UNIVERSITY OF CAMBRIDGE

CALPHAD enhances machine learning for alloy design

Gareth Conduit

Cambridge 2022

Hosted Zi-Kui Liu and his wife at Gonville & Caius College, Cambridge, UK, during summer 2022

Many discussions of zentropy in the gardens adjacent to Professor Hawking's old office

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Further discussions about CALPHAD at Dinner

Machine learning to

Model datasets where the data is sparse

Exploit property-property relationships

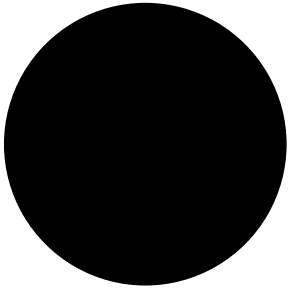
Merge data, computer simulations, and physical laws

Reduce costly experiments to accelerate discovery

Black box machine learning for materials design

Properties

Composition

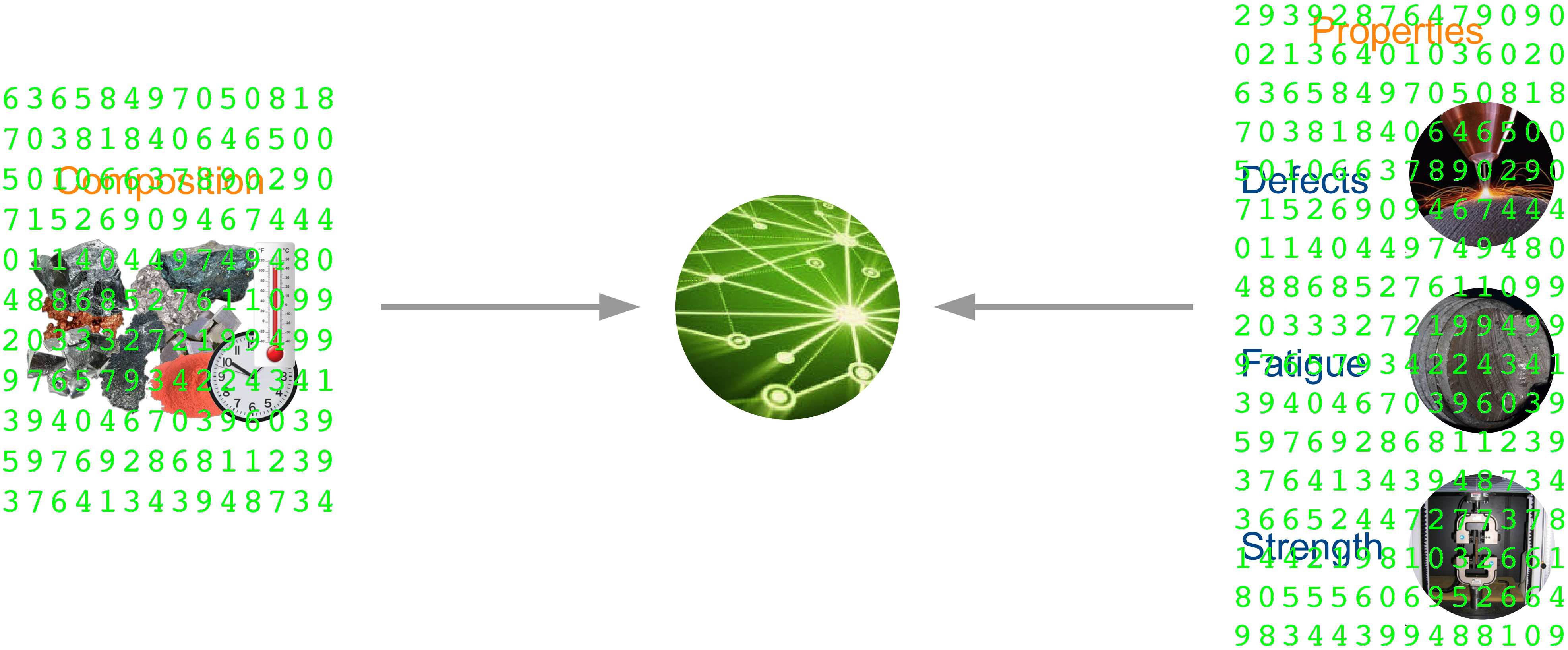


Defects

Fatigue

Strength

Train the machine learning



Machine learning predicts material properties

Composition

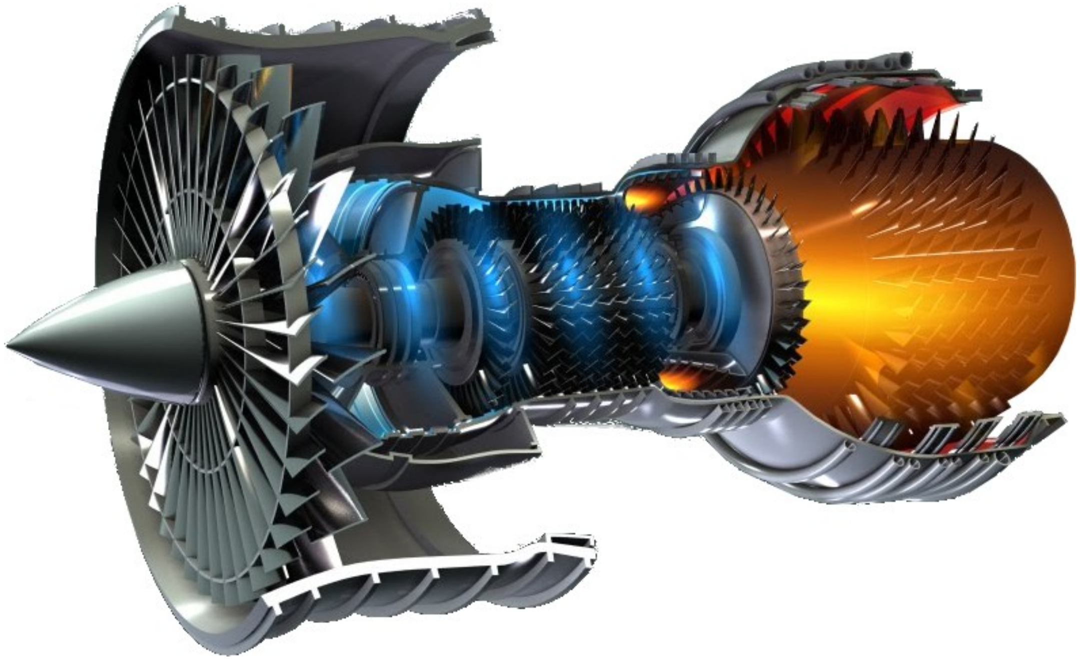
Properties

Defects

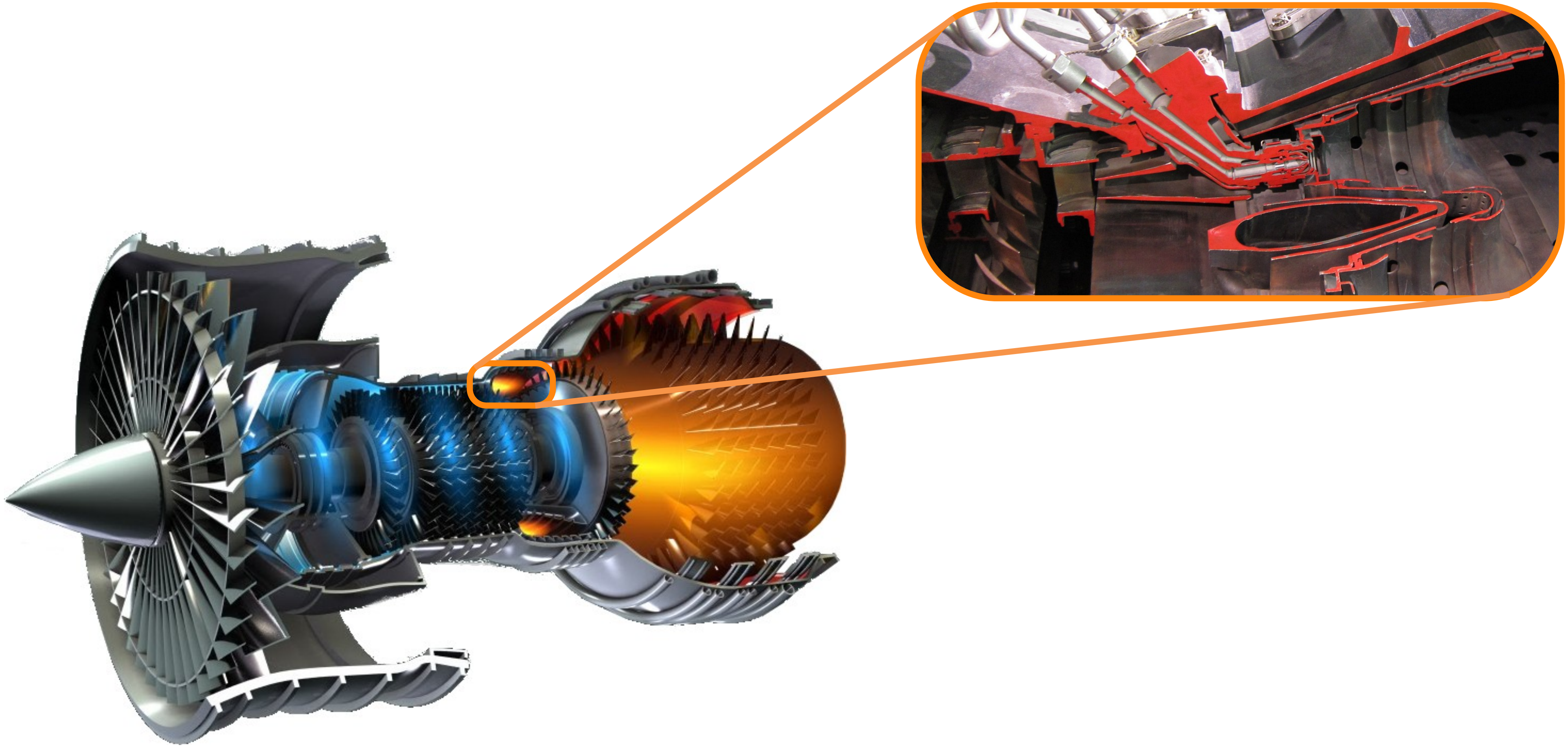
Fatigue

Strength

Jet engine schematic



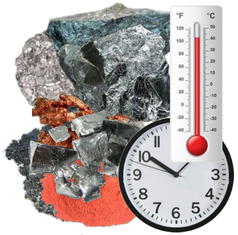
Combustor in a jet engine



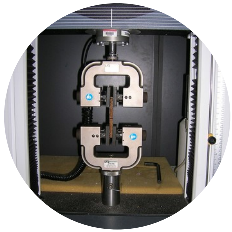
Strength

Strength

Data available to model strength



100 entries



Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

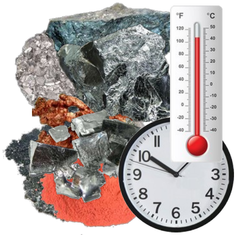
Just 100 data entries available to model strength

Strength and phase behavior are correlated

Strength

Phase behavior

First predict phase behavior



100,000 entries

Use 100,000 CALPHAD results to model complex composition → phase behavior

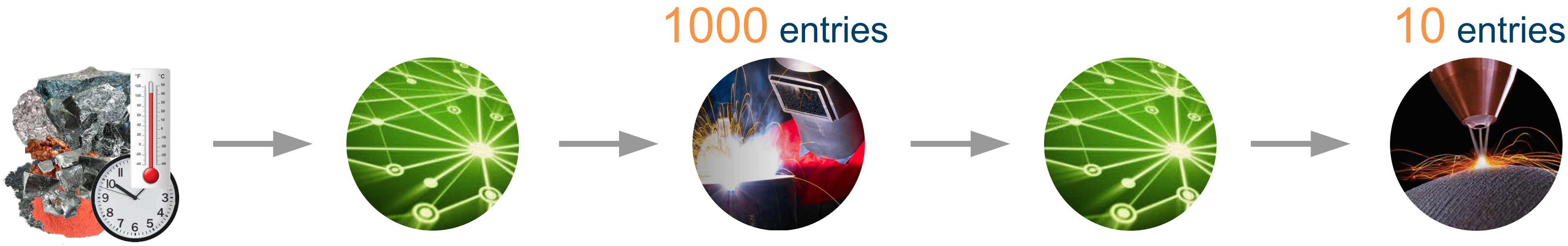
Use CALPHAD to predict strength

Use 100,000 CALPHAD results to model complex composition → phase behavior

100 strength entries capture the phase behavior → strength relationship

Two interpolations aid the composition → strength extrapolation

Use weldability to predict defects formed



Use 1000 weldability entries to understand complex composition → weldability model

10 defects entries capture the simple weldability → defect relationship

Two interpolations aid composition → defects extrapolation

Target properties

Elemental cost	< 25 $\$kg^{-1}$
Density	< 8500 kgm^{-3}
γ’ content	< 25 wt%
Oxidation resistance	< 0.3 $mgcm^{-2}$
Defects	< 0.15% defects
Phase stability	> 99.0 wt%
γ’ solvus	> 1000˚C
Thermal resistance	> 0.04 $K\Omega^{-1}m^{-3}$
Yield stress at 900˚C	> 200 MPa
Tensile strength at 900˚C	> 300 MPa
Tensile elongation at 700˚C	> 8%
1000hr stress rupture at 800˚C	> 100 MPa
Fatigue life at 500 MPa, 700˚C	> 10^5 cycles

Composition and processing variables

Cr 19%

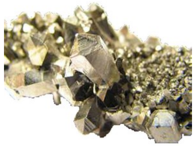
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



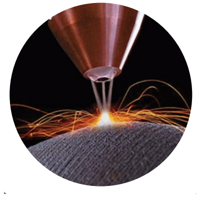
Al 2.9%

C 0.04%

B 0.01%

Ni

Expose 0.8



T_{HT} 1300ºC

Phase behavior targets

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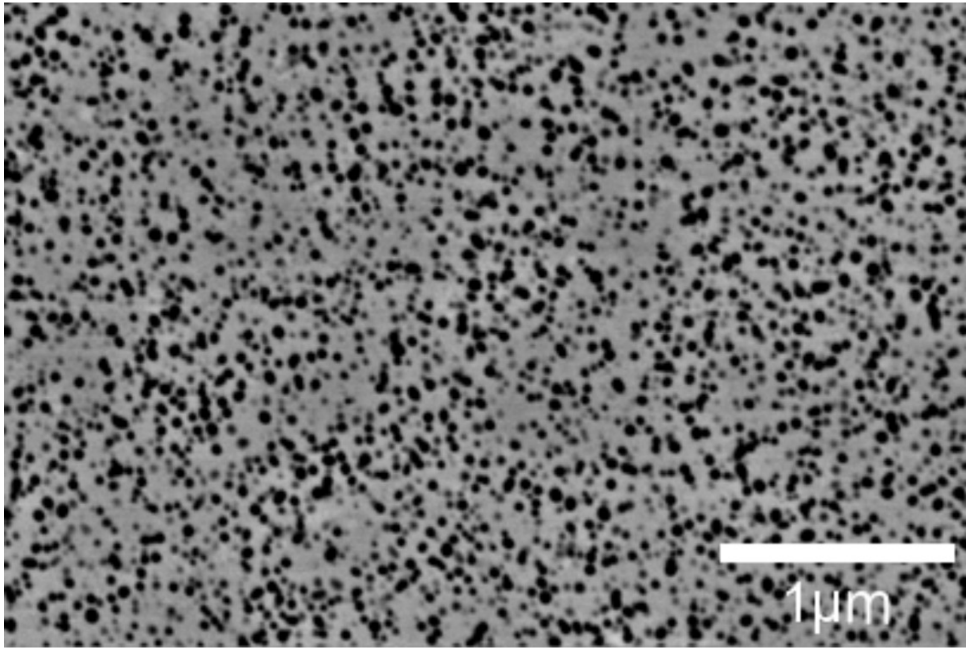
Microstructure



Probabilistic neural network identification of an alloy for direct laser deposition
B. Conduit, T. Illston, S. Baker, D. Vadegadde Duggappa, S. Harding, H. Stone & GJC
Materials & Design **168**, 107644 (2019)

Strength target

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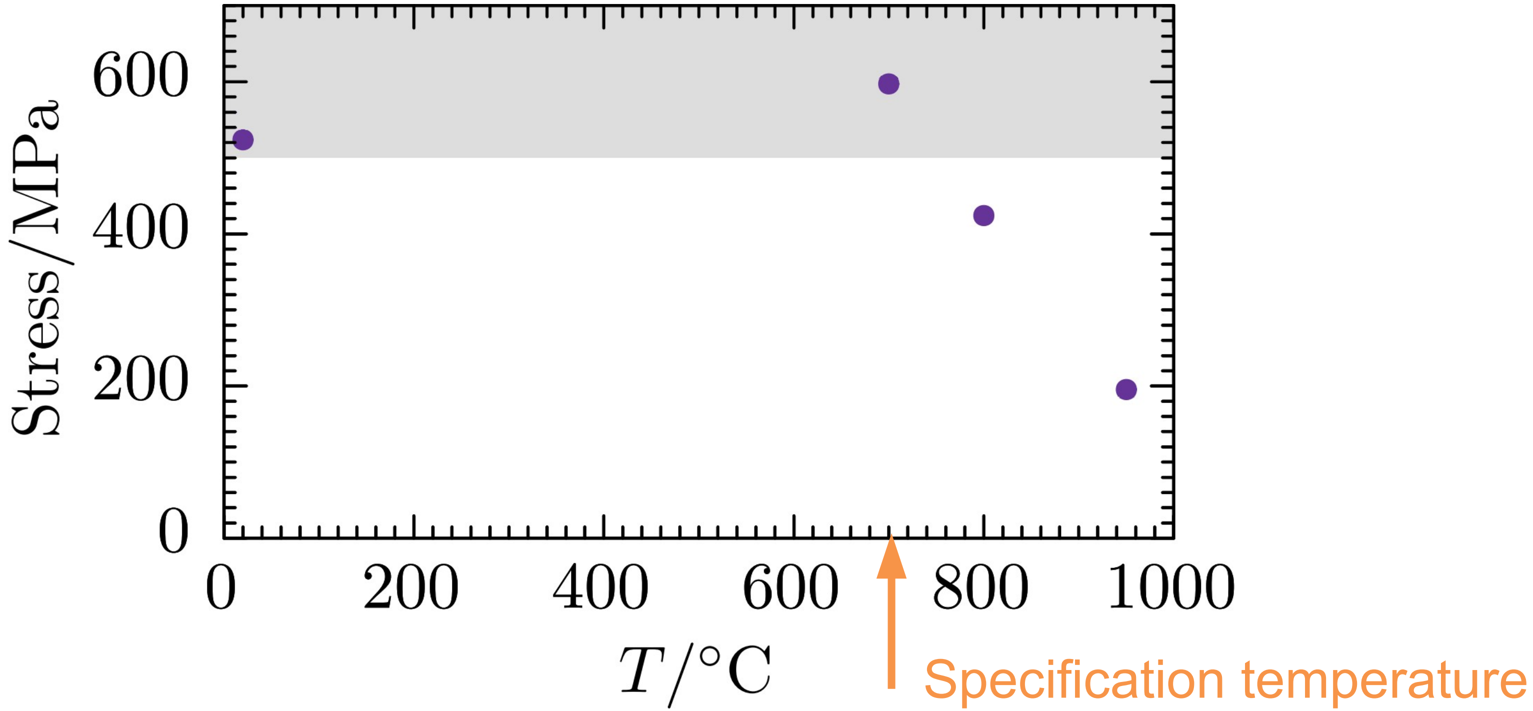
Test the high cycle fatigue stress



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Defects target

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Thermal resistance	$> 0.04\ K\Omega^{-1}m^{-3}$
Yield stress at 900˚C	$>$ 200 MPa
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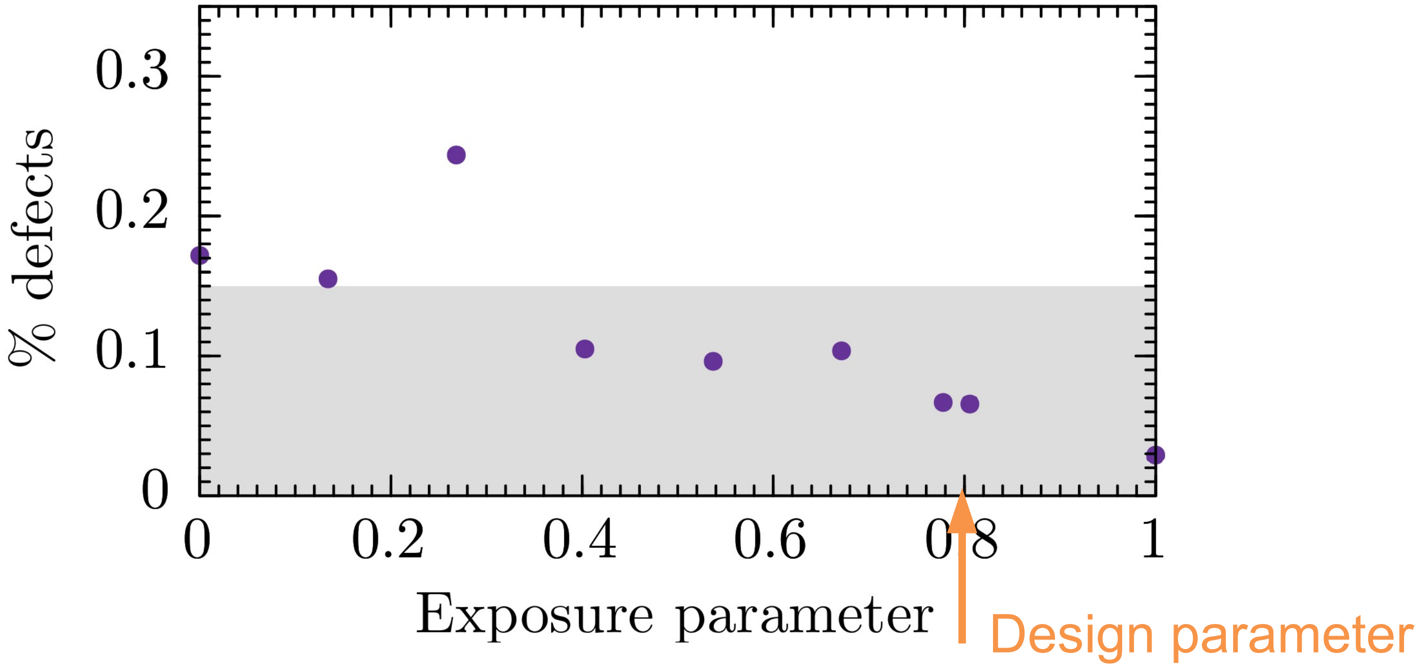
Tensile elongation at 700˚C	$>$ 8%
1000hr stress rupture at 800˚C	$>$ 100 MPa
Fatigue life at 500 MPa, 700˚C	$> 10^5$ cycles

Test the defect density



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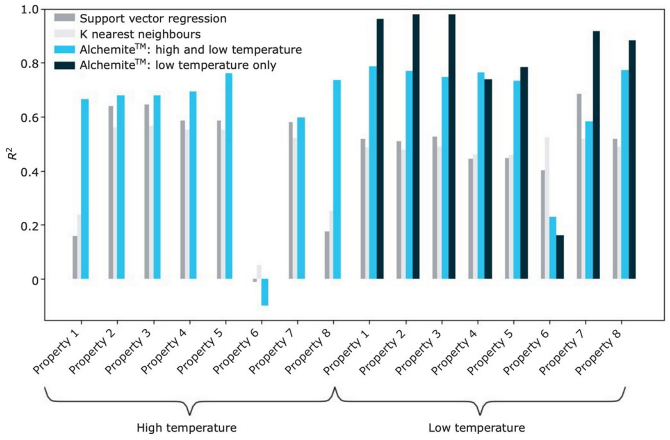
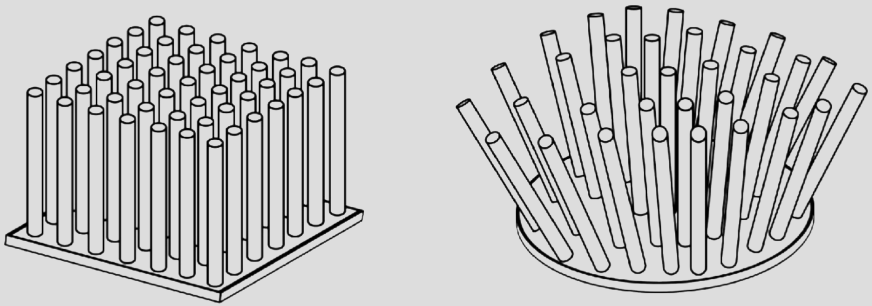
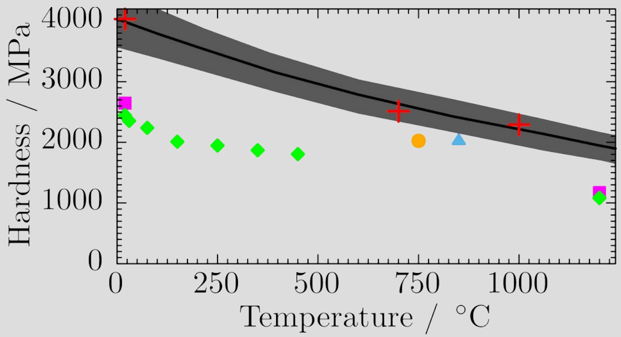


Johnson Matthey Technology Review
66, 130 (2022)



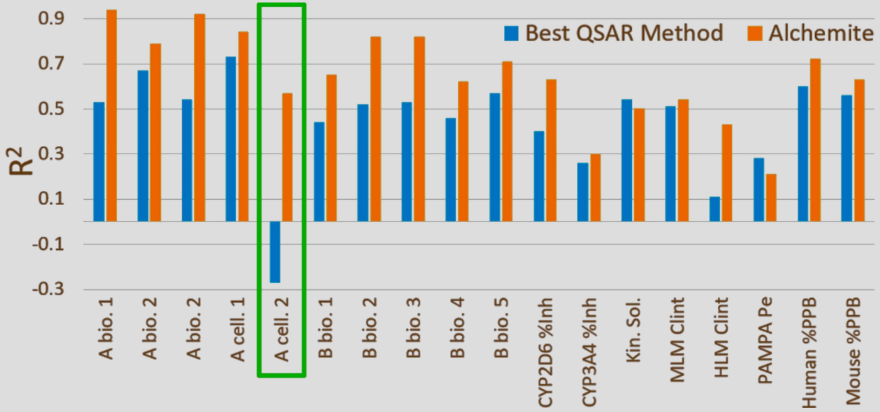
NASA Technical Memorandum
20220008637



Materials & Design **131**, 358 (2017)
Scripta Materialia **146**, 82 (2018)
Data Centric Engineering **3**, e30 (2022)

Alloy	Source	ANN	Δ_σ	Actual
Steel AISI 301L	193	269	5	238[23]
Steel AISI 301	193	267	5	221[23]
Al 1080 H18	51	124	5	120[23]
Al 5083 wrought	117	191	14	300,190[4, 23]
Al 5086 wrought	110	172	11	269,131[4, 23]
Al 5454 wrought	102	149	14	124[23]
Al 5456 wrought	130	201	11	165[23]
INCONEL600	223	278	10	≥550[23]

Computational Materials
Science **147**, 176 (2018)

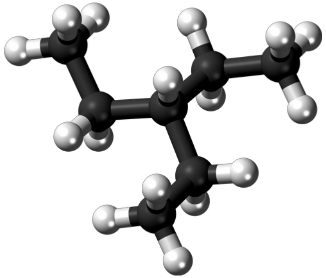


J. of Chem. Info. & Model. **60**, 2848 (2020)
Applied AI Letters **2**, e31 (2021)
Molecular Pharmaceutics **19**, 1488 (2022)

Constellation PHARMACEUTICALS
Takeda
AstraZeneca

optibrium™
iff

Journal of Computer-Aided
Molecular Design **35**, 112501140 (2021)



Fluid Phase Equilibria **501**, 112259 (2019)
Journal of Chemical Physics **153**, 014102 (2020)

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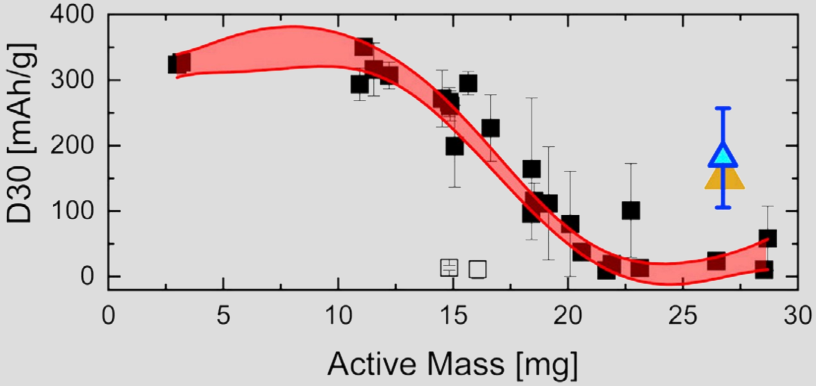

Cell Reports
Physical Science
2, 100683 (2021)

UNIVERSITY OF BIRMINGHAM
Ansys
GRANTA

Summary

Merge computer simulations with experimental data and exploit property-property relationships to circumvent missing data

Designed and experimentally verified alloy for direct laser deposition

Generic approach applied to alloys, batteries, pharmaceuticals, and beyond

Taken to market through startup Intellegens