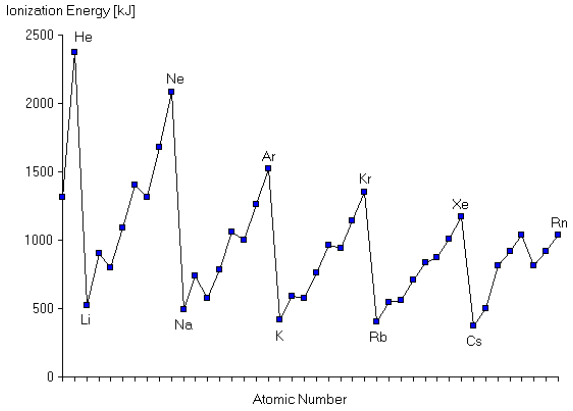
UNIVERSITY OF CAMBRIDGE

Materials design with artificial intelligence

Gareth Conduit

TCM Group, Department of Physics

Approaches to materials design



Experiment

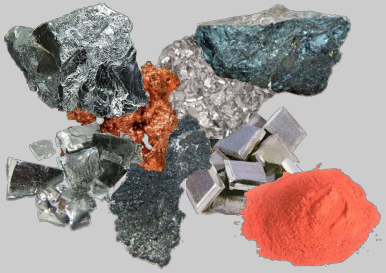
Physical laws

Computer simulation

Materials design

Neural networks for materials design

Composition



Artificial intelligence

Properties

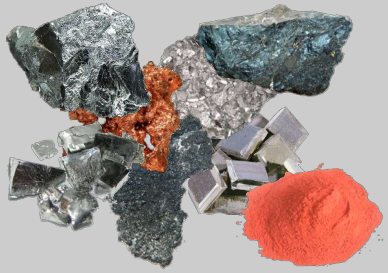
UTS

Hardness

Cost

Neural networks for materials design

Composition



Artificial intelligence

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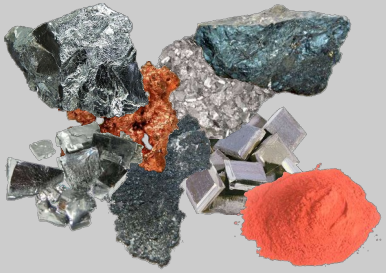

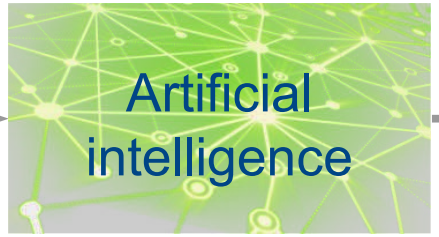

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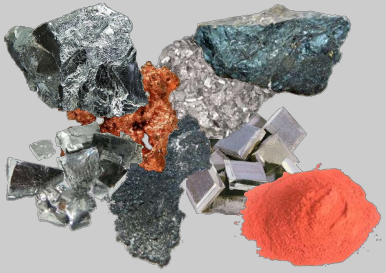


Properties

UTS

Hardness

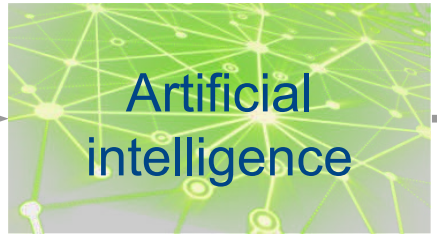
Cost

Simulations

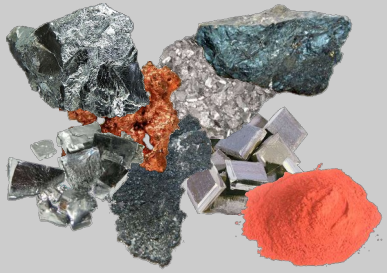
Density Functional

Molecular dynamics

Finite element



Composition



Properties

UTS

Hardness

Cost

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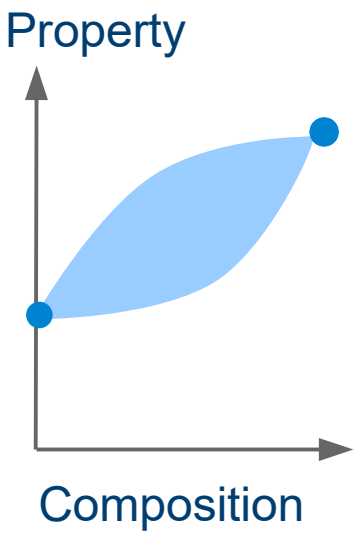
Density Functional

Molecular dynamics

Finite element

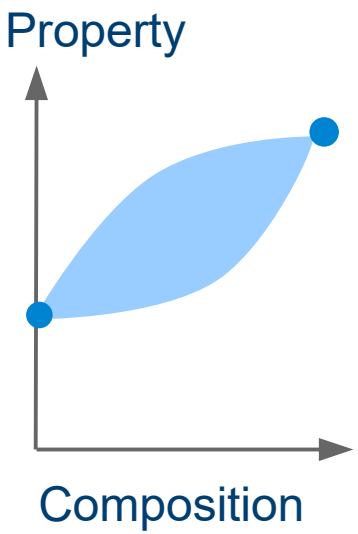
Combine databases with neural networks

Experiment

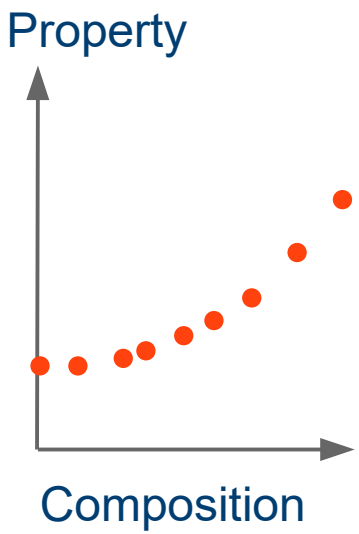


Combine databases with neural networks

Experiment



Simulation

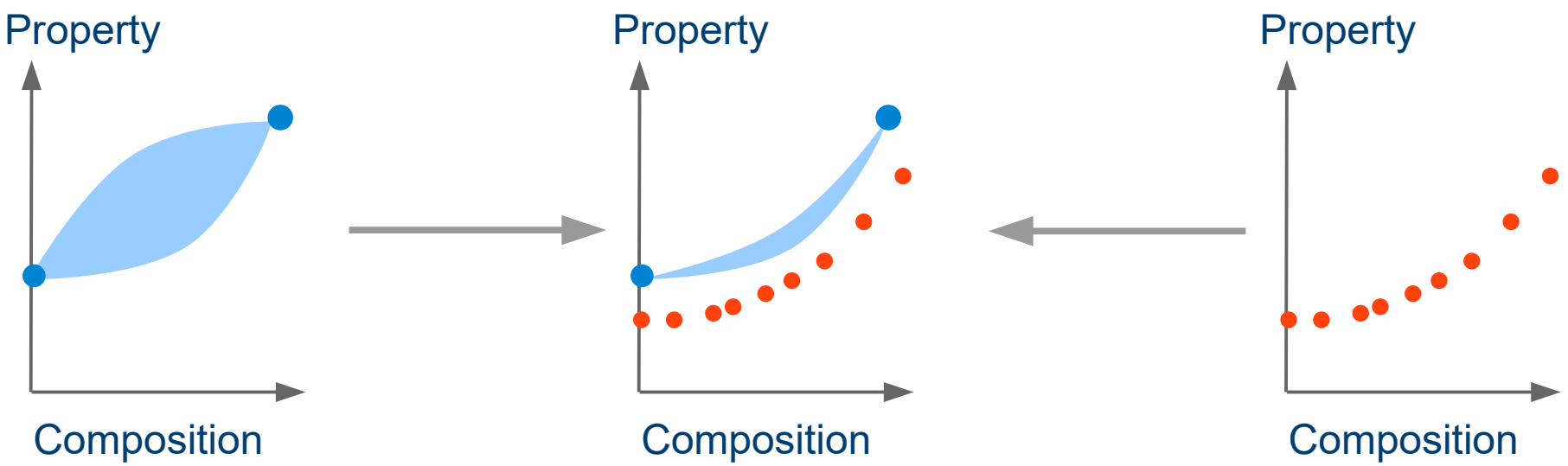


Combine databases with neural networks

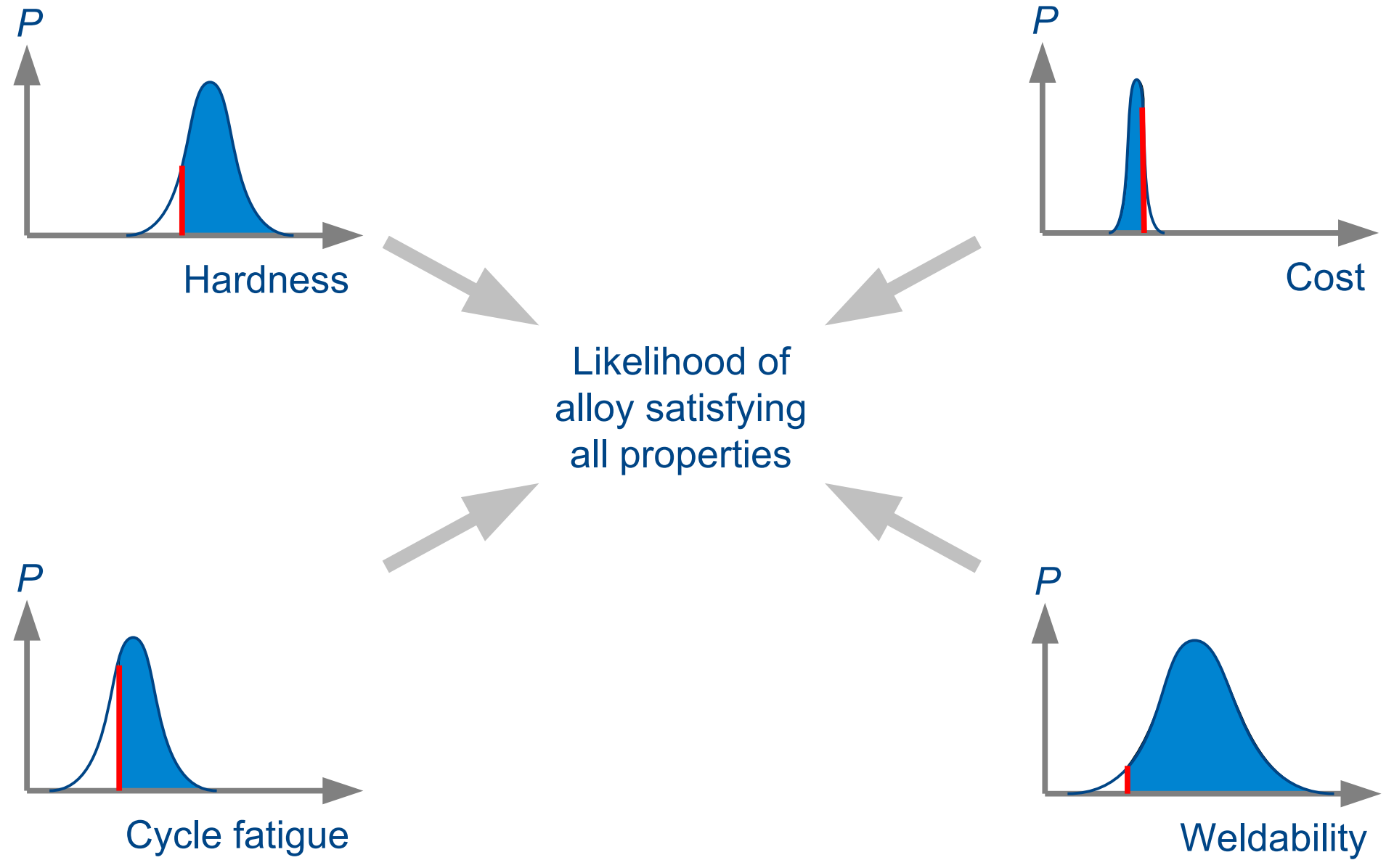
Experiment

Combined

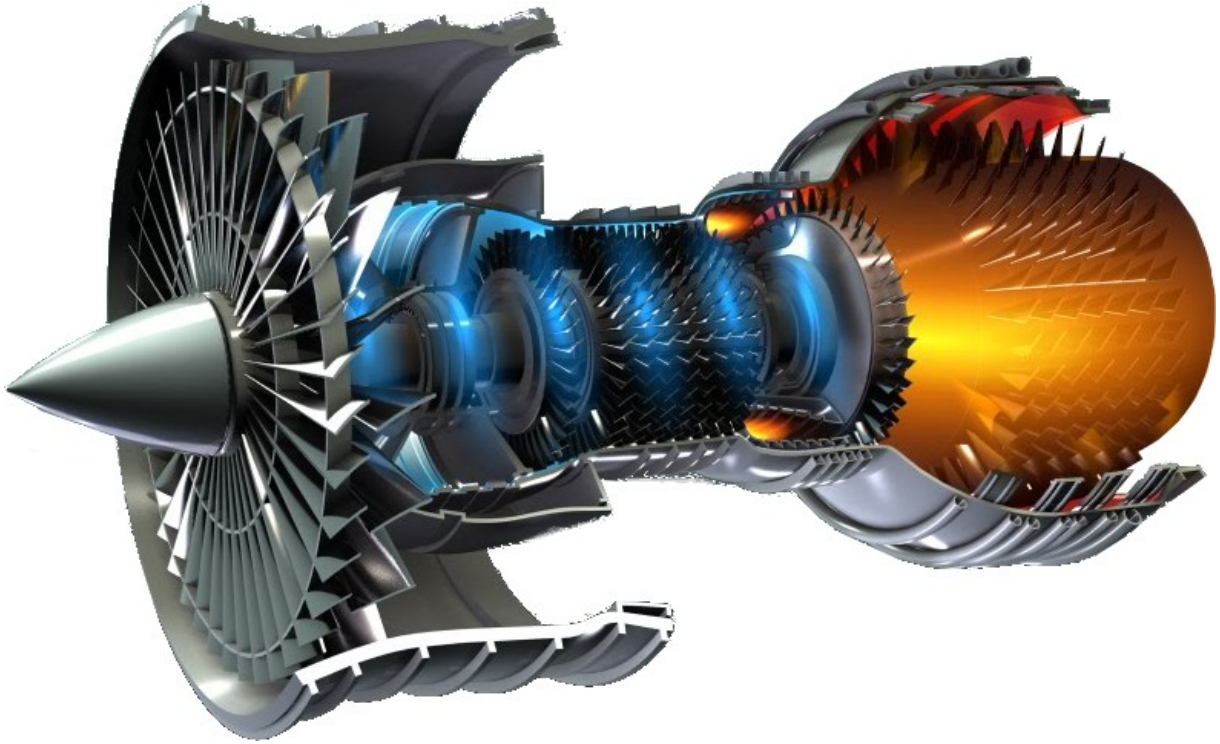
Simulation



Combining likelihood



Schematic of an engine



In press for Materials & Design (2017)

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

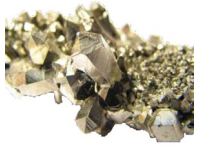
Co: 20.0

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

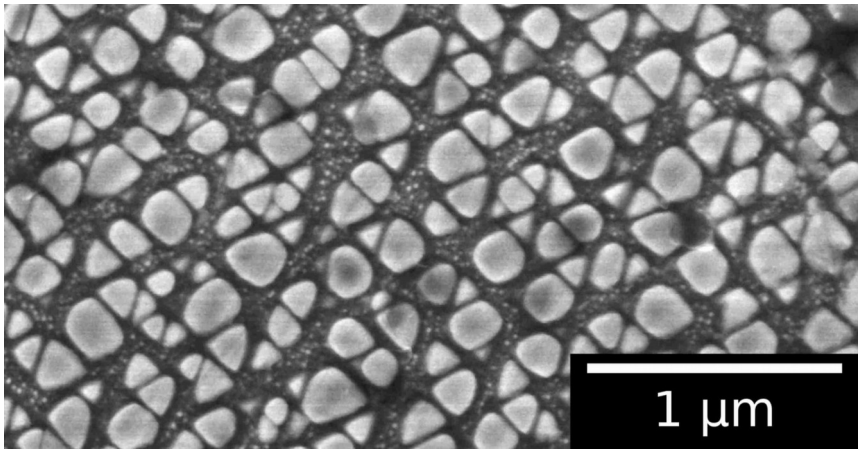
Zr: 0.18

Ni: 47.2

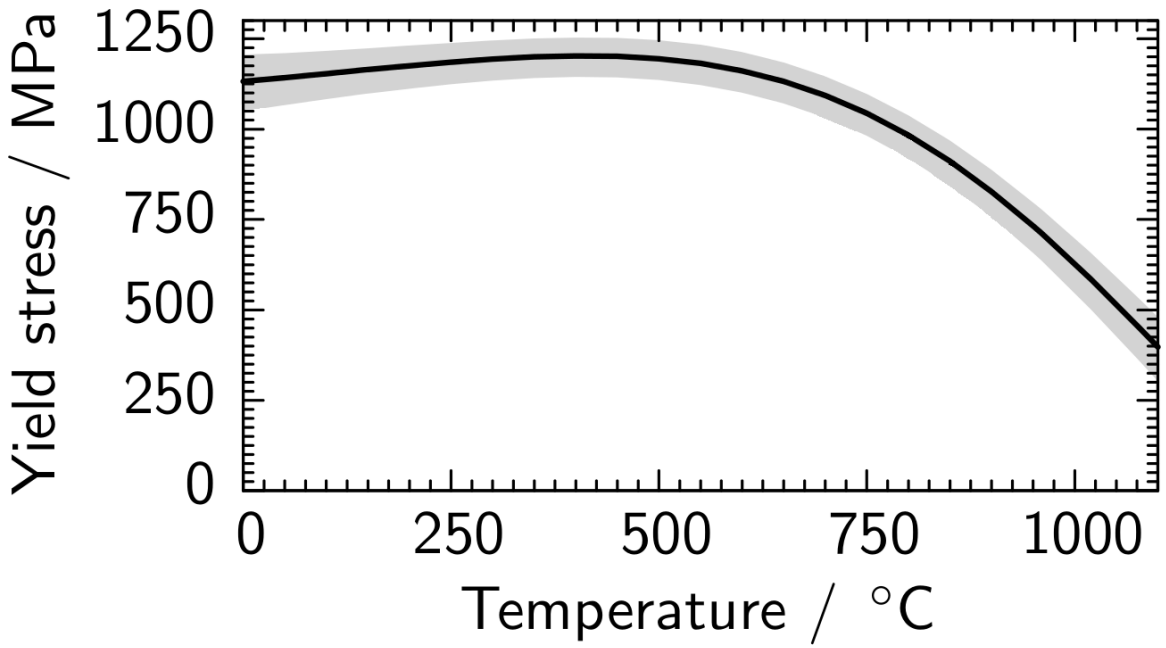
900ºC

30 hours

Microstructure

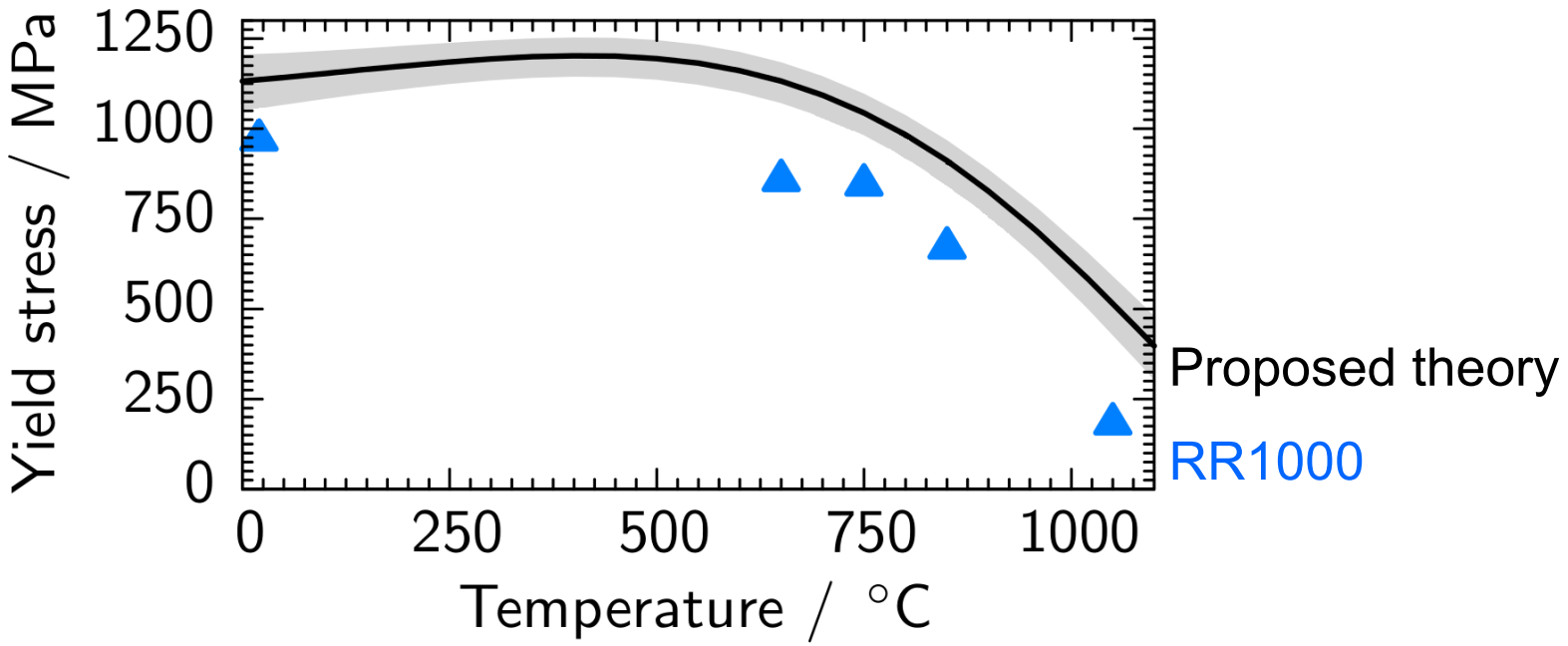


Testing the yield stress

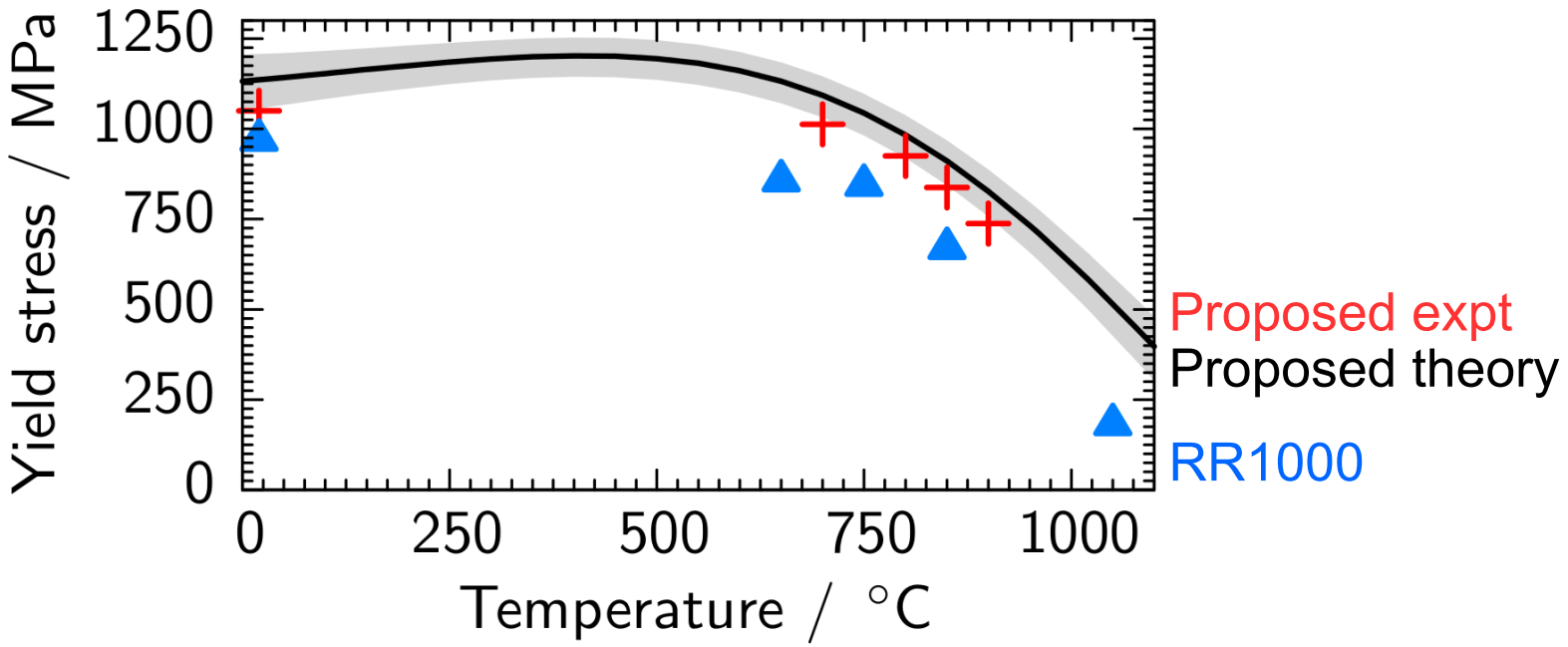


Proposed theory

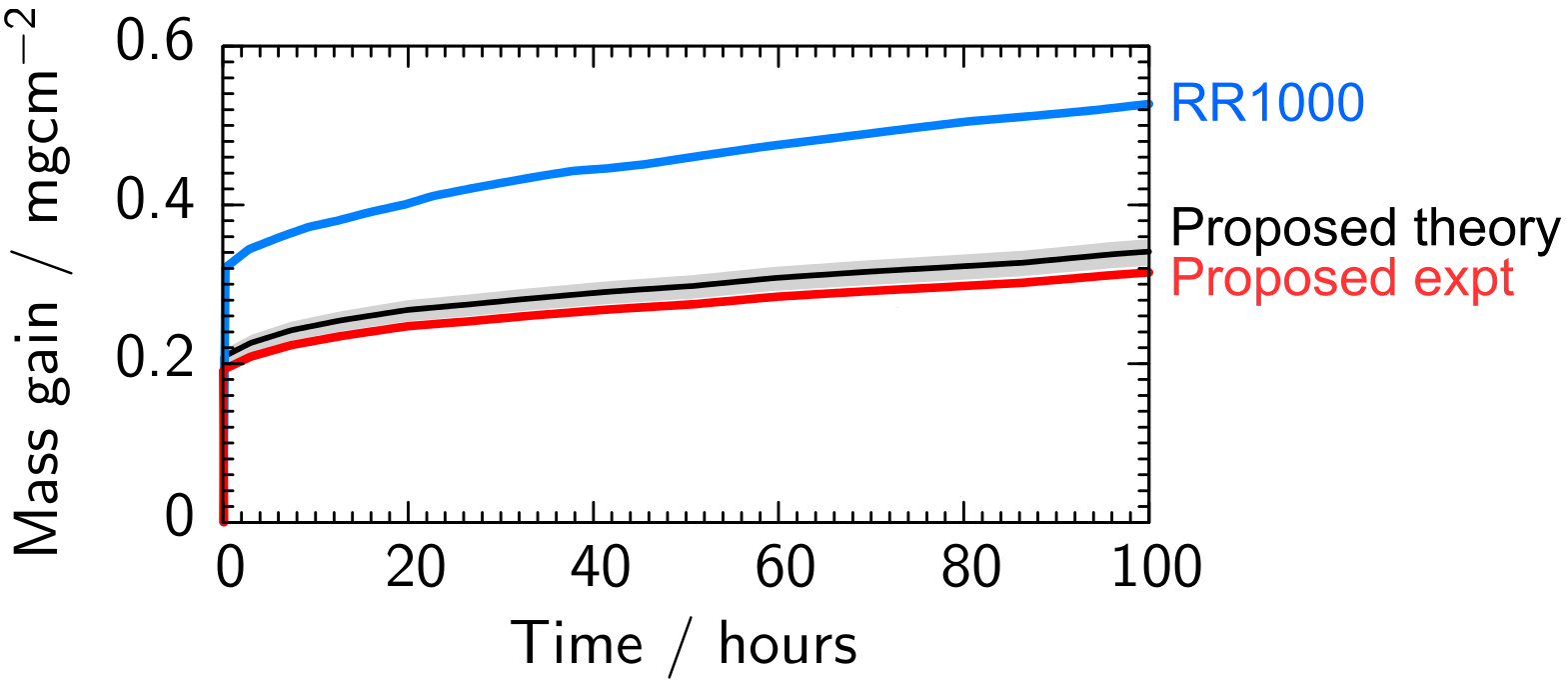
Testing the yield stress



Testing the yield stress

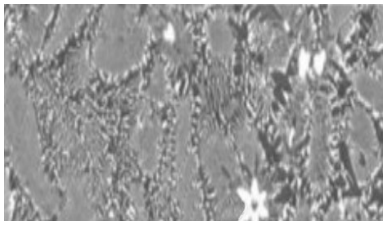


Testing the oxidation resistance

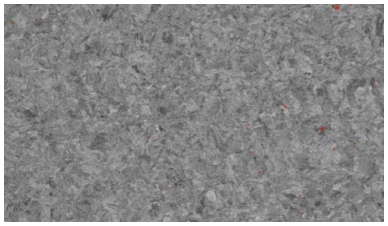


High temperature alloys discovered

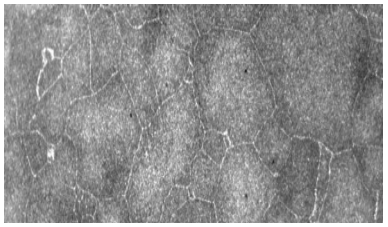
Cr-Cr_2Ta alloys
Intermetallics, 48, 62



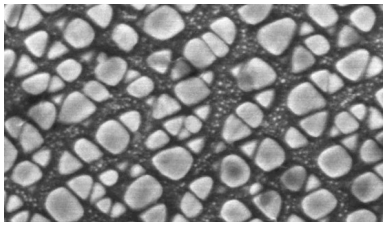
Combustor alloy
GB1408536



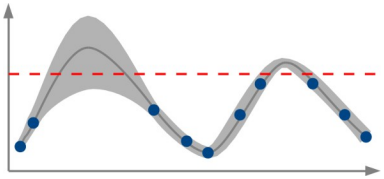
RR1000 grain growth
Acta Materialia, 61, 3378



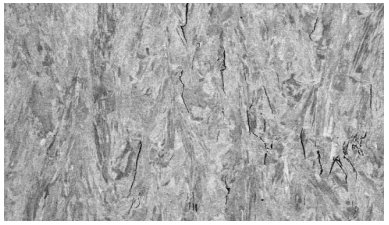
Ni alloy
In press for
Materials & Design (2017)



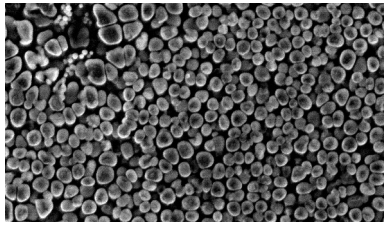
Discovery algorithm
EP14153898
US 2014/177578



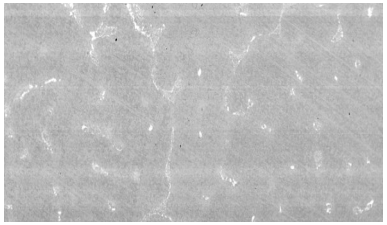
Ni alloy for additive manufacture



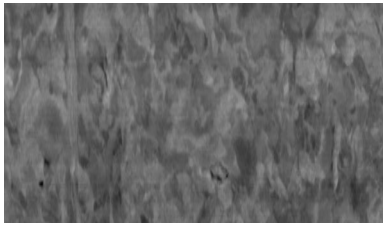
Ni disc alloy
EP14157622
US 2013/0052077 A2



Mo-Hf forging alloy
EP14161255
US 2014/223465

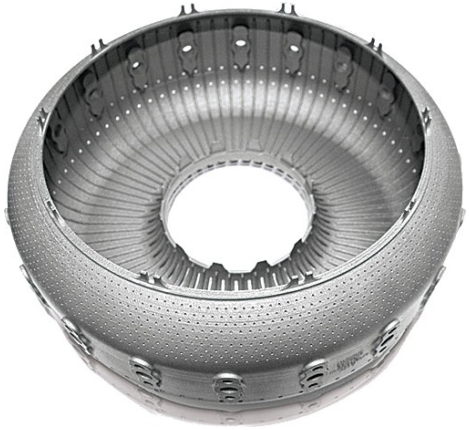


Mo-Nb forging alloy
EP14161529
US 2014/224885

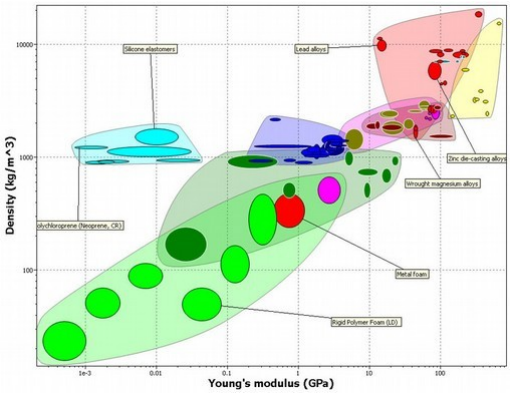


Materials design

3D printed alloy
for combustors
Designed from
7 data points

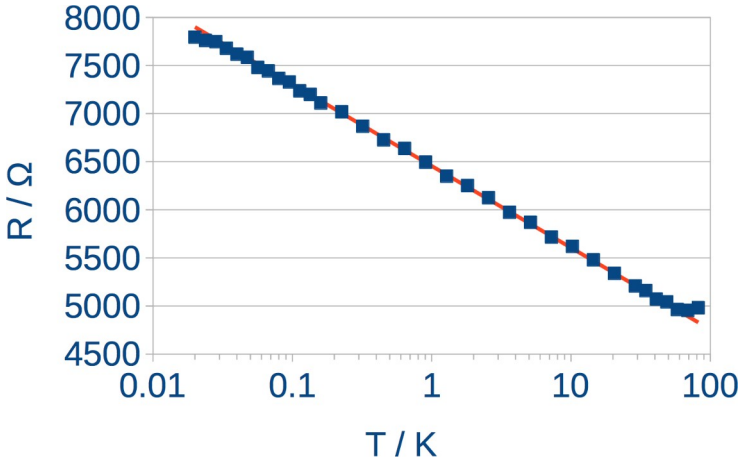


Materials databases
Found 792 errors



Materials design

Low temperature thermometer



Lake Shore CRYOTRONICS

Increased drug data available 200-times

e-Therapeutics plc
The Network Pharmacology Company

Materials design

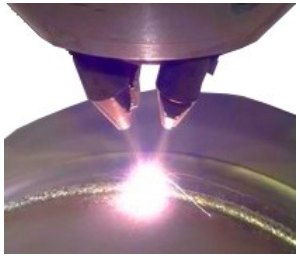
Battery design
with DFT and
experimental data

SAMSUNG

Designing lubricants
with DFT and
experimental data

bp

Additive manufacturing
from molecular dynamics
and experimental data



DASSAULT SYSTEMES

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