インテレジェンズ

intellegens

Applied machine learning

応用機械学習

材料・化学品・製造業などのセクターで

イノベーションの加速をお手伝いします

Dr Gareth Conduit

ギャレス・コンデュイット / 博士

Machine learning to

Model datasets where the data is sparse

Exploit property-property relationships

Merge data, computer simulations, and physical laws

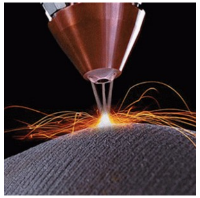
Reduce costly experiments to accelerate discovery

Black box machine learning for materials design

Properties

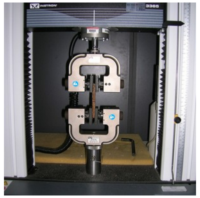
Composition

Defects

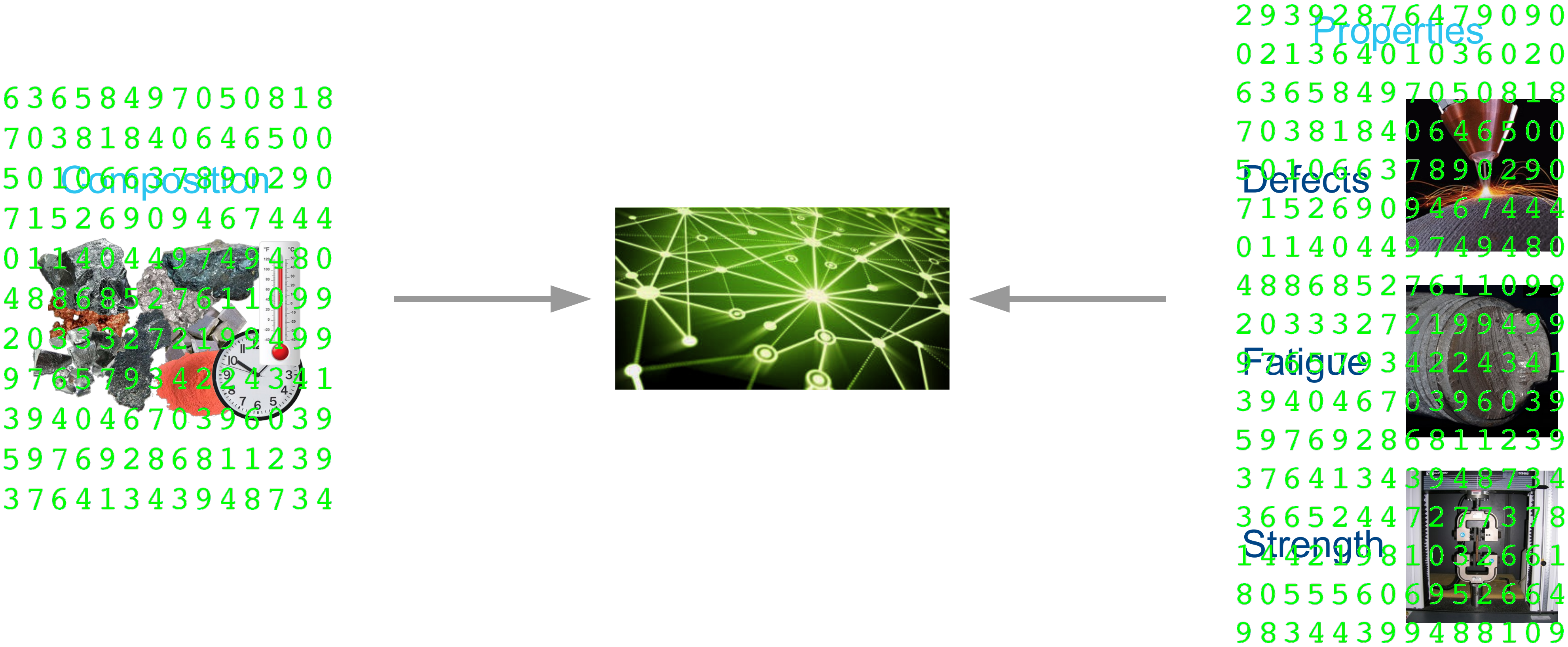


Fatigue

Strength



Train the machine learning

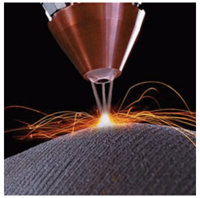


Machine learning predicts material properties

Properties

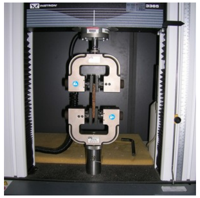
Composition

Defects

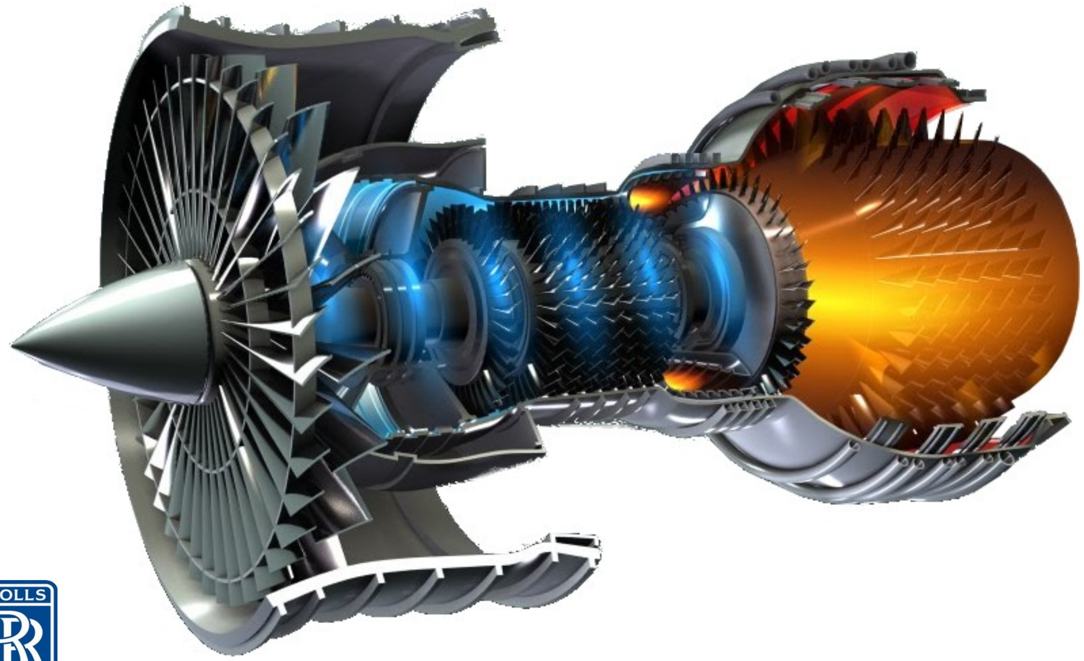


Fatigue

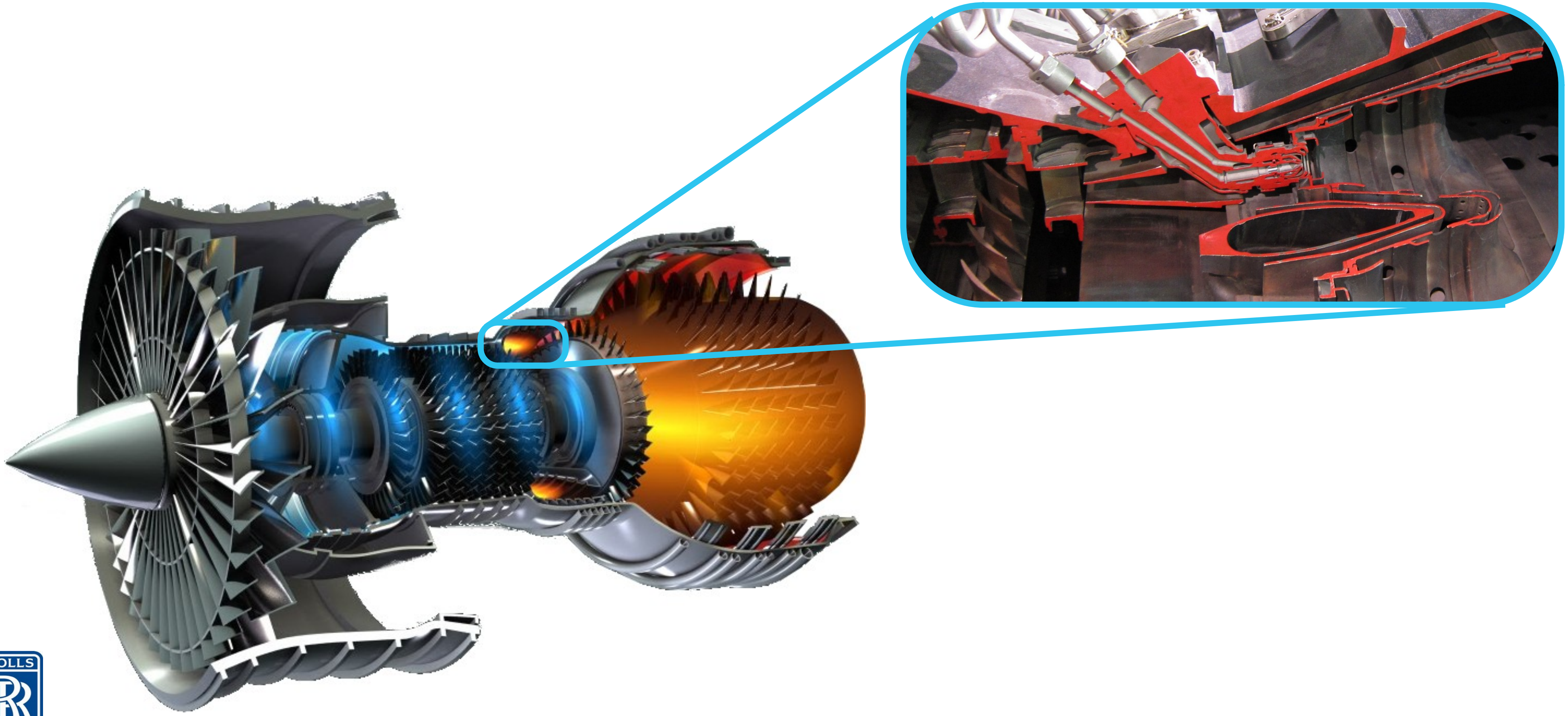
Strength



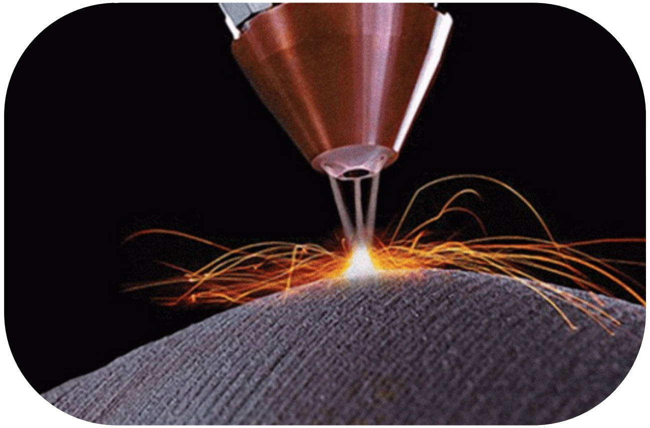
Jet engine schematic



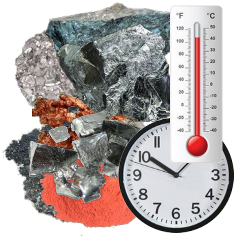
Combustor in a jet engine



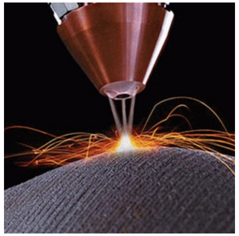
Direct laser deposition



Data available to model defect density



10 entries

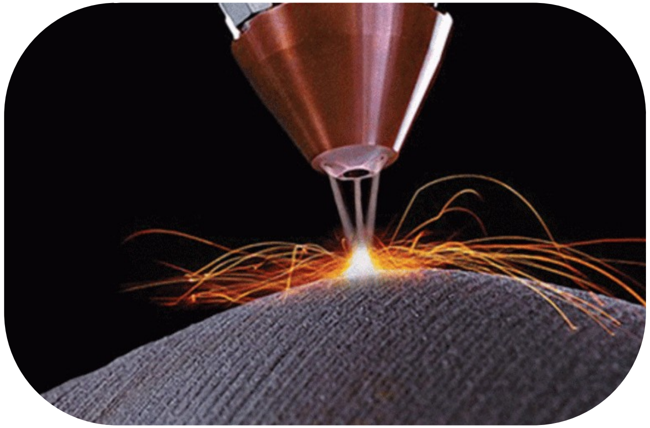


Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

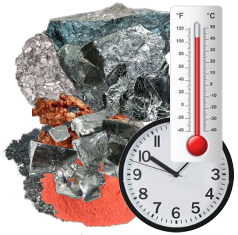
Ability for printing and welding are strongly correlated



Laser

Electricity

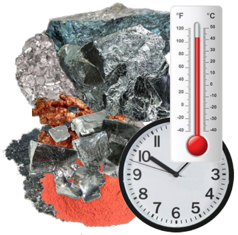
First predict weldability



1000 entries

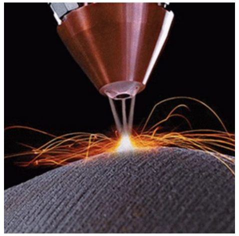
Use 1000 weldability entries to understand complex composition → weldability model

Use weldability to predict defects formed



1000 entries

10 entries



Use 1000 weldability entries to understand complex composition → weldability model

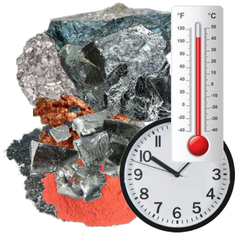
10 defects entries capture the simple weldability → defect relationship

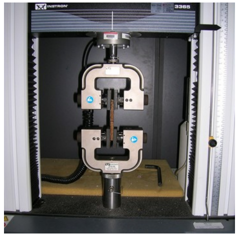
Two interpolations aid composition → defects extrapolation

Use CALPHAD to predict strength

100,000 entries

500 entries





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	$> 0.04\ \mathrm{K}\Omega^{-1}\mathrm{m}^{-3}$
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%

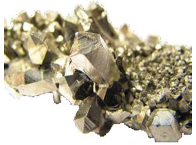
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



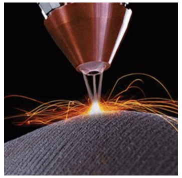
Al 2.9%

C 0.04%

B 0.01%

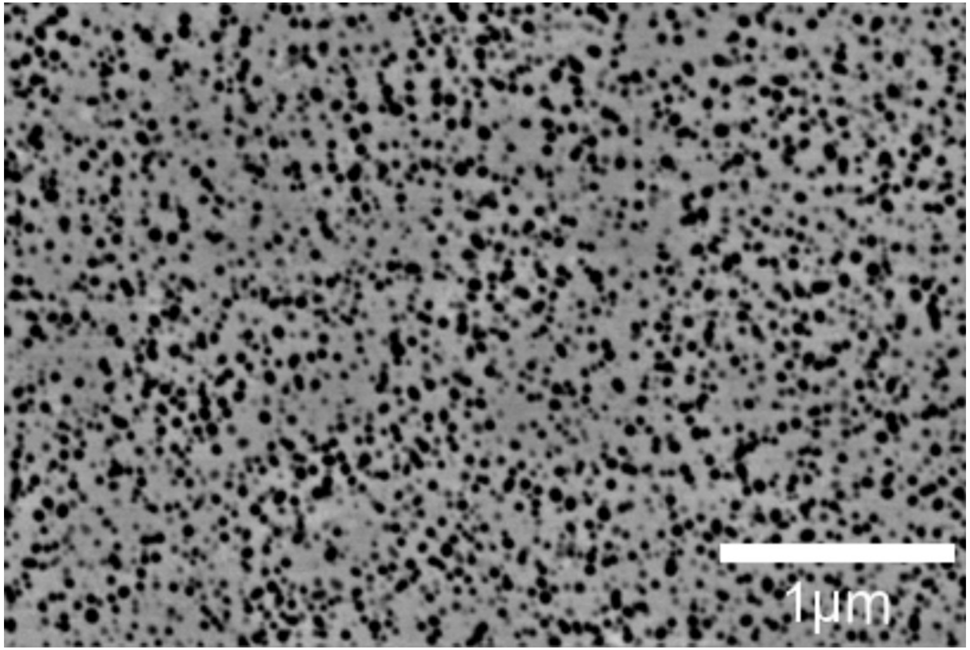
Ni

Expose 0.8



T_{HT} 1300ºC

Microstructure



Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design 168, 107644 (2019)

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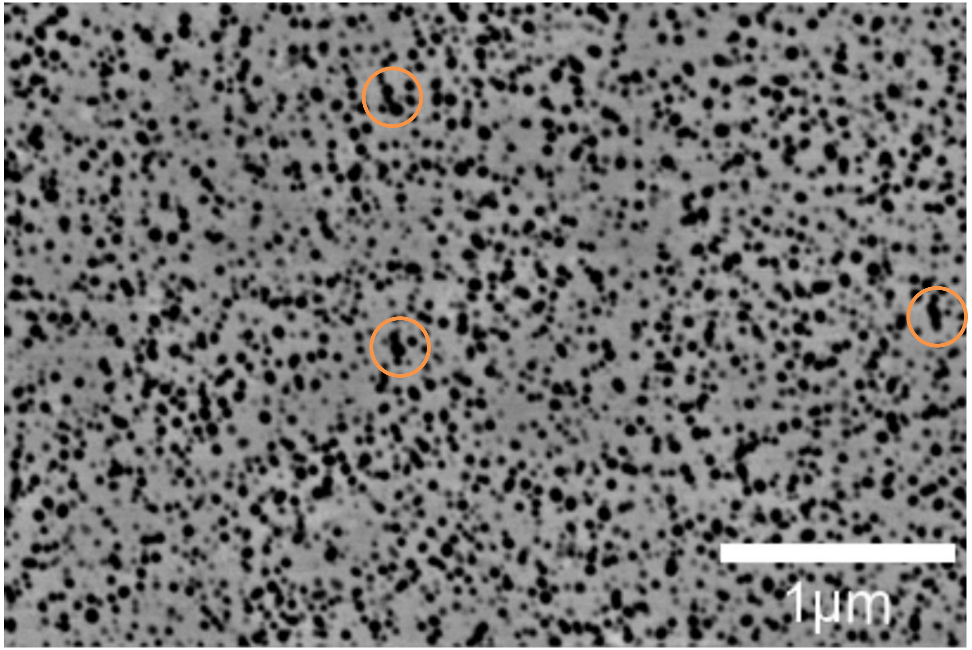

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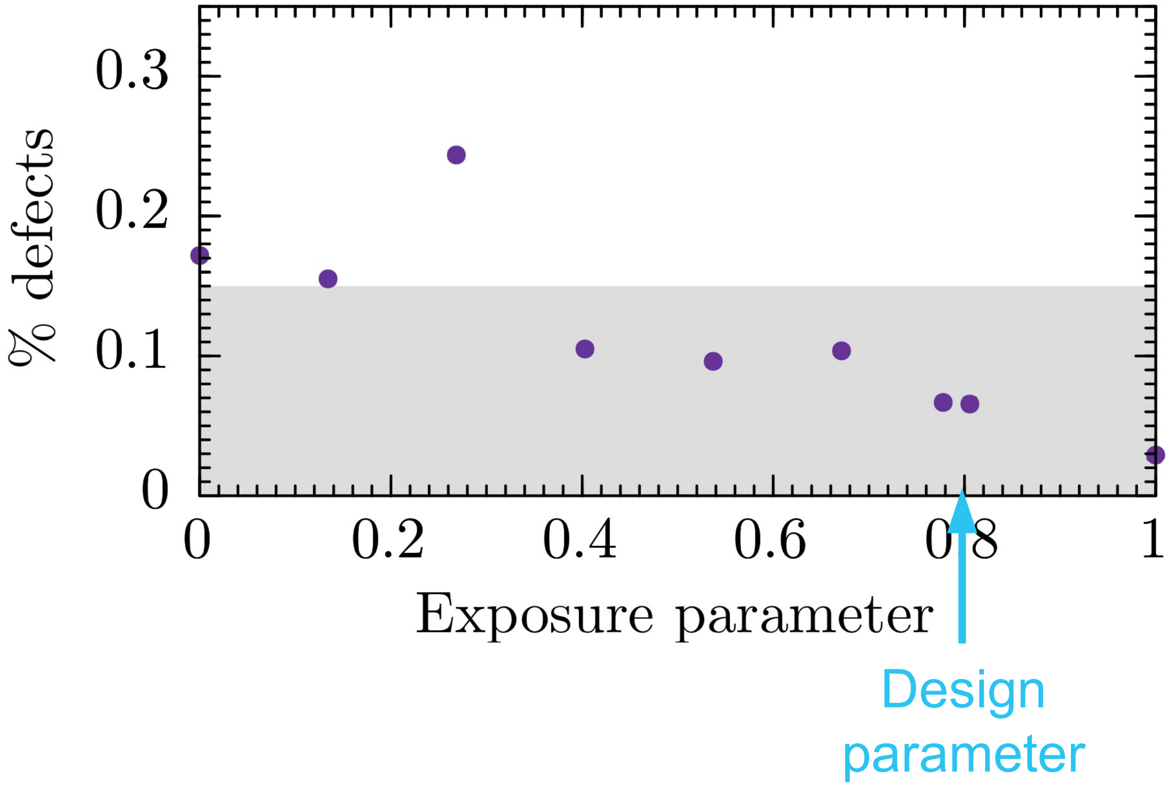
Testing the defect density



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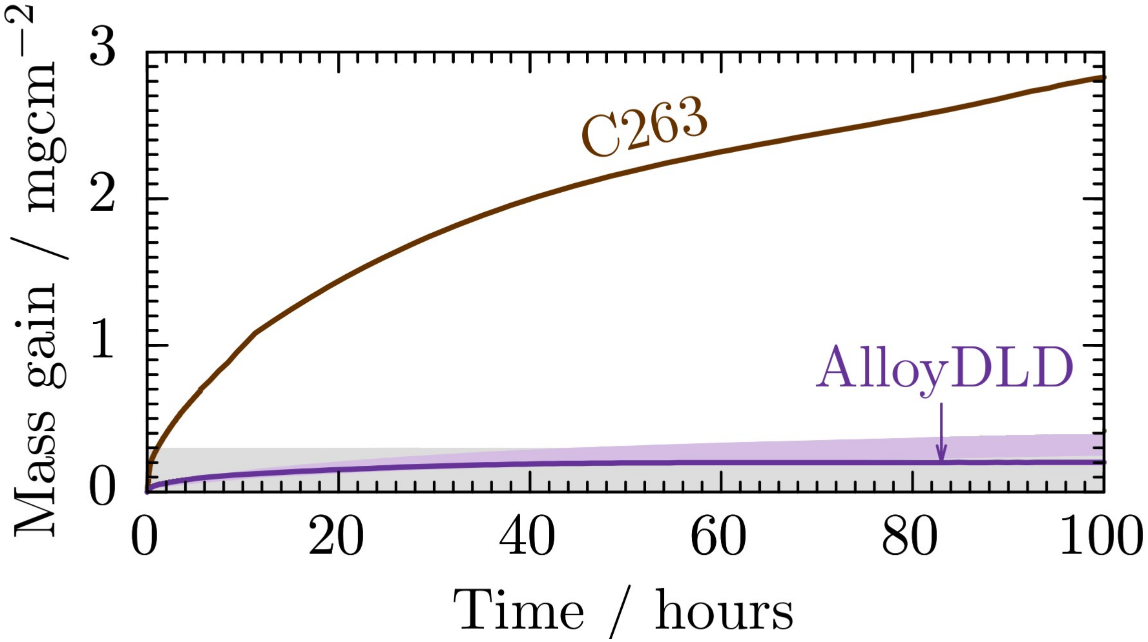
Testing the oxidation resistance



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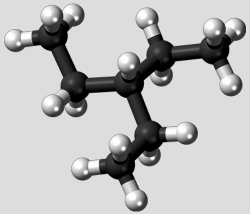
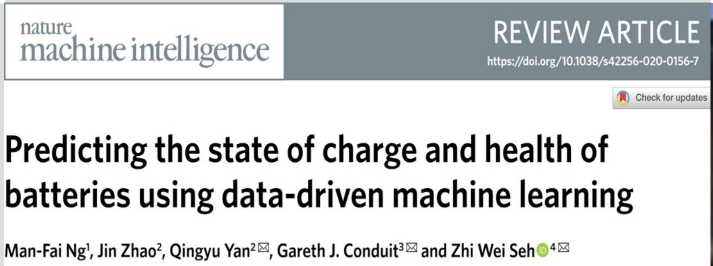
Materials & Design 168, 107644 (2019)

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



Fluid Phase Equilibria
501, 112259 (2019)

Journal of Chemical Physics
153, 014102 (2020)



nature machine intelligence

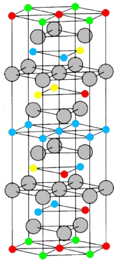
REVIEW ARTICLE

https://doi.org/10.1038/s42256-020-0156-7

Check for updates

Predicting the state of charge and health of batteries using data-driven machine learning

Man-Fai Ng[1], Jin Zhao[2], Qingyu Yan[2]✉, Gareth J. Conduit[3]✉ and Zhi Wei Seh[4]✉



Johnson Matthey
Technology Review
66, 130 (2022)

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 materials, batteries, pharmaceuticals, and beyond

Taken to market through by Intellegens as Alchemite Analytics™