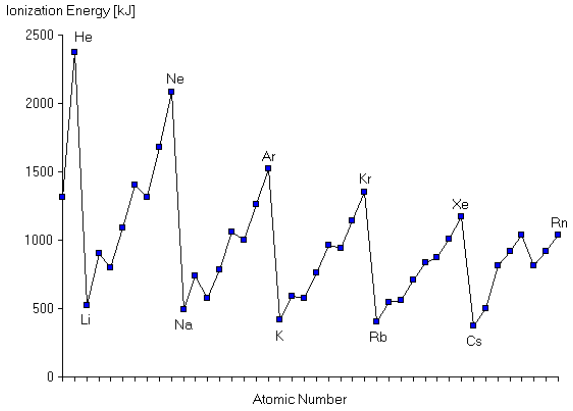
UNIVERSITY OF CAMBRIDGE

Who needs atoms to design materials?

Gareth Conduit

Theory of Condensed Matter Group, Department of Physics

Approaches to materials design



Experiment

Physical laws

Computer simulation

Materials design

A deep neural network algorithm that

Reduces product development costs

Accelerates product to market

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

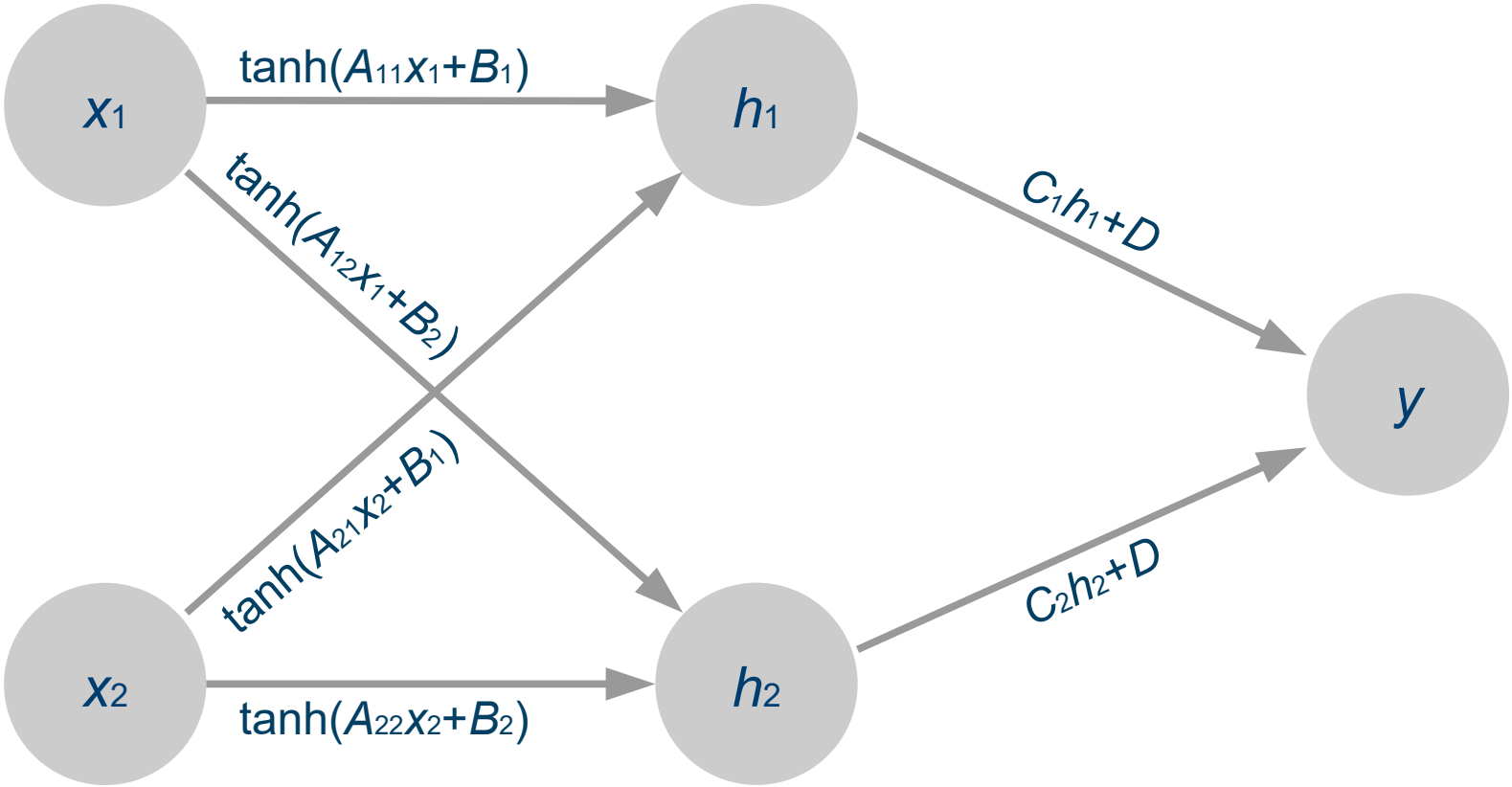
Neural networks: first train

Neural networks: then predict

Unique neural network: train on fragmented data

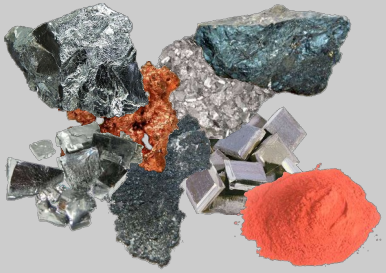
Unique neural network: predict on fragmented data

Neural networks: mathematical form



Neural networks for materials design

Composition



Artificial intelligence

Properties

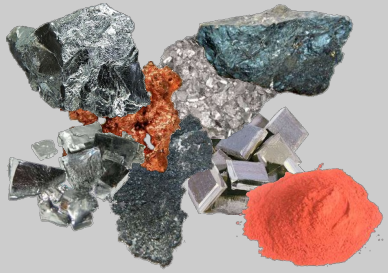
UTS

Hardness

Cost

Neural networks for materials design

Composition



Artificial intelligence

Properties

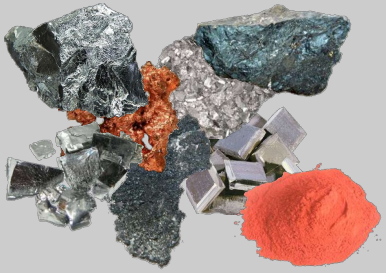
UTS

Hardness

Cost

Neural networks for materials design

Composition



Properties

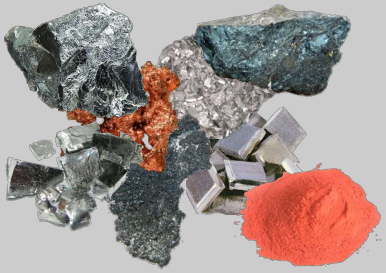
UTS

Hardness

Cost

Neural networks for materials design

Composition



Properties

UTS

Hardness

Cost

Simulations

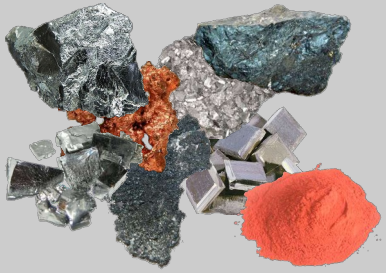
Density Functional

Molecular dynamics

Finite element

Artificial intelligence

Composition



Properties

UTS

Hardness

Cost

Simulations

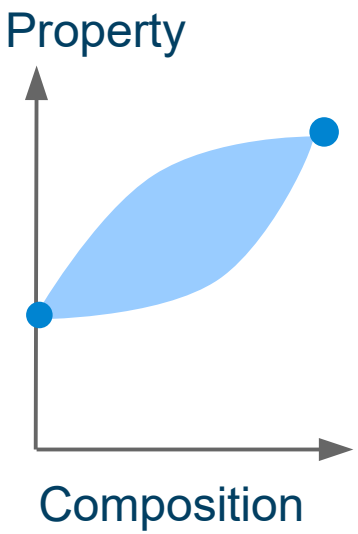
Density Functional

Molecular dynamics

Finite element

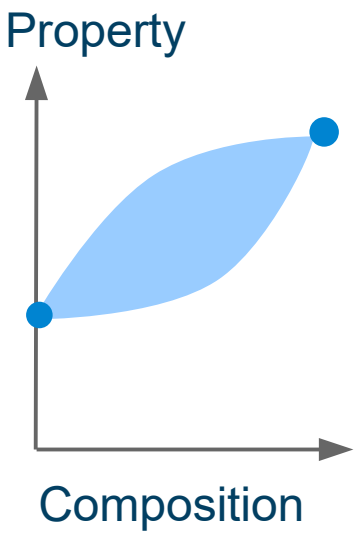
Combine databases with neural networks

Experiment

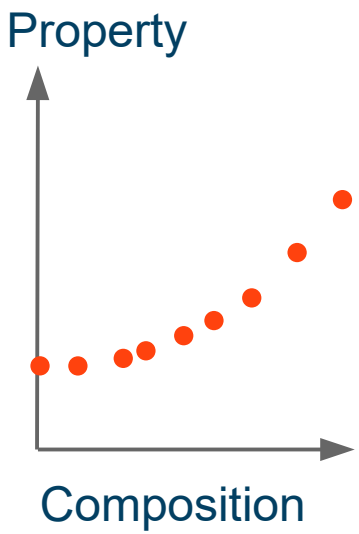


Combine databases with neural networks

Experiment



Simulation

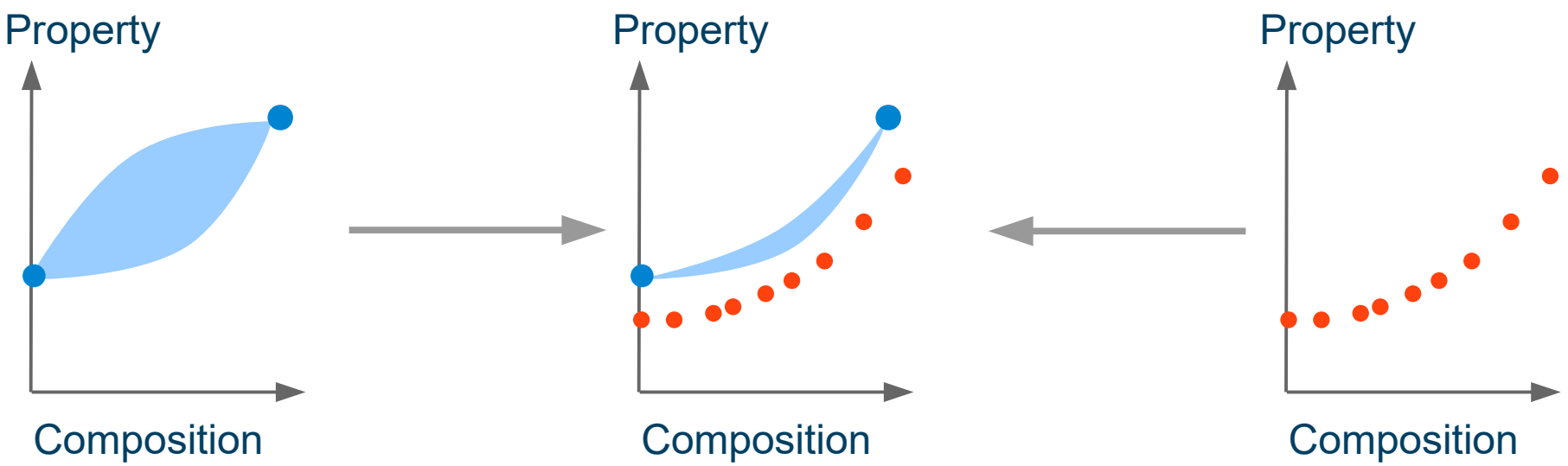


Combine databases with neural networks

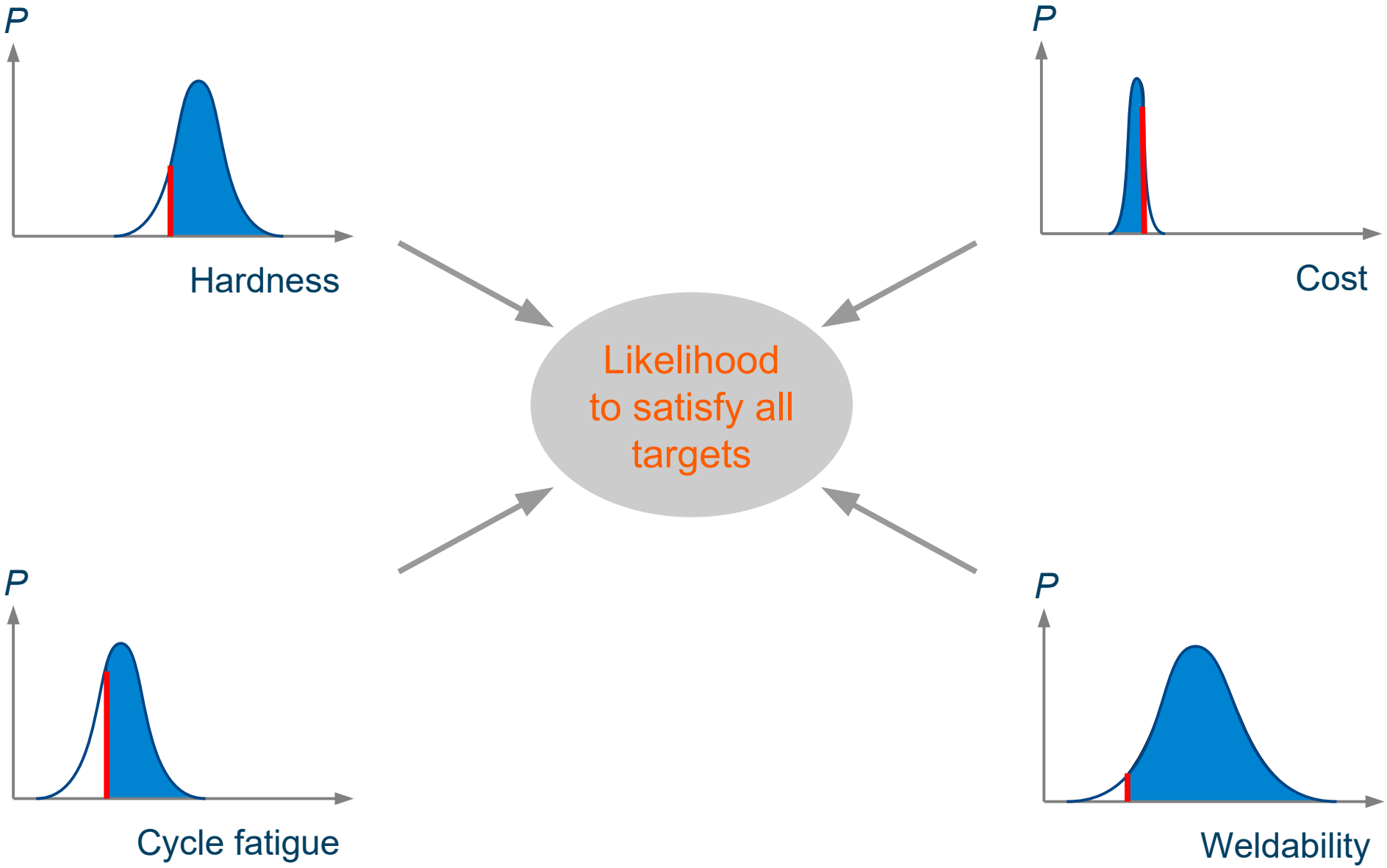
Experiment

Combined

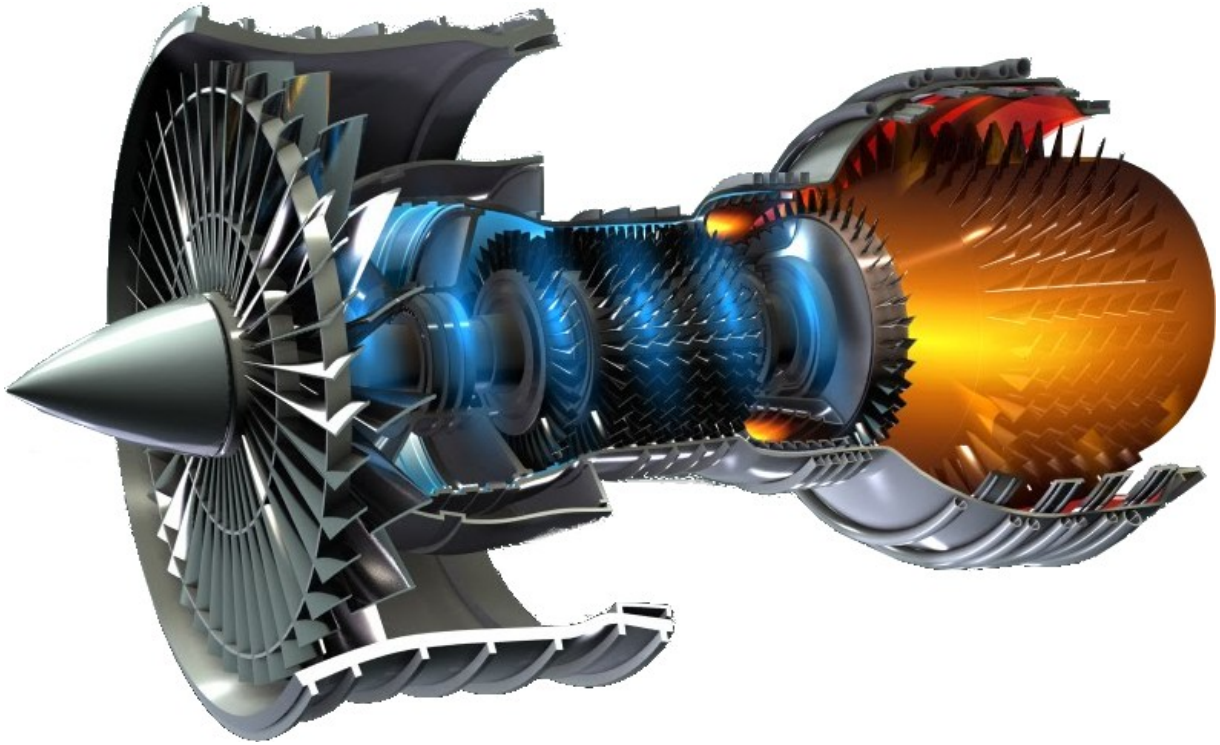
Simulation



Combining likelihood



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

Cr:15.8

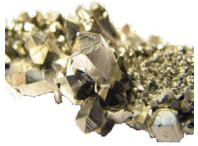
Co: 20.0

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

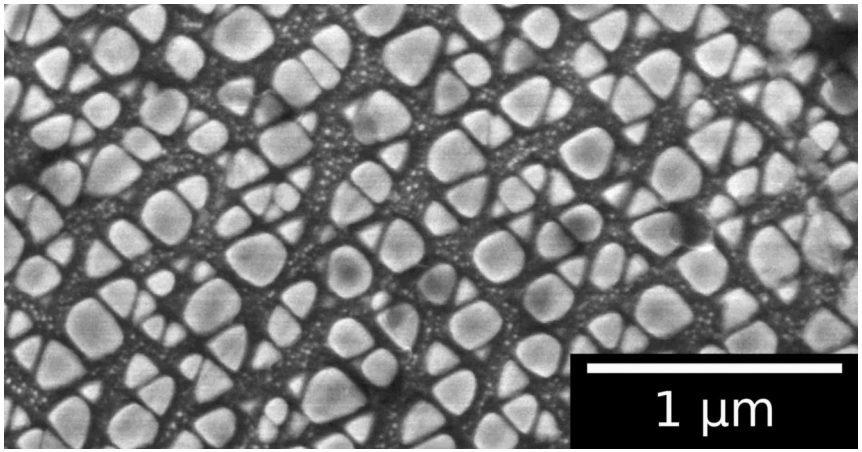
Zr: 0.18

Ni: 47.2

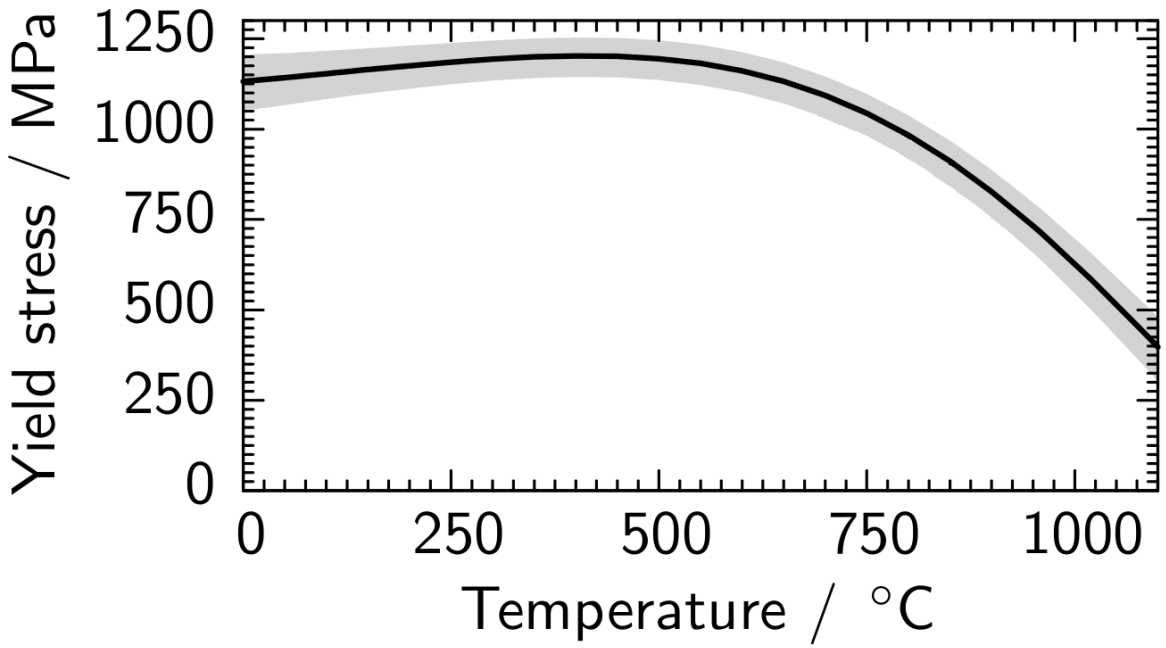
900ºC

30 hours

Microstructure

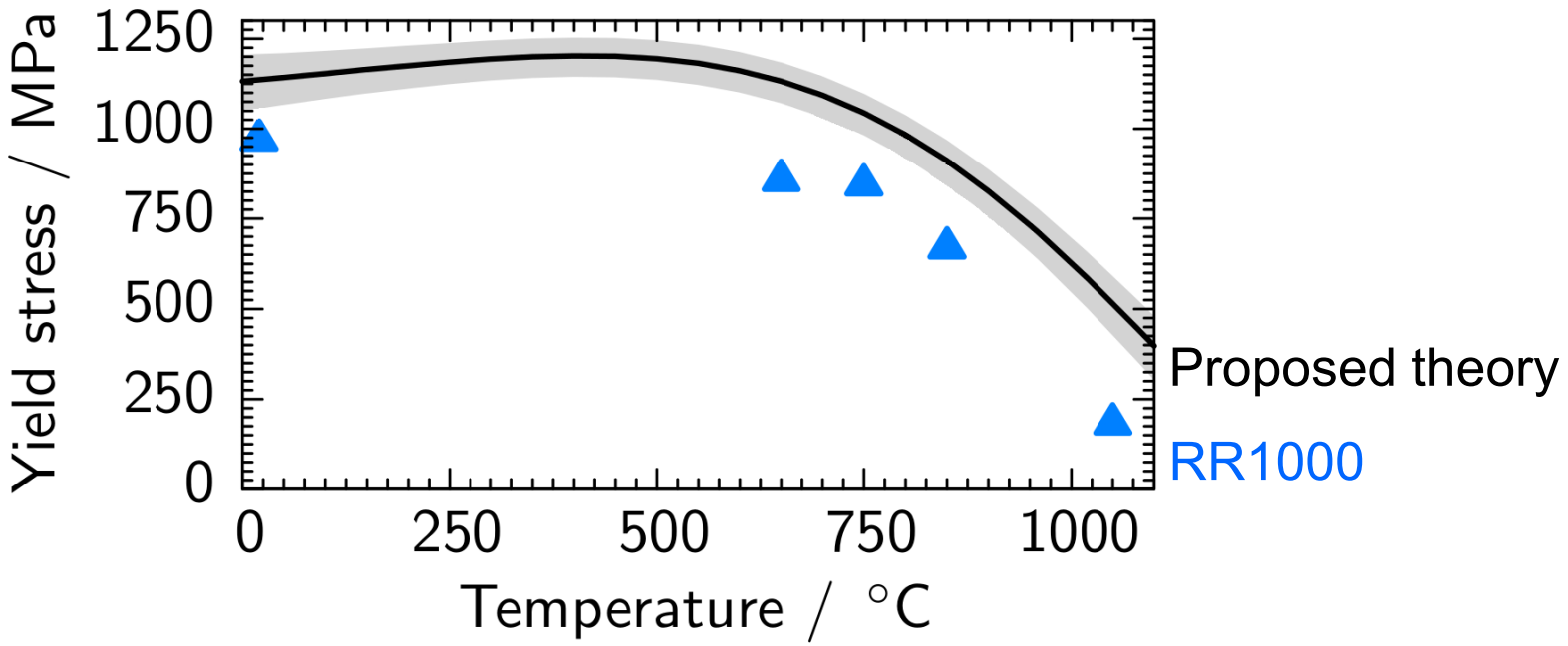


Testing the yield stress

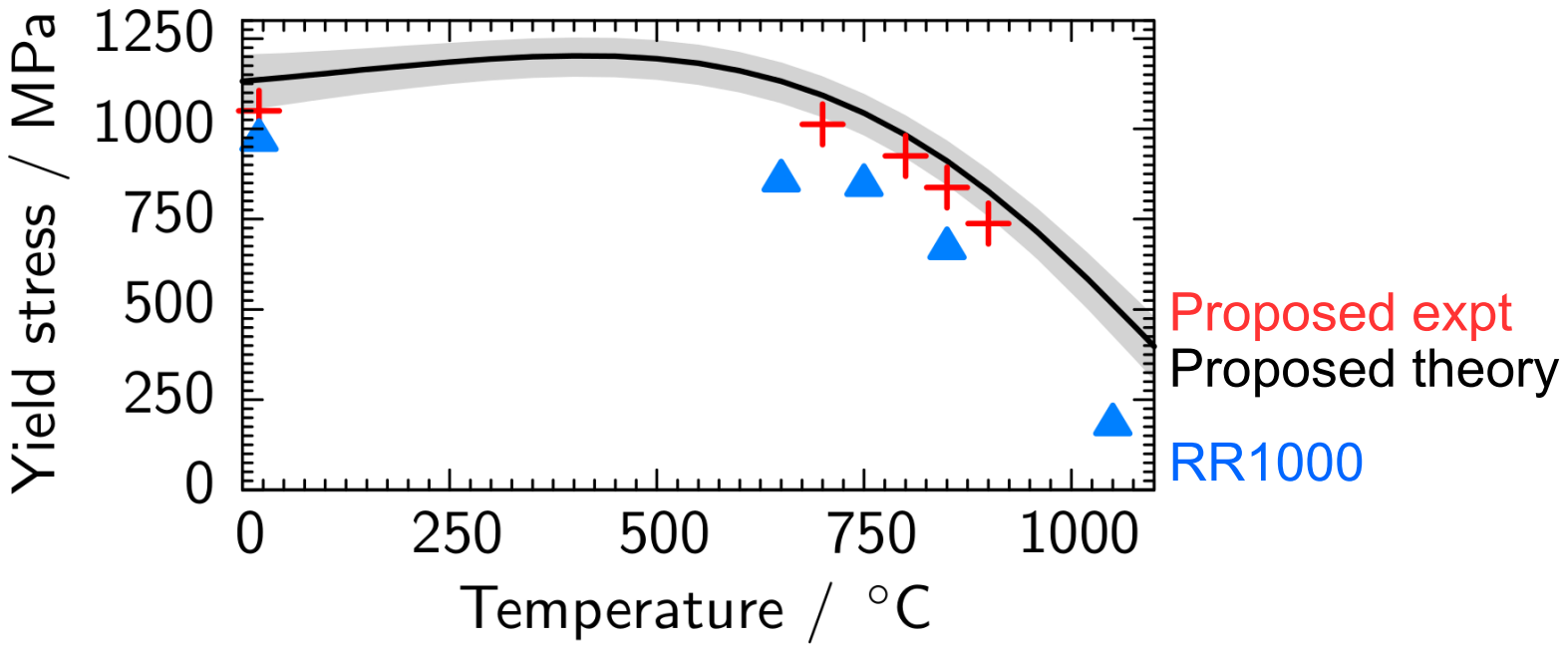


Proposed theory

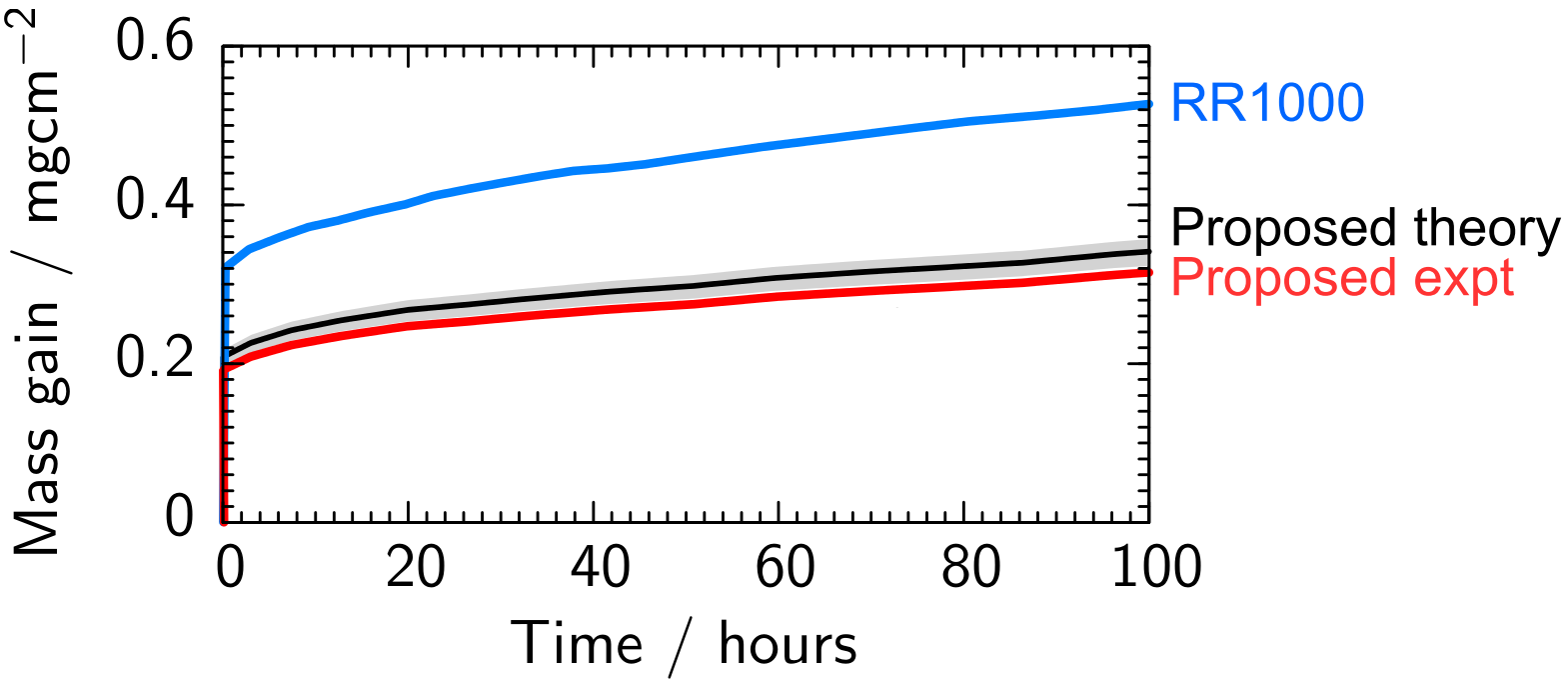
Testing the yield stress



Testing the yield stress

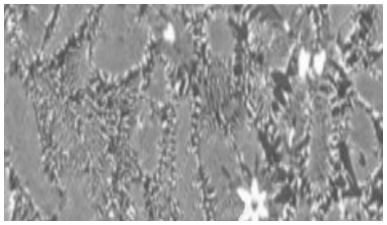


Testing the oxidation resistance

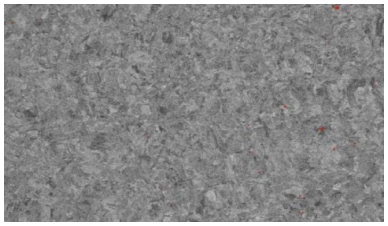


High temperature alloys discovered

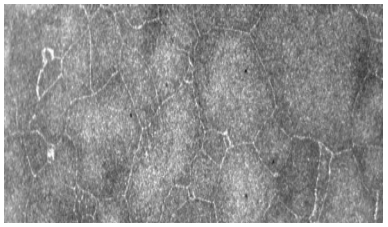
Cr-Cr_2Ta alloys
Intermetallics, 48, 62



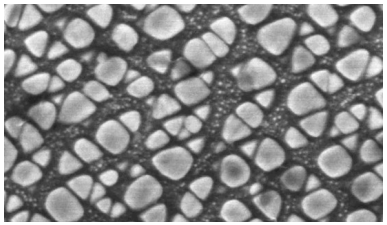
Combustor alloy
GB1408536



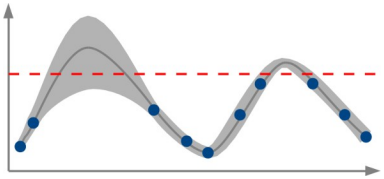
RR1000 grain growth
Acta Materialia, 61, 3378



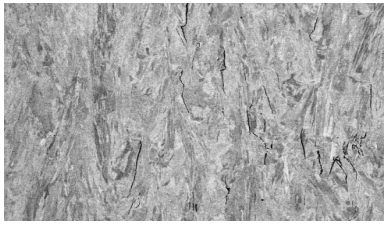
Ni alloy
Materials & Design, 131, 258



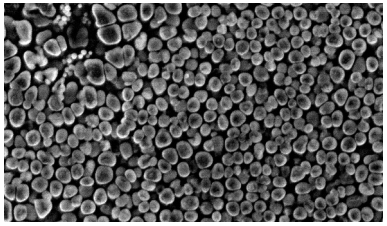
Discovery algorithm
EP14153898
US 2014/177578



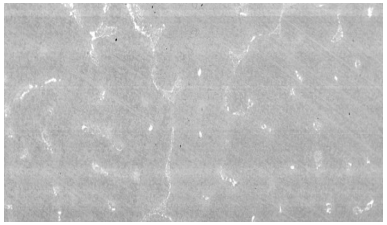
Ni alloy for additive manufacture



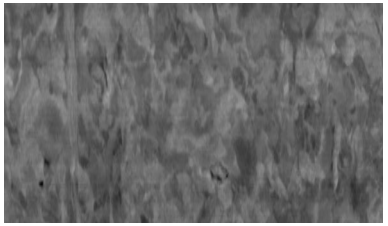
Ni disc alloy
EP14157622
US 2013/0052077 A2



Mo-Hf forging alloy
EP14161255
US 2014/223465

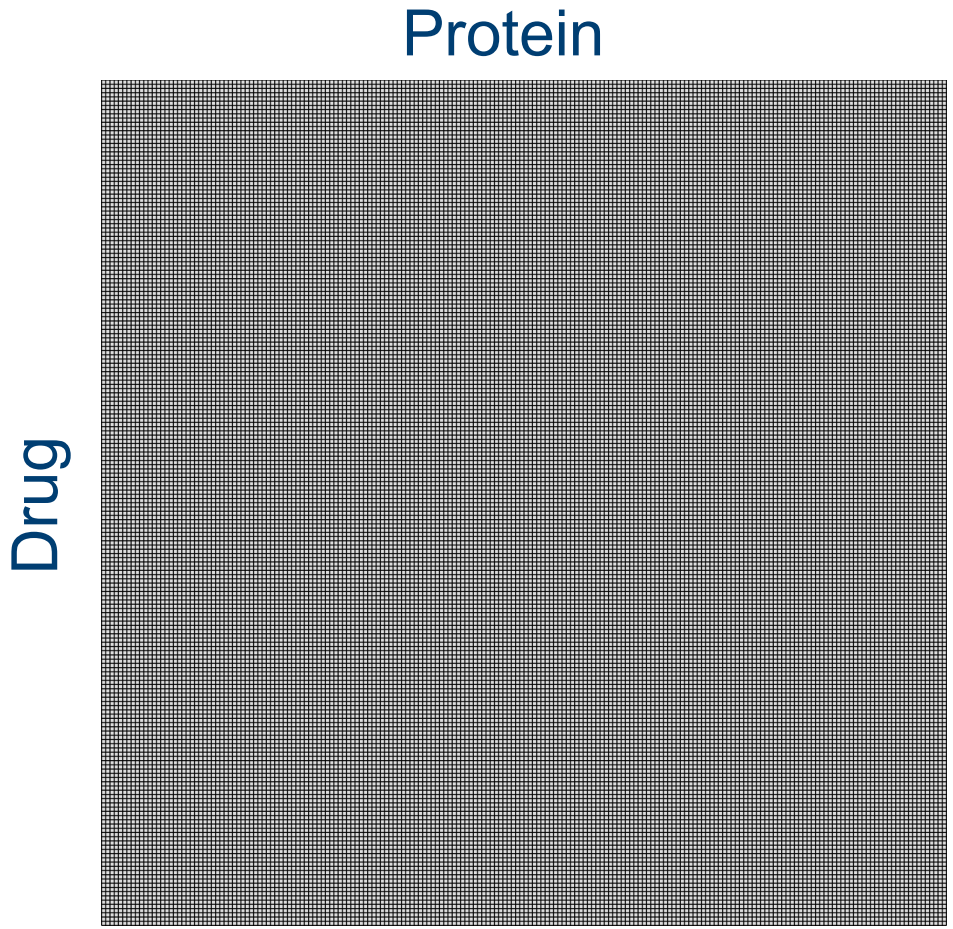


Mo-Nb forging alloy
EP14161529
US 2014/224885



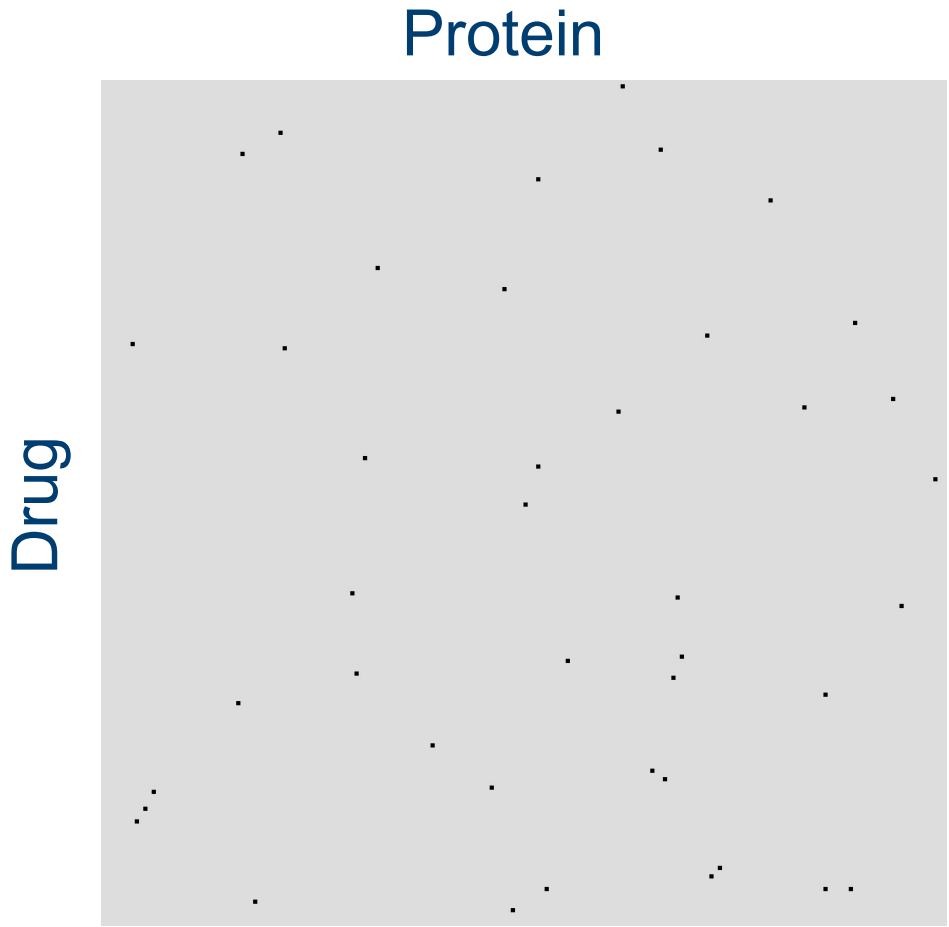
Protein activity database

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



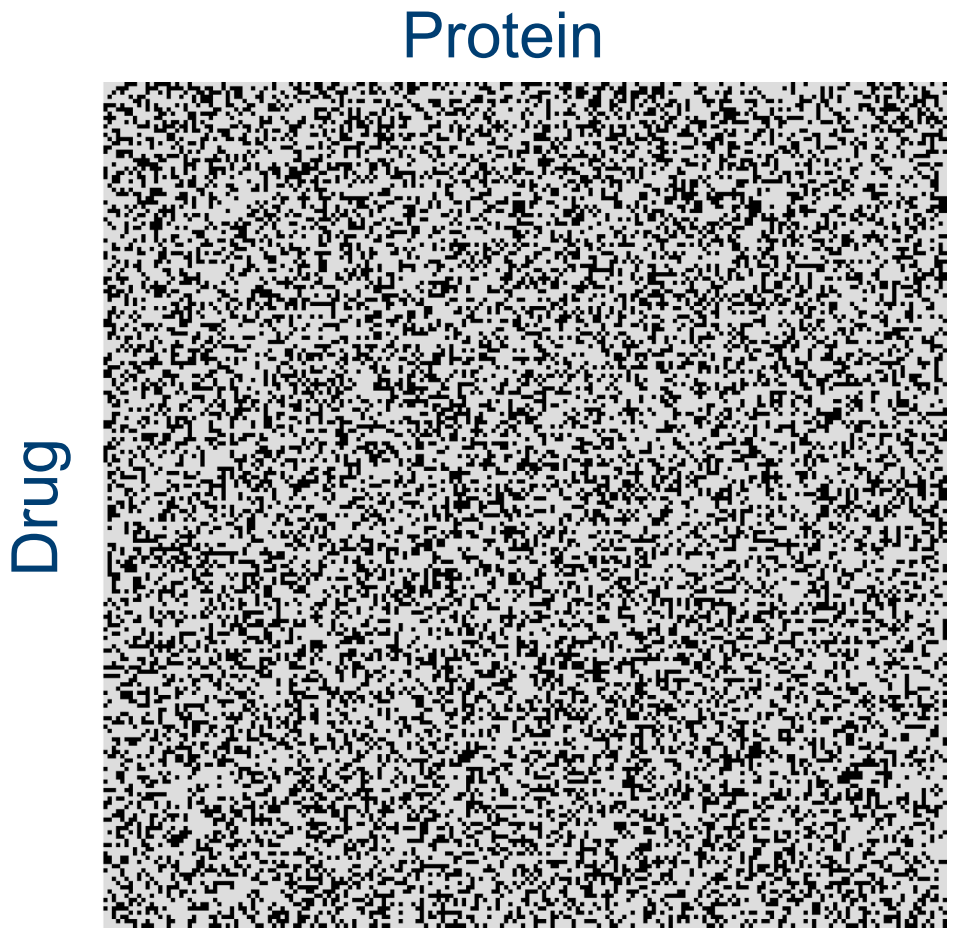
Protein activity data

Database has protein activity for 0.1% of entries



Protein activity data

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



Drug discovery

Data for protein activity with compound

e-therapeutics

Drug discovery

Data for protein activity with compound

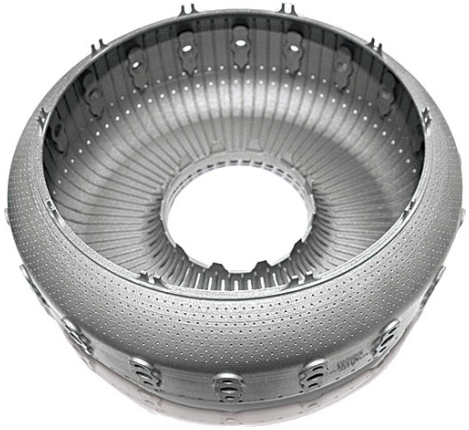
Include additional information about drug structure

Increased drug data available 400-times,
saving $1billion in experimental costs

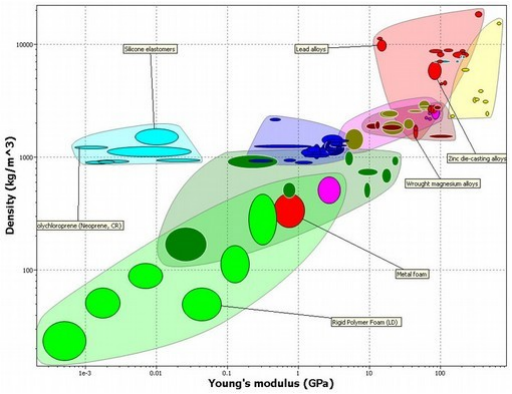
e-therapeutics

Materials design

3D printed alloy
for combustors
Designed from
7 data points



Materials databases
Found 792 errors

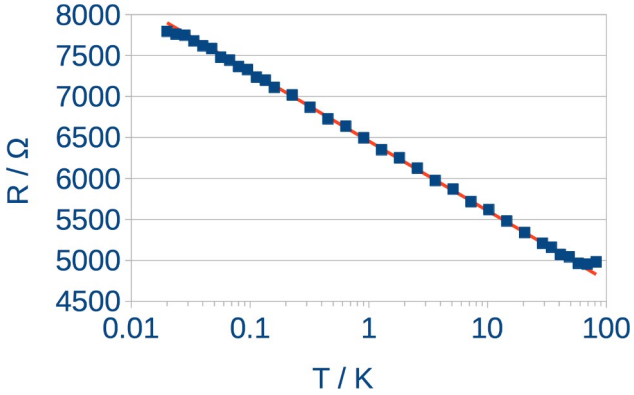


Materials design

Battery design with DFT and experimental data

Designing lubricants with DFT and experimental data

Low temperature thermometer



Summary

Apply deep learning to high-value fragmented data

Cut costs by reducing need for expensive experiments

Discovery and verification in materials and drug discovery

Merge experiments and simulations into holistic design tool

Worked with 7 companies, founded startup intellegens