

intellegens

Applied machine learning

Synthetic alchemy: unleash the power of
multimodal machine learning for materials design

Dr Gareth Conduit

Alchemite™ machine learning

Use case of machine learning to extract information **beyond data**

Applications of **generic** Alchemite™ to **materials** design



Introducing Alchemite™ applied machine learning



Developed at [University of Cambridge](#)

Key use cases: [chemicals](#), [materials](#), [life sciences](#), and [manufacturing](#)

Innovative method extracts value from [sparse, noisy data](#) to solve complex, high-dimensional problems

Focus on ease-of-deployment for [immediate return on investment](#)

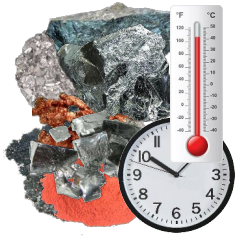
Machine learning beyond data



Strength and phase behavior are correlated



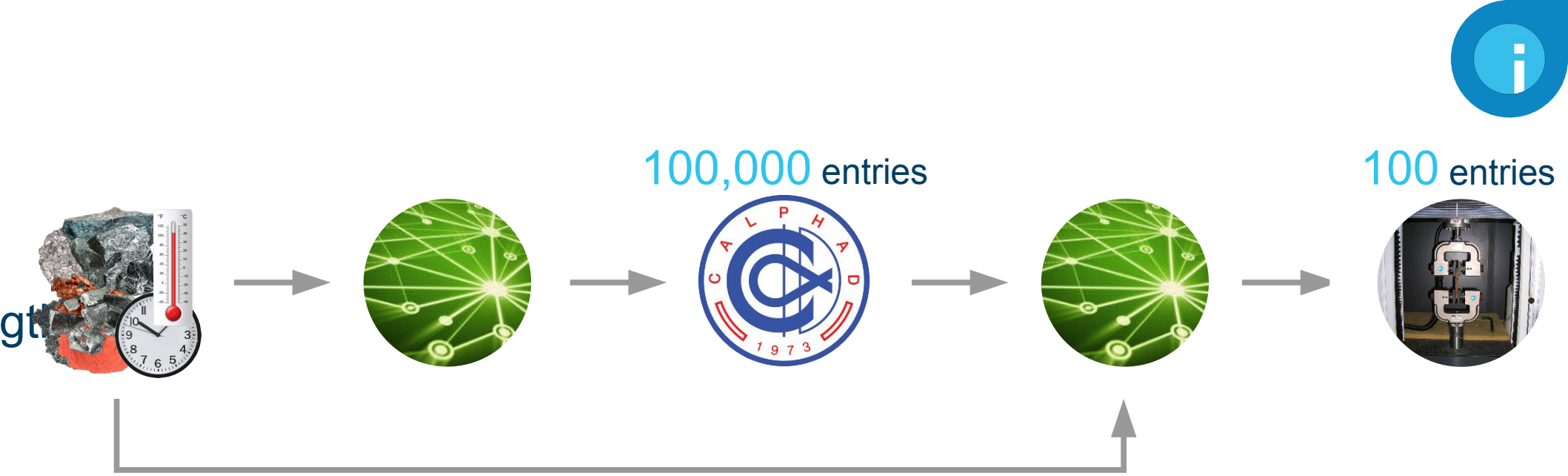
First predict phase behavior



100,000 entries



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



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

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 KΩ ⁻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%



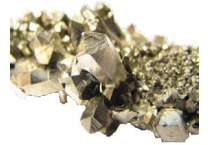
W 1.2%



Zr 0.05%



Nb 3%



Al 2.9%



C 0.04%



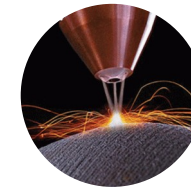
B 0.01%



Ni



Expose 0.8



T_{HT} 1300°C



Phase behavior targets



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 Ω ⁻¹m⁻³

Yield stress at 900 °C > 200 MPa

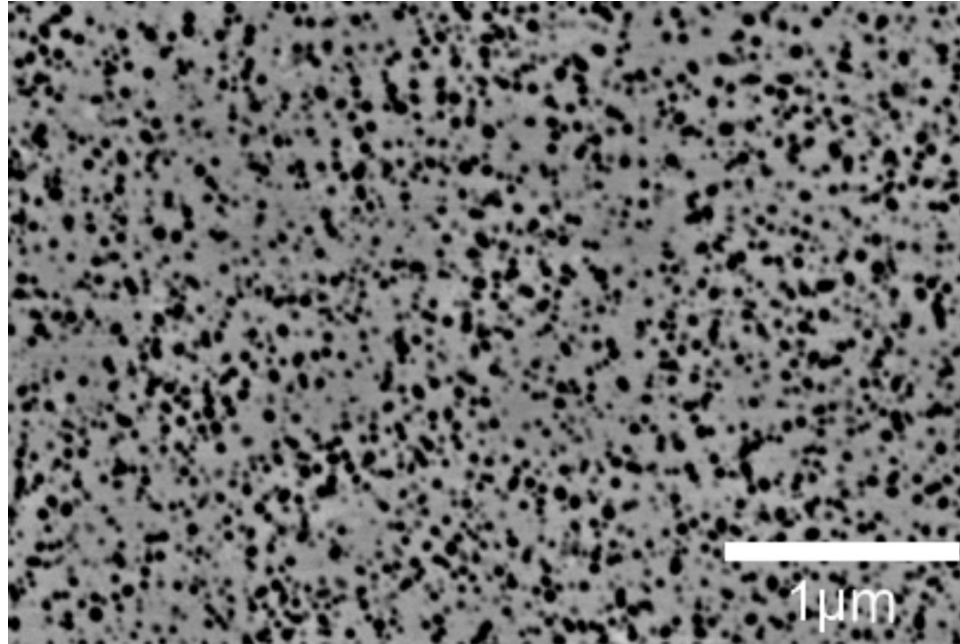
Tensile strength at 900 °C > 300 MPa

Tensile elongation at 700 °C > 8%

1000hr stress rupture at 800 °C > 100 MPa

Fatigue life at 500 MPa, 700 °C > 10⁵ cycles

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

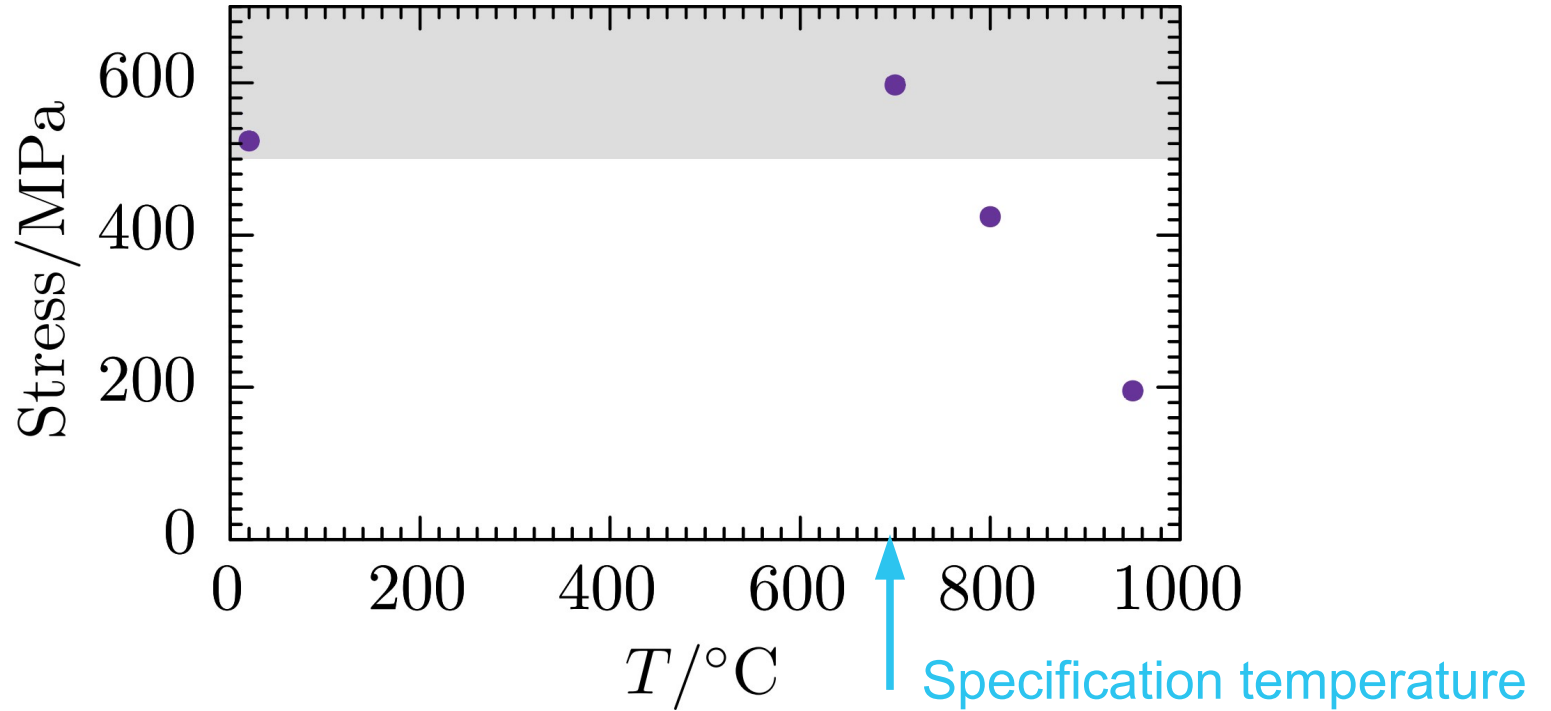
Materials & Design **168**, 107644 (2019)

Strength target



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 KΩ ⁻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

Test the high cycle fatigue stress

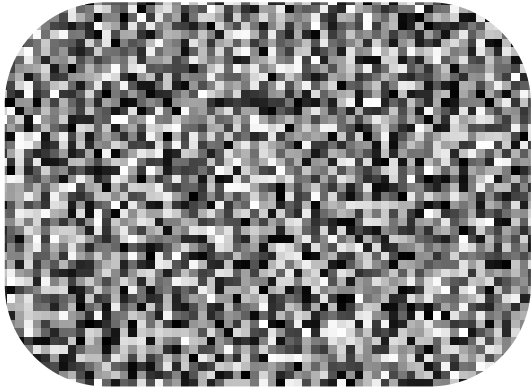


Probabilistic neural network identification of an alloy for direct laser deposition

B. Conduit, T. Illston, S. Baker, D. Vadegadde Duggappa, S. Harding, H. Stone & GJC

Materials & Design **168**, 107644 (2019)

Extract information from noise



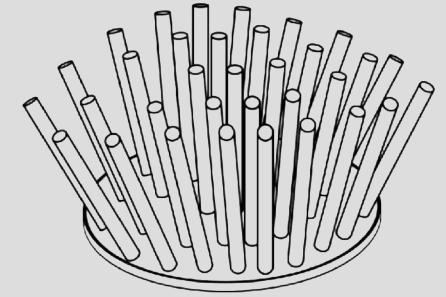
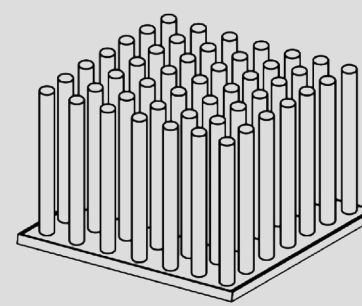
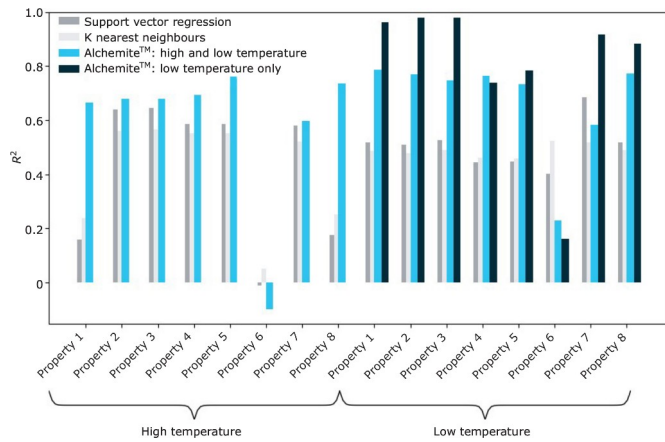
Machine learning approach to the formulation problem



Probabilistic selection and design of concrete using machine learning
Data-Centric Engineering 4, e9 (2023)

Real-life use of Alchemite™

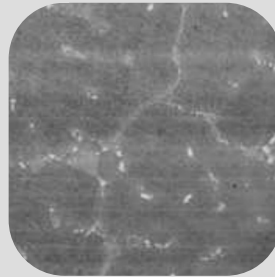
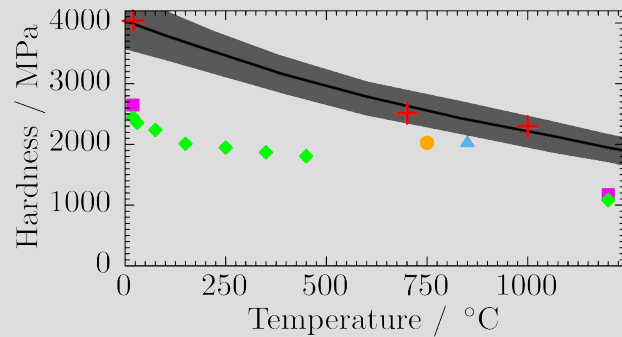




Johnson Matthey Technology Review
66, 130 (2022)



NASA Technical Memorandum
20220008637



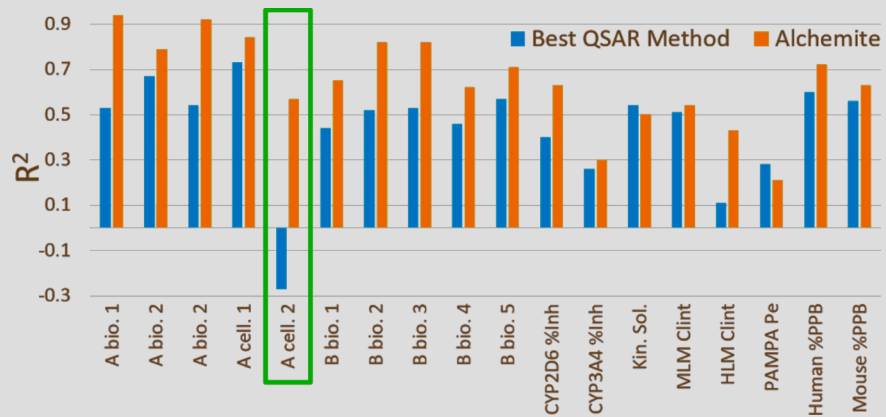
Alloy	Source	ANN	$\Delta\sigma$	Actual
Steel AISI 301L	193	269	5	238[23]
Steel AISI 301	193	267	5	221[23]
Al 1080 H18	51	124	5	120[23]
Al 5083 wrought	117	191	14	300,190[4, 23]
Al 5086 wrought	110	172	11	269,131[4, 23]
Al 5454 wrought	102	149	14	124[23]
Al 5456 wrought	130	201	11	165[23]
INCONEL600	223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

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



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

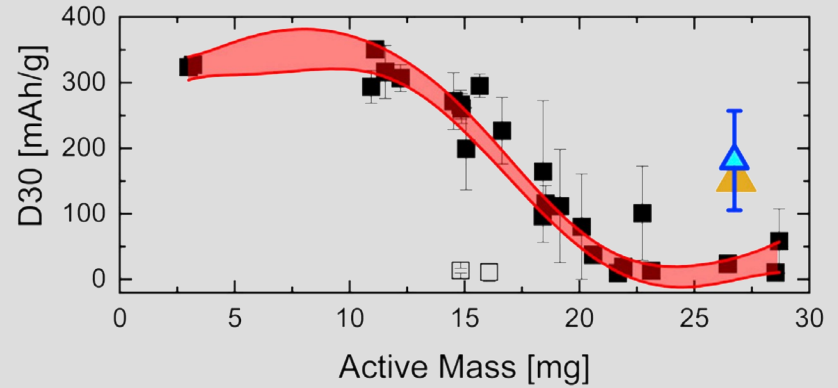
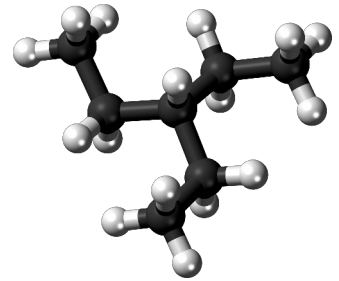




J. of Chem. Info. & Model. **60**, 2848 (2020)
 Applied AI Letters **2**, e31 (2021)
 Molecular Pharmaceutics **19**, 1488 (2022)



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 **2**, 161 (2020)
 Cell Reports Physical Science **2**, 100683 (2021)

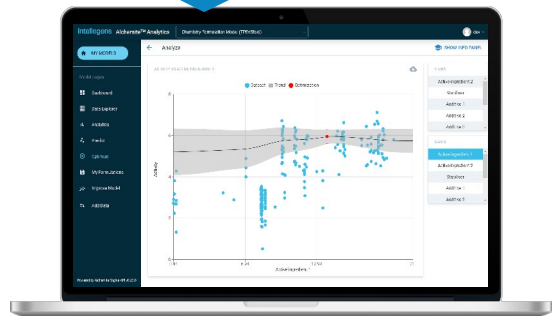


Intellegens offers the Alchemite™ product family



Scientists & engineers

Fast start, easy-to-use, visual



←
*Option to
deploy models*

Alchemite™ Analytics

Deep data insights on your desktop
Guide experiments, predict, design, optimize

Data scientists

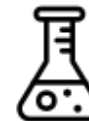
Add to your ML toolkit



Alchemite™ Engine

Integrate into your workflow (API, Python)
Advanced configuration, enterprise deployment

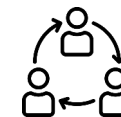
*Optional
connectors*



Lab systems



*Software &
scripts*



*Sharing &
collaboration*

**Alchemite™
Success**

Apply Intellegens deep learning expertise
Advice to your data science team or full project management

Alchemite™ enables machine learning **beyond data**

Include **first principles** simulations and extract **information from noise**

Generic approach applied to many physical, chemical, and biological sciences

