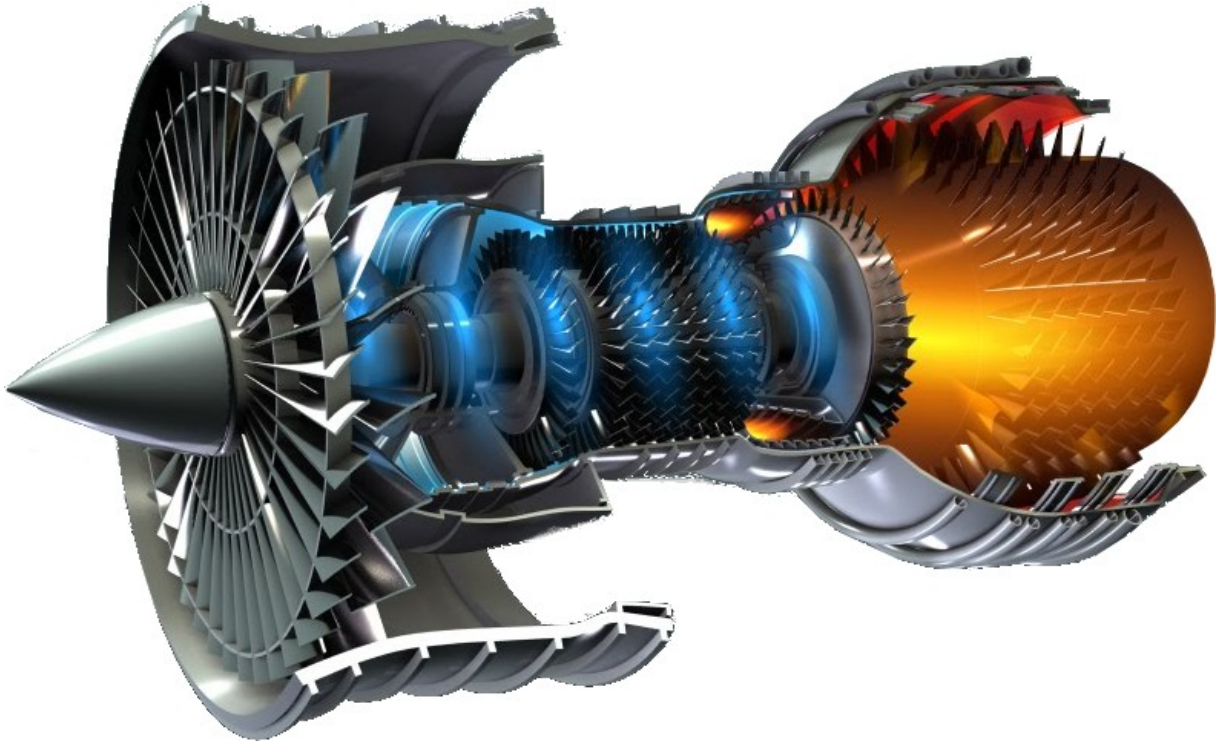


Experimental



Structural and experimental

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%

Proposed alloy composition

Cr:15.8

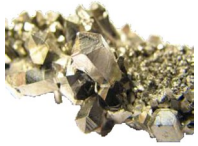
Co: 20.0

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

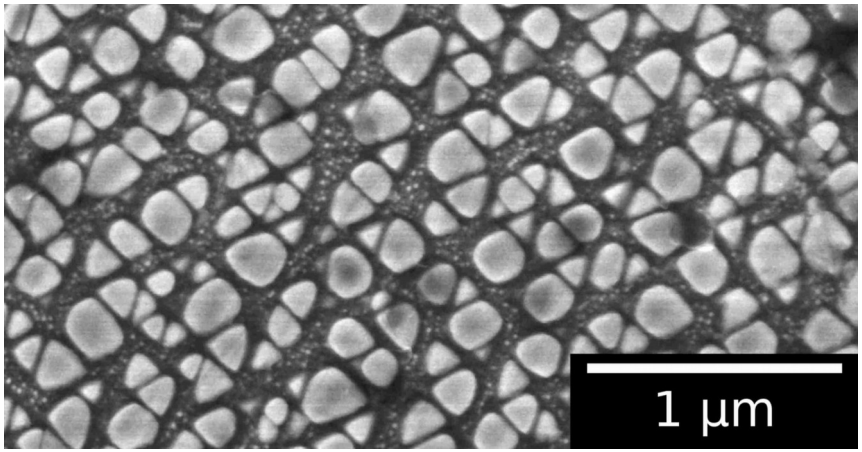
Zr: 0.18

Ni: 47.2

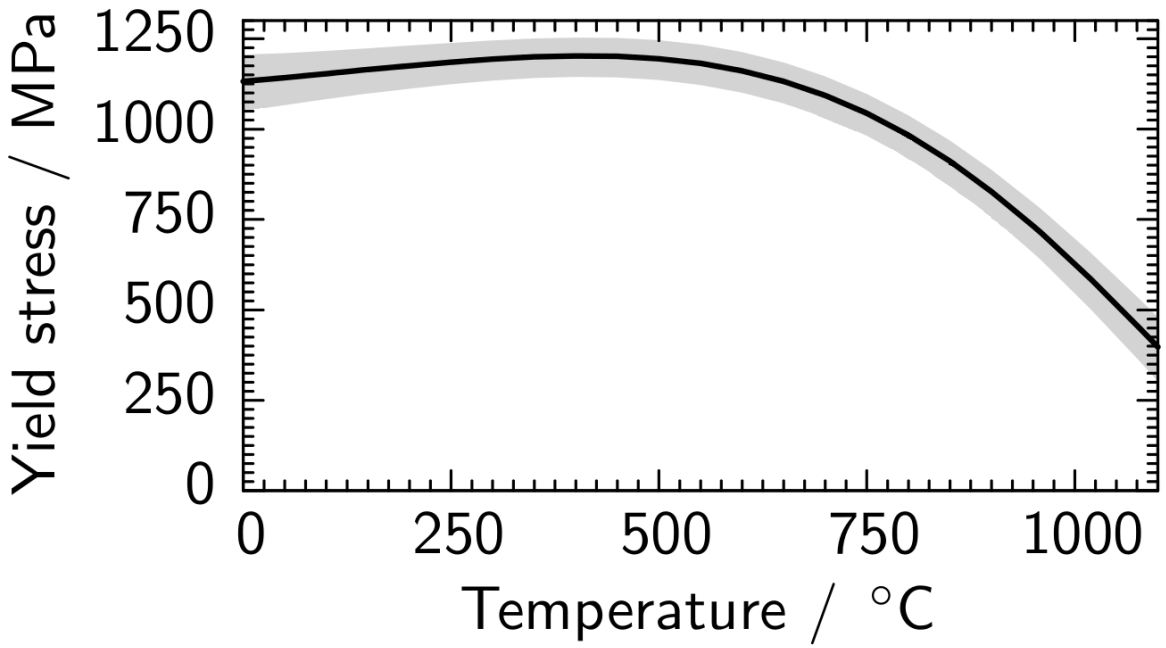
900ºC

30 hours

Microstructure

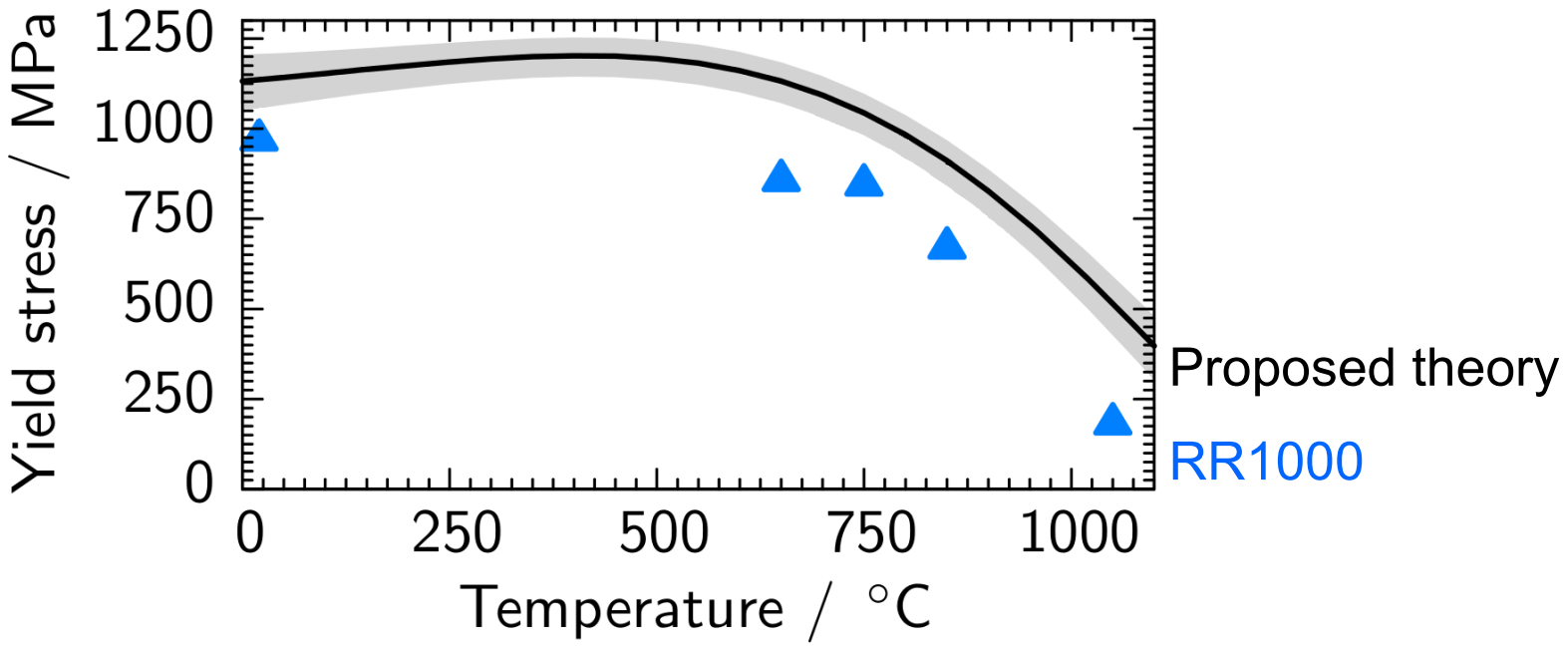


Testing the yield stress

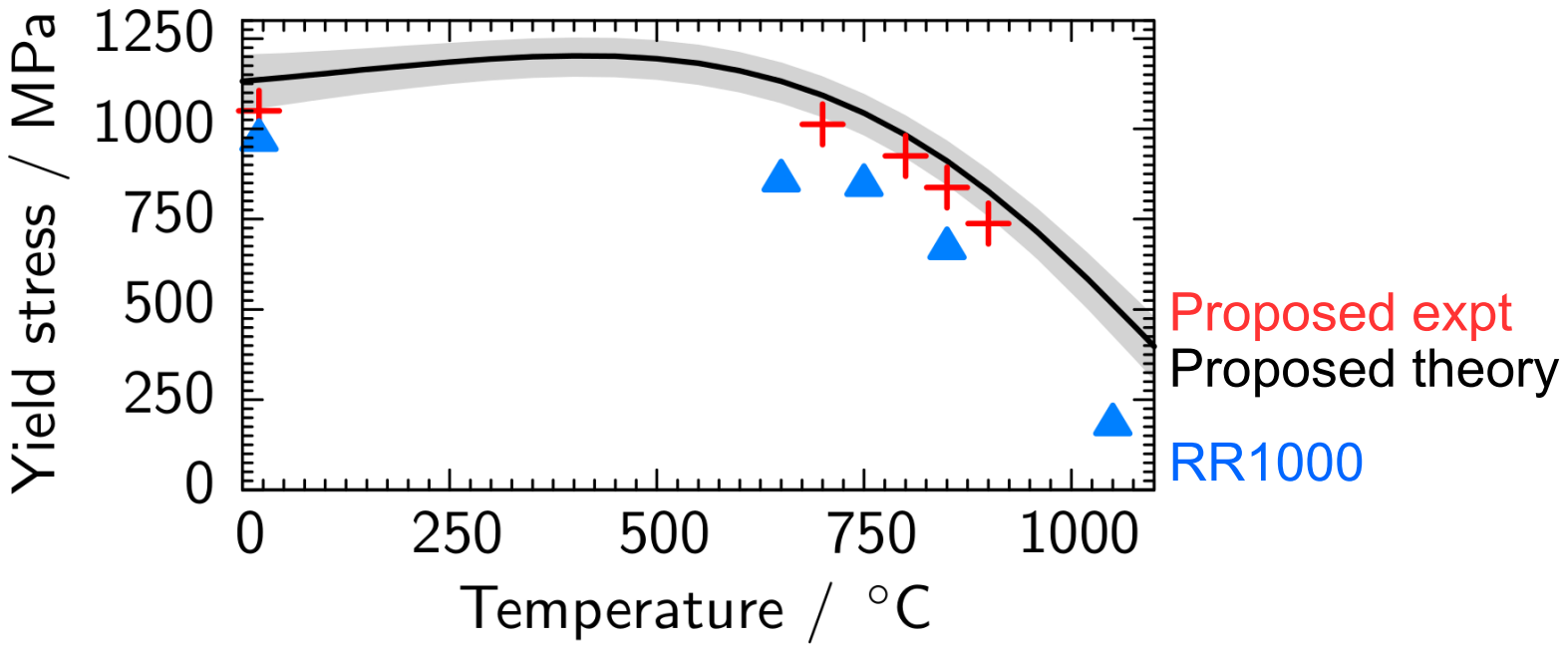


Proposed theory

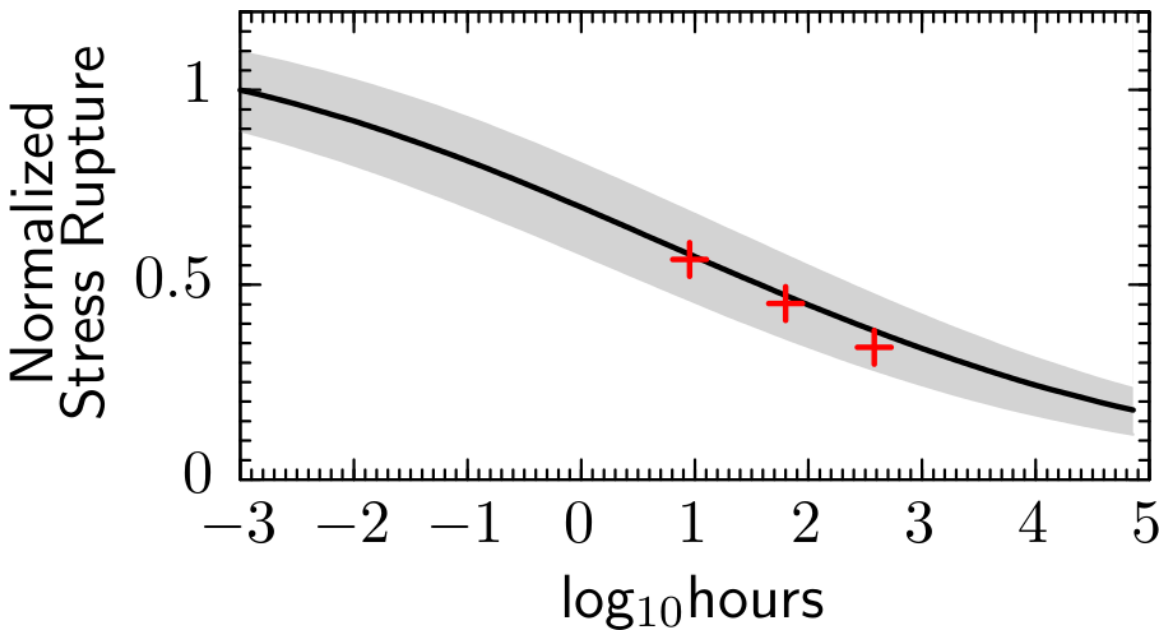
Testing the yield stress



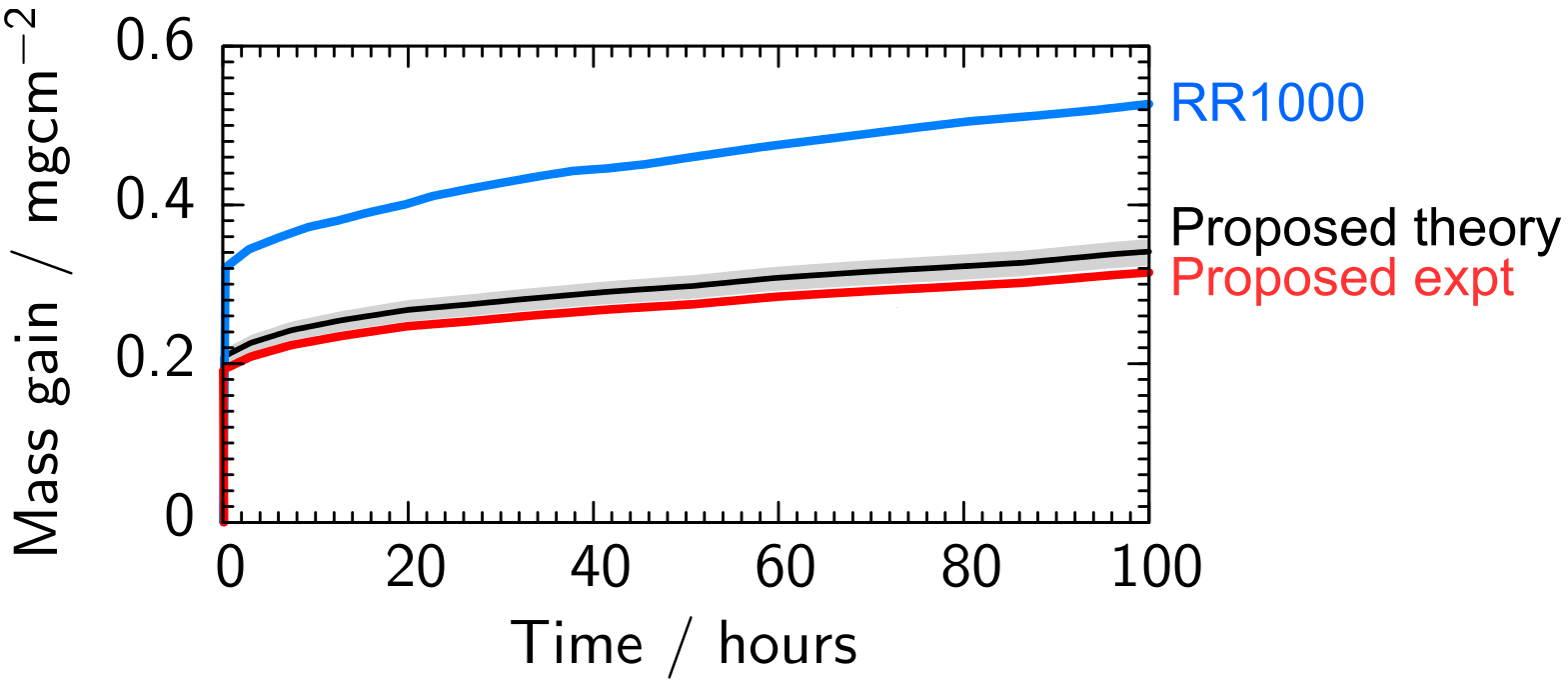
Testing the yield stress



Testing stress rupture

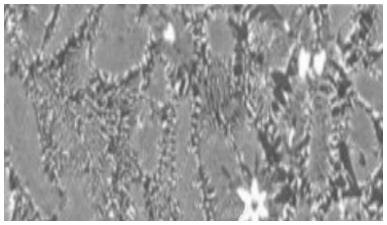


Testing the oxidation resistance

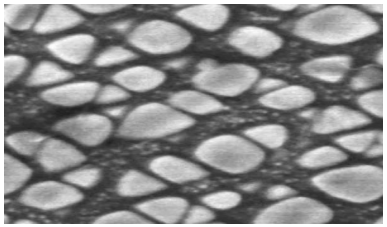


Alloys discovered

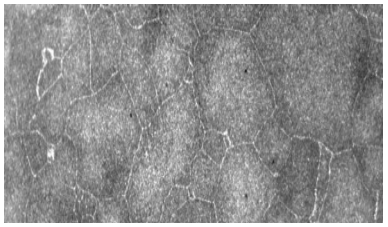
Cr-Cr_2Ta alloys
Intermetallics, 48, 62



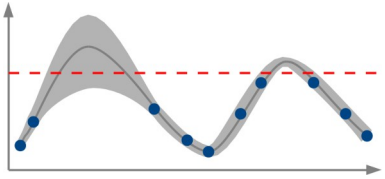
Combustor alloy
GB1408536



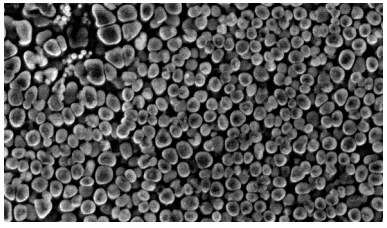
RR1000 grain growth
Acta Materialia, 61, 3378



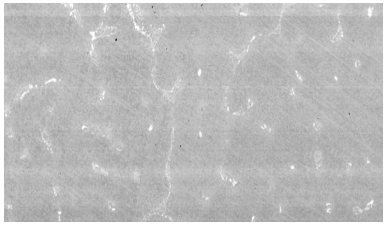
Discovery algorithm
EP14153898
US 2014/177578



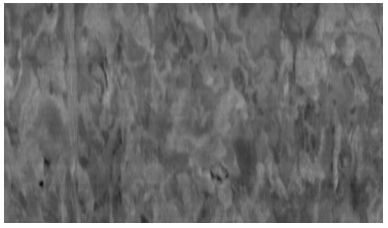
Ni disc alloy
EP14157622
US 2013/0052077 A2



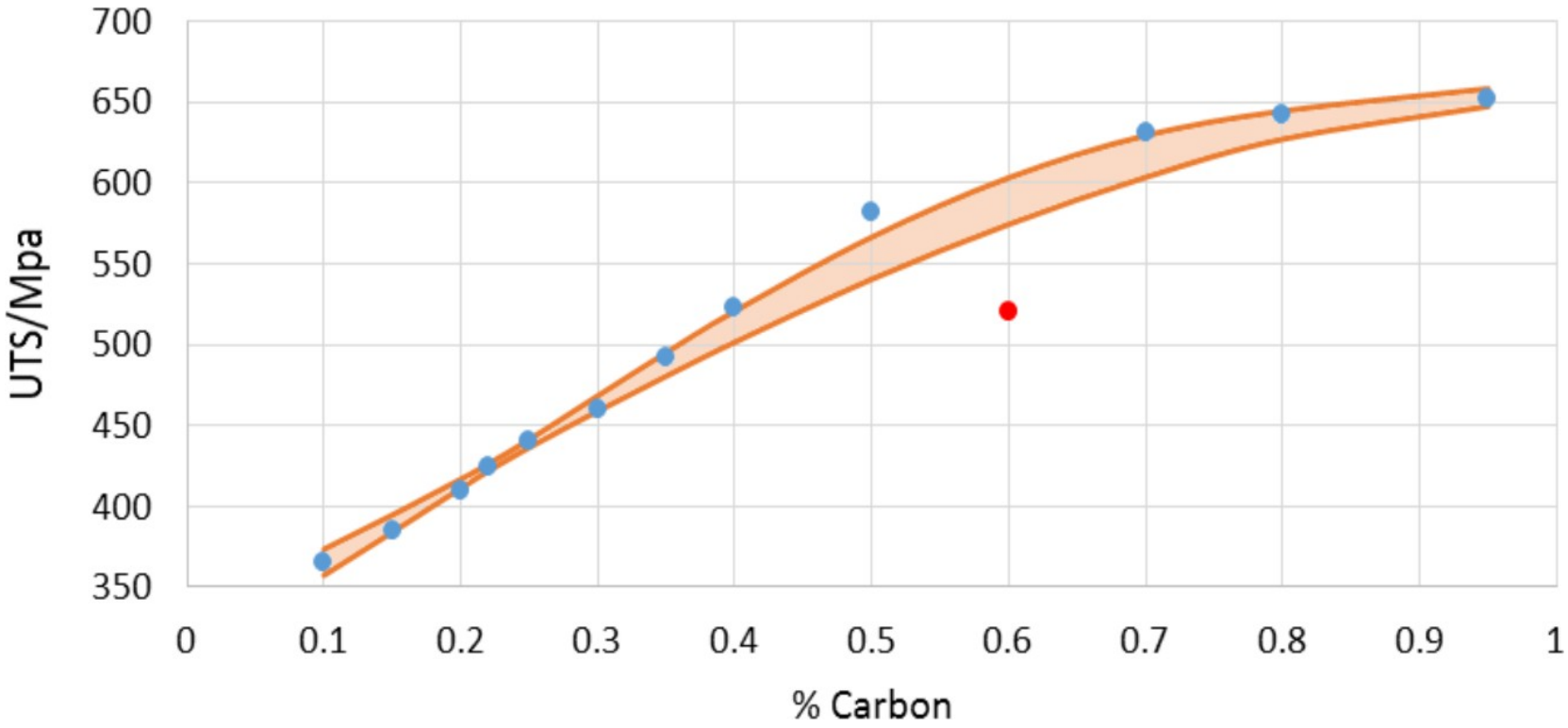
Mo-Hf forging alloy
EP14161255
US 2014/223465



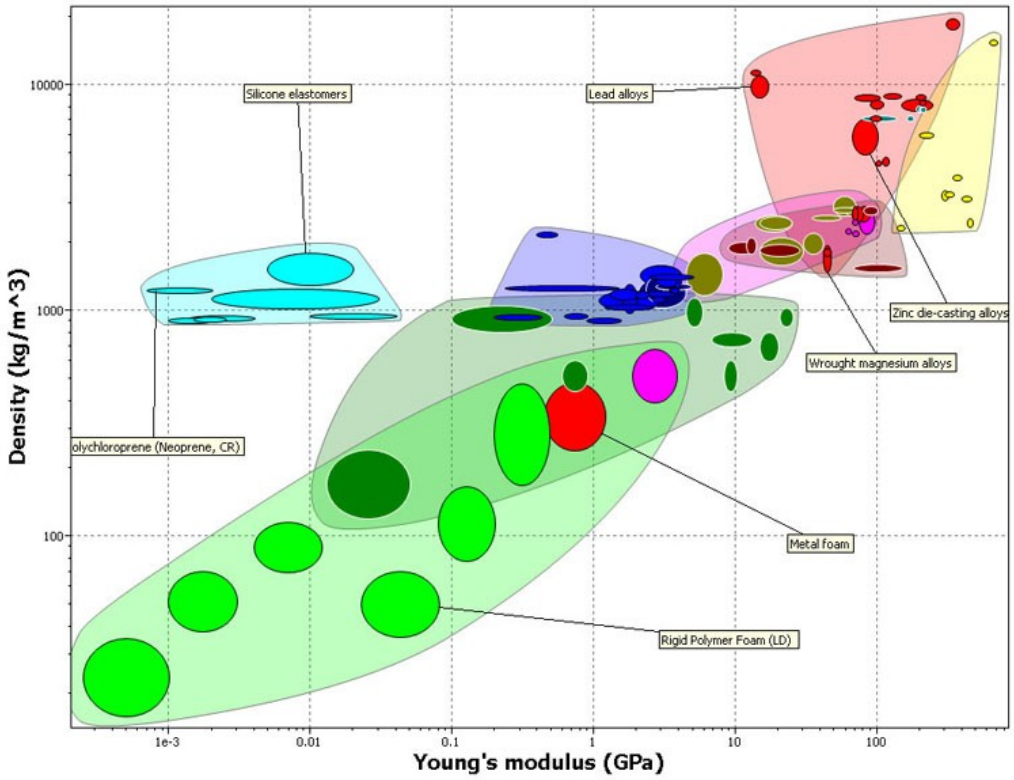
Mo-Nb forging alloy
EP14161529
US 2014/224885



Database integrity



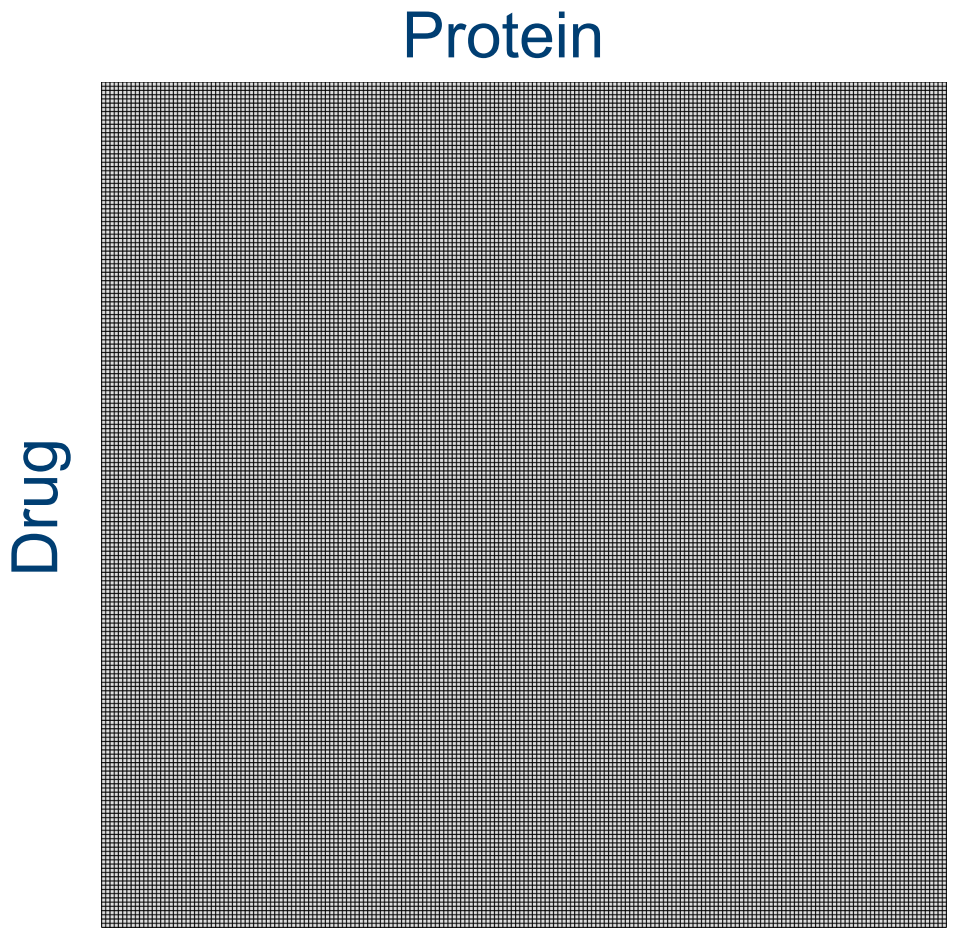
Database integrity



Found 792 erroneous points confirmed against primary sources

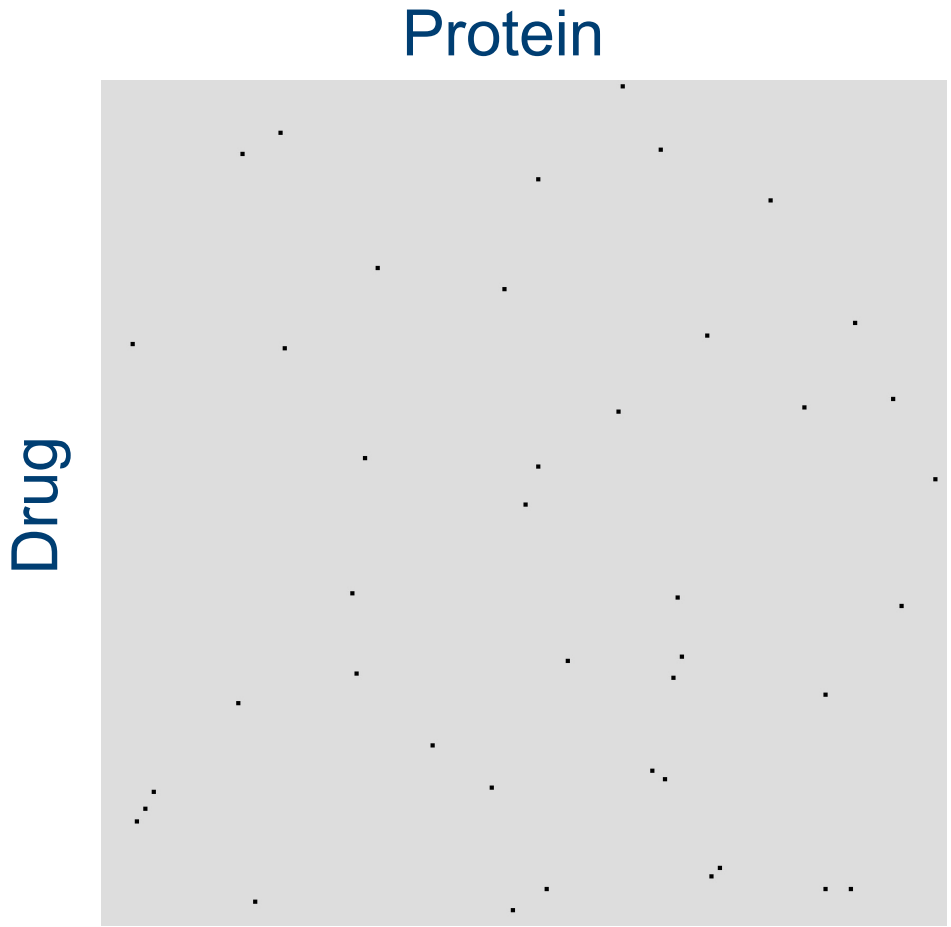
Protein activity database

Database contains 10,000 proteins and 2,000,000 compounds



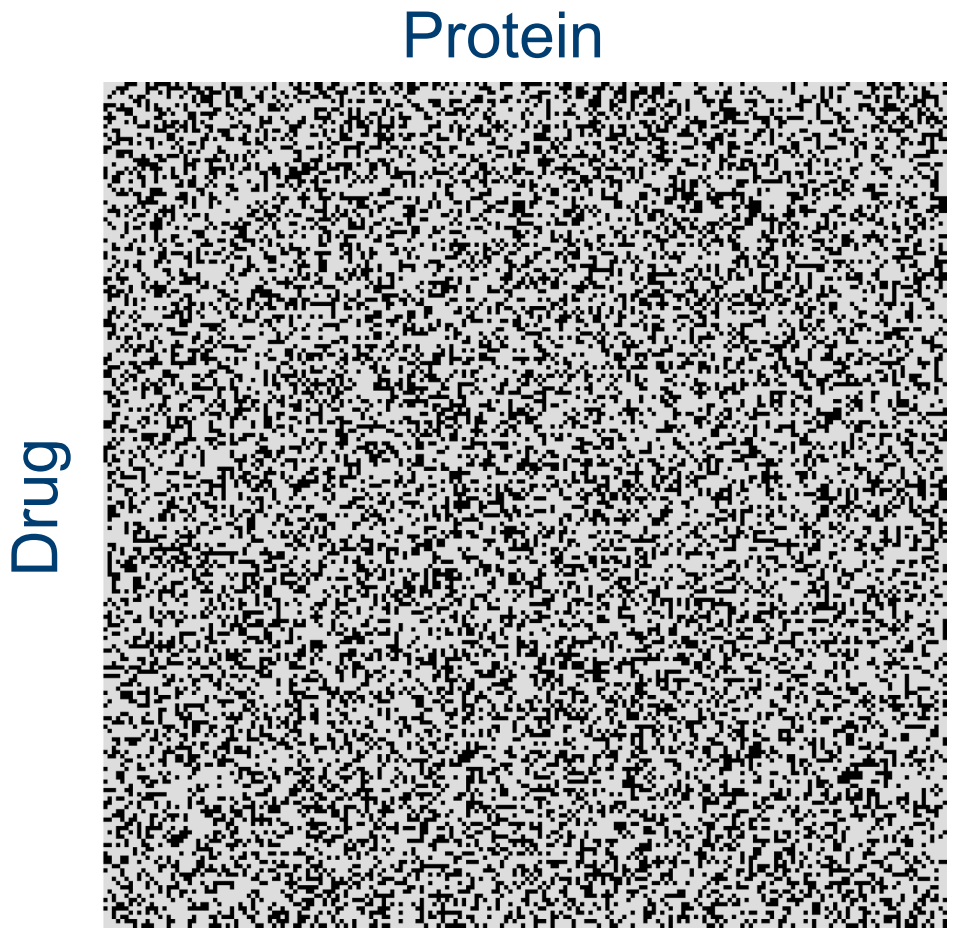
Protein activity data

Database has protein activity for 0.1% of entries



Protein activity data

Filled in 32% of the data points with 75% accuracy



Summary

Used artificial intelligence to discover materials and drugs

Handle fragmented data

Merge experiments and simulations into holistic design tool

Worked with 7 different companies, formed startup intellegens