UNIVERSITY OF CAMBRIDGE

Machine learning for data-driven design of AM materials and processes

Gareth Conduit

Machine learning to

Model datasets where the data is sparse

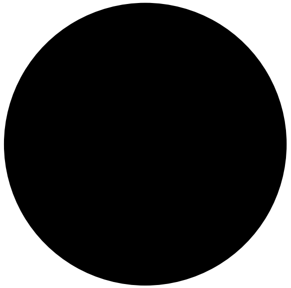
Exploit property-property relationships

Merge data, computer simulations, and physical laws

Reduce costly experiments to accelerate discovery

Black box machine learning for materials design

Composition



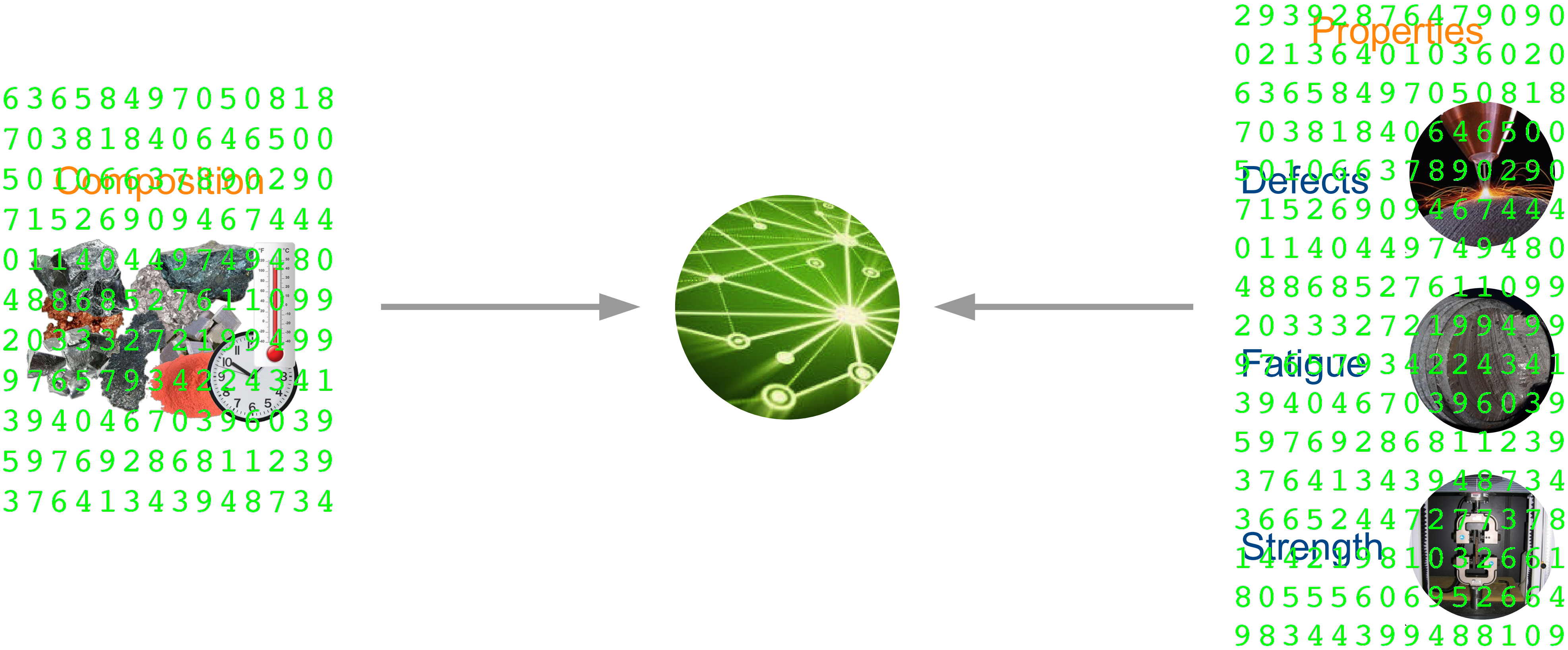
Properties

Defects

Fatigue

Strength

Train the machine learning



Machine learning predicts material properties

Composition

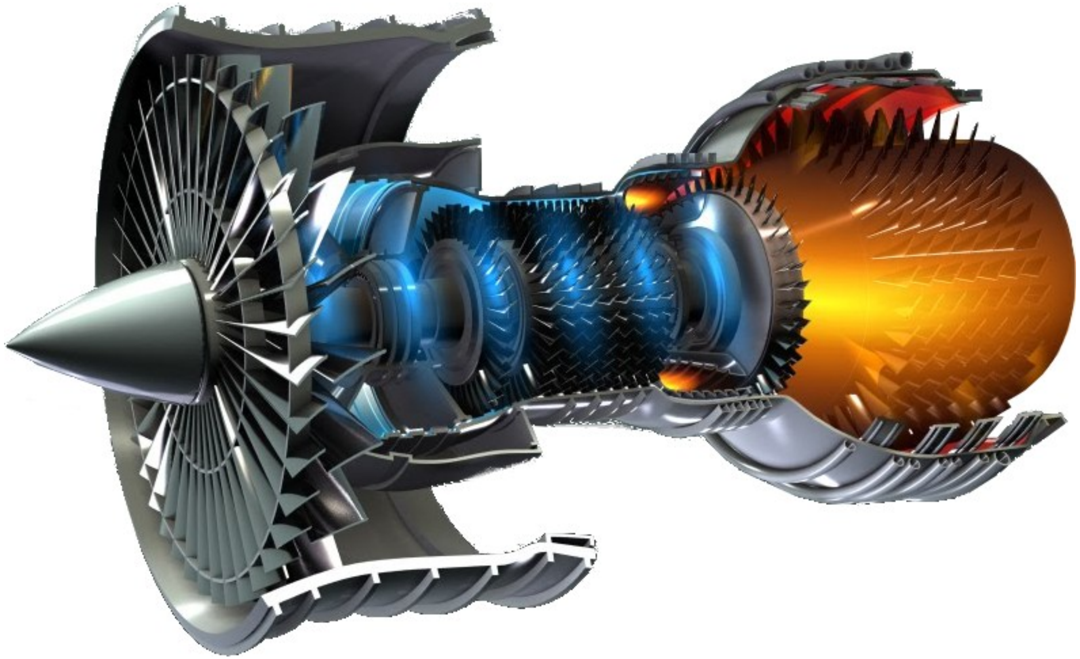
Properties

Defects

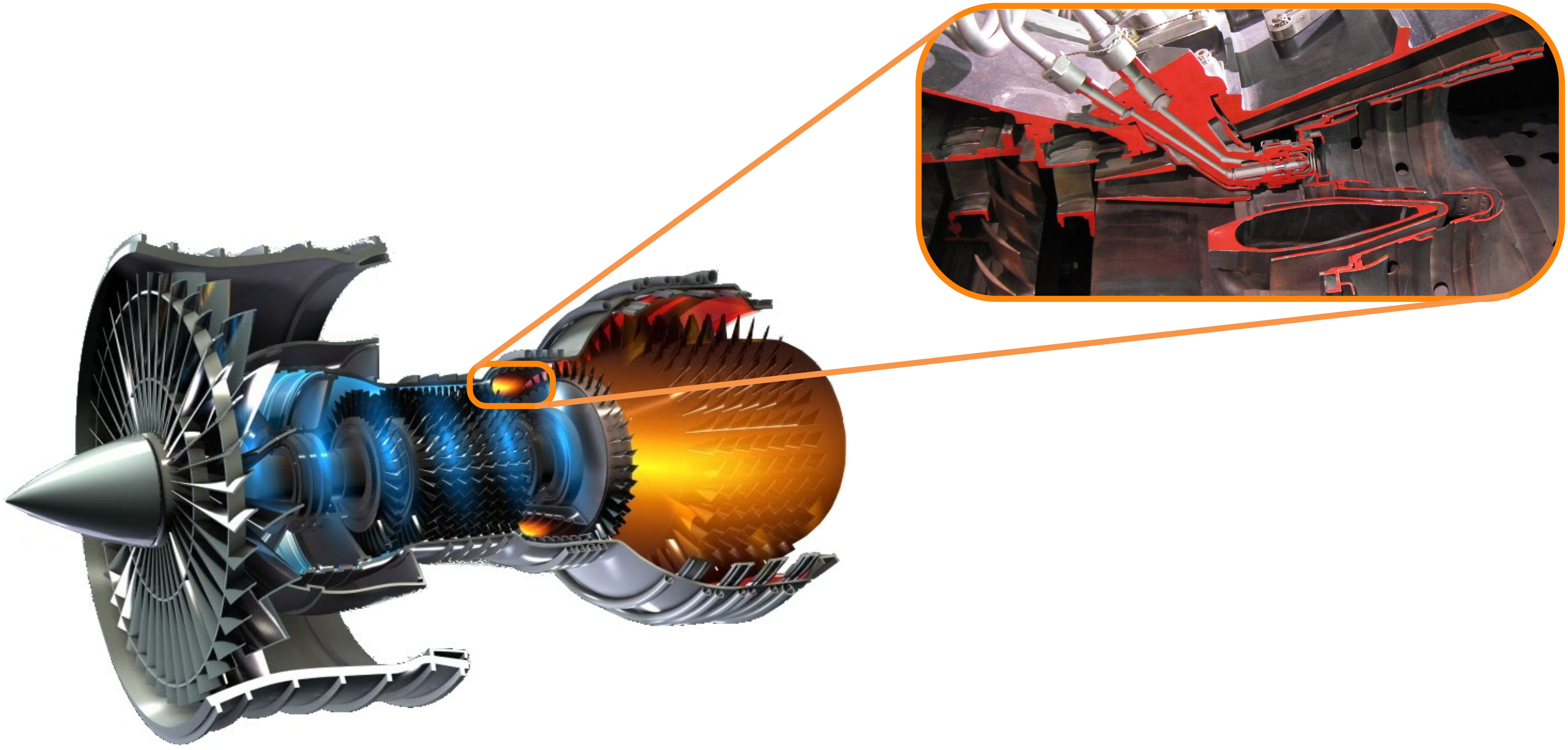
Fatigue

Strength

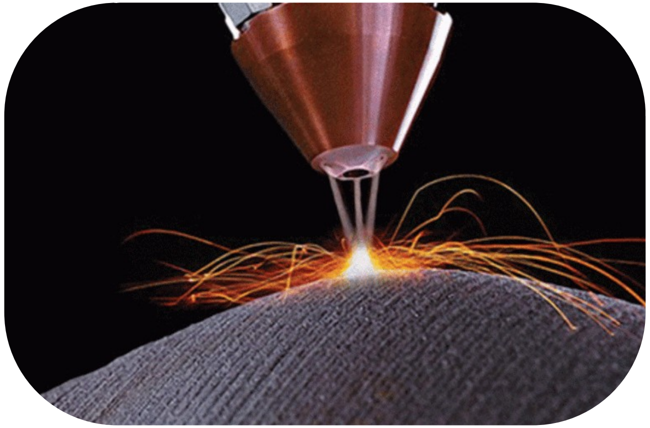
Jet engine schematic



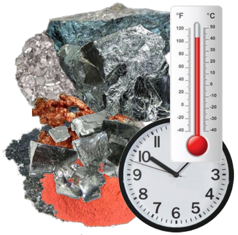
Combustor in a jet engine



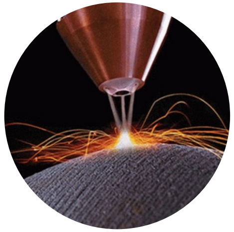
Direct laser deposition



Data available to model defect density



10 entries

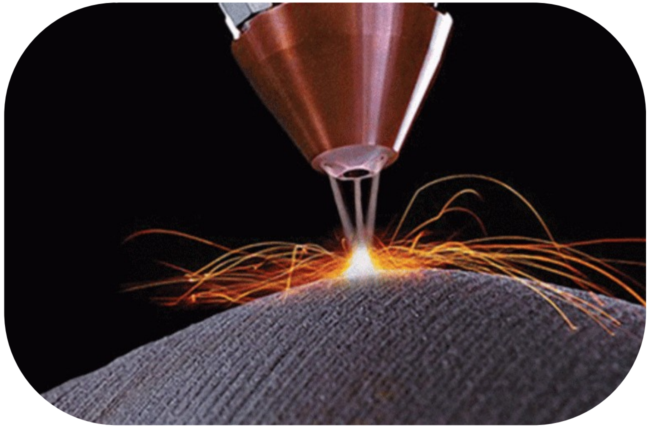


Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

Ability for printing and welding are strongly correlated



Laser

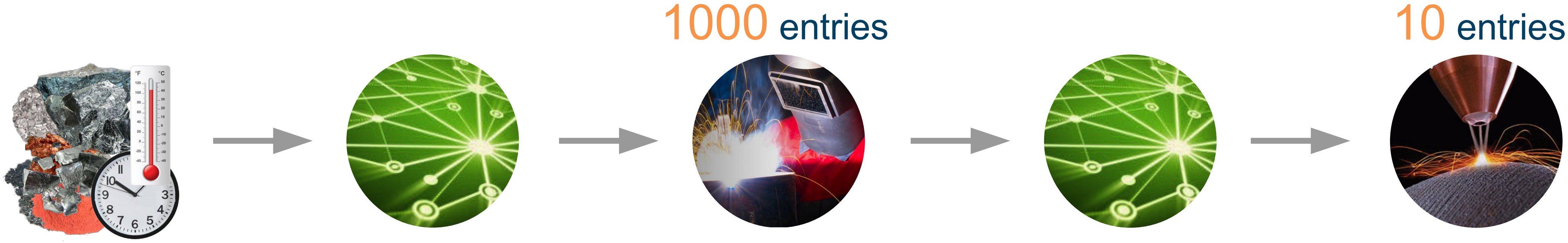
Electricity

First predict weldability

1000 entries

Use 1000 weldability entries to understand complex composition → weldability model

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

Use CALPHAD to predict strength

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

500 strength entries capture the phase behavior → strength relationship

Two interpolations aid the composition → strength extrapolation

Target properties

Elemental cost	$< 25\ \$\mathrm{kg}^{-1}$
Density	$< 8500\ \mathrm{kgm}^{-3}$
γ’ content	< 25 wt%
Oxidation resistance	$< 0.3\ \mathrm{mgcm}^{-2}$
Defects	$< 0.15\%$ defects
Phase stability	> 99.0 wt%
γ’ solvus	$> 1000^{\circ}\mathrm{C}$
Thermal resistance	$> 0.04\ \mathrm{K\Omega^{-1}m^{-3}}$
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%

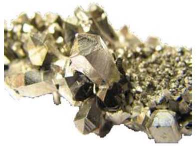
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



Al 2.9%

C 0.04%

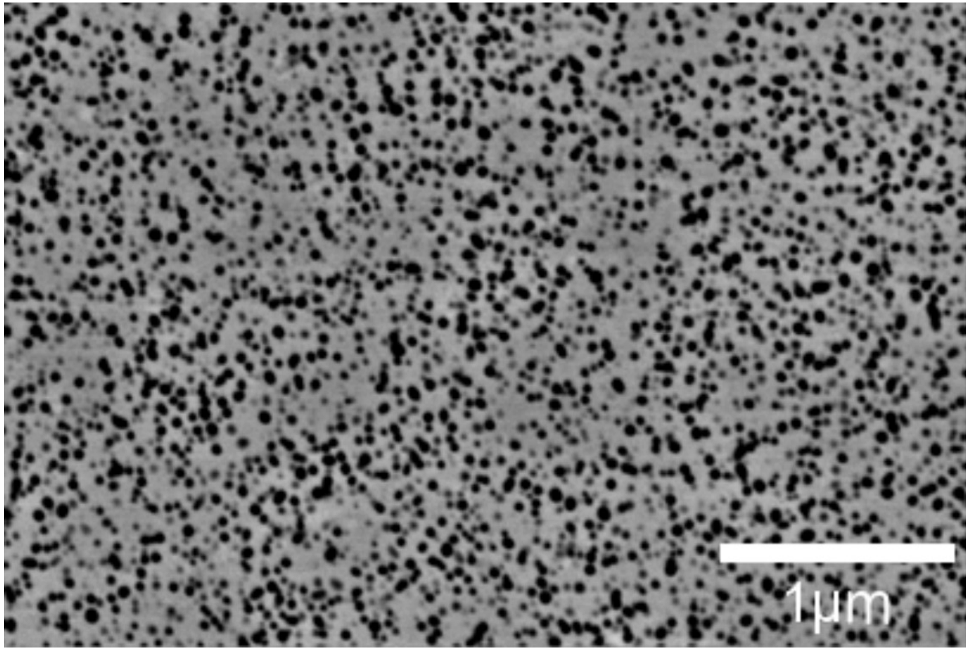
B 0.01%

Ni

Expose 0.8

T_{HT} 1300ºC

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)

Defects target

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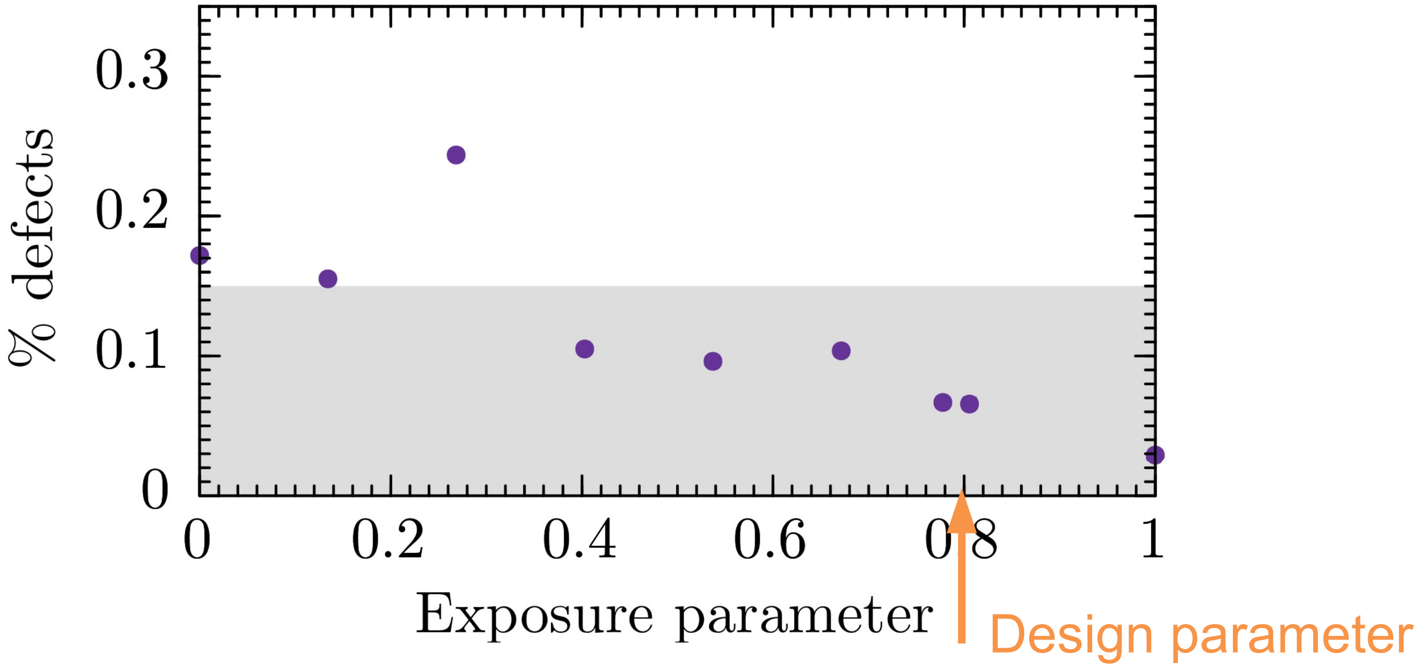
Testing the defect density



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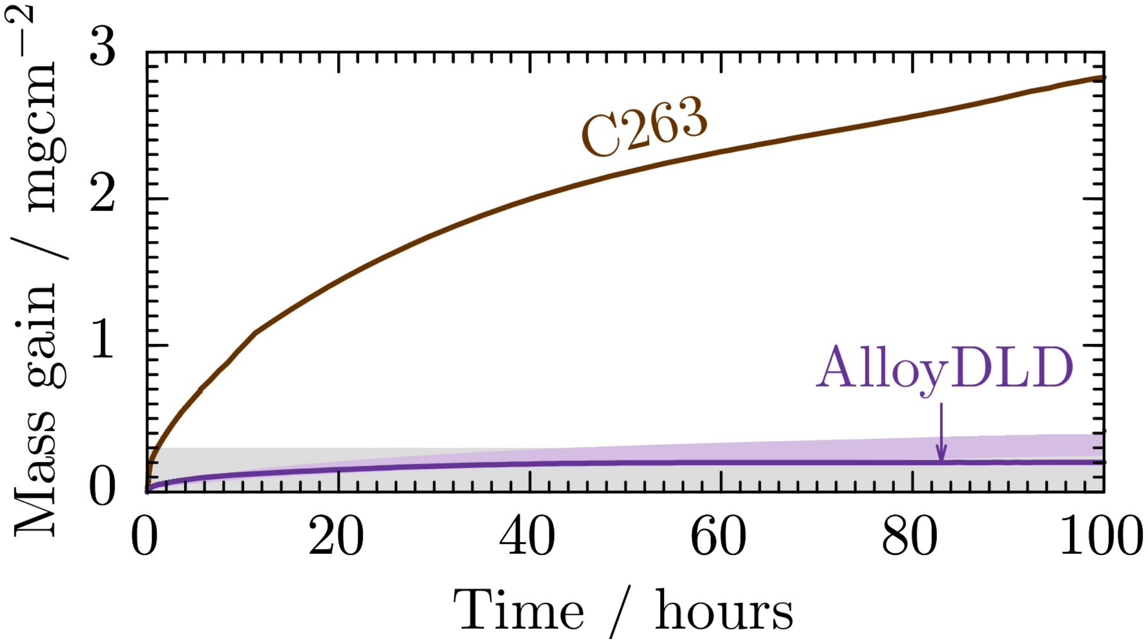
Testing the oxidation resistance



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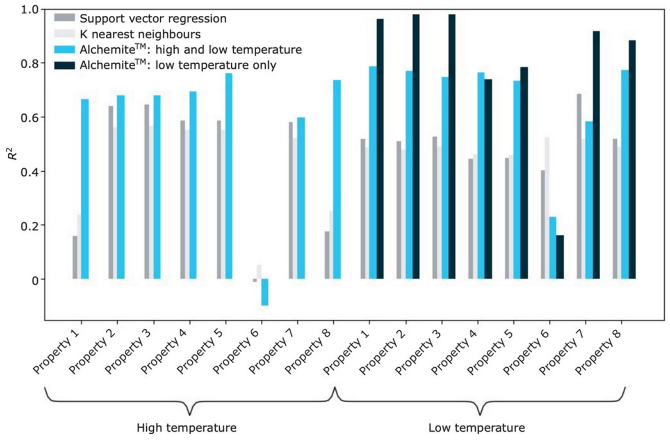
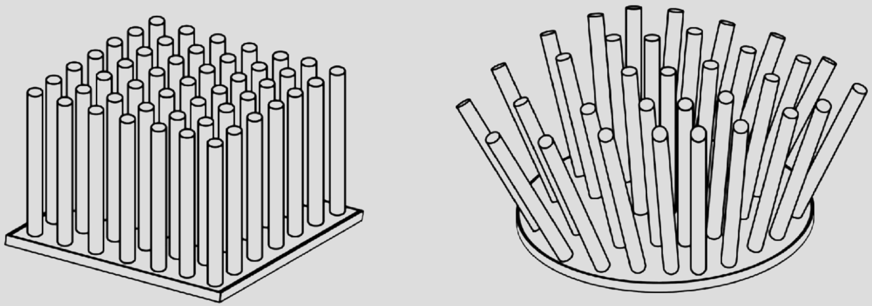
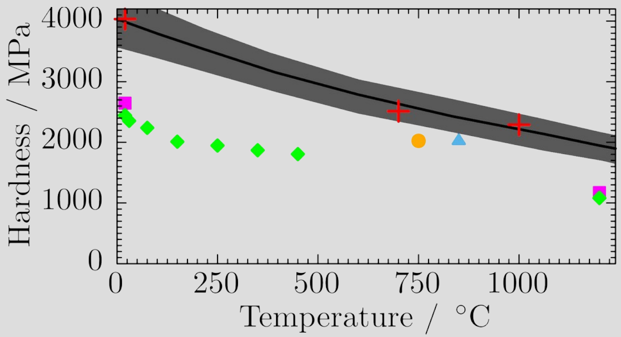


Johnson Matthey Technology Review
66, 130 (2022)



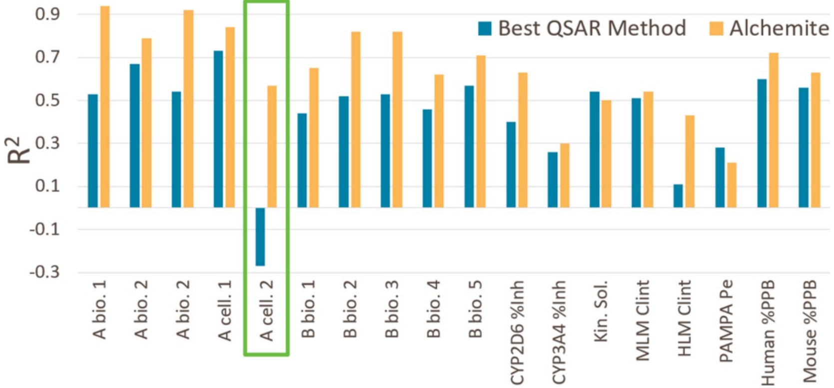
NASA Technical Memorandum
20220008637



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

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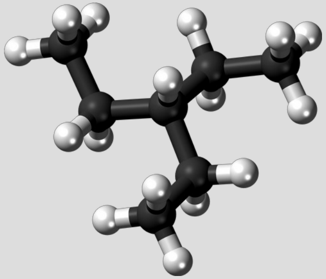

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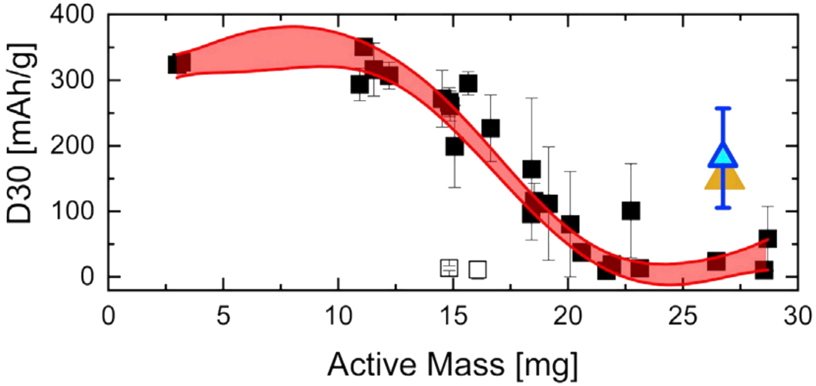
Fluid Phase Equilibria **501**, 112259 (2019)
Journal of Chemical Physics **153**, 014102 (2020)



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

intellegens