



Advanced material design
using deep learning

Alchemite™ optimized design process

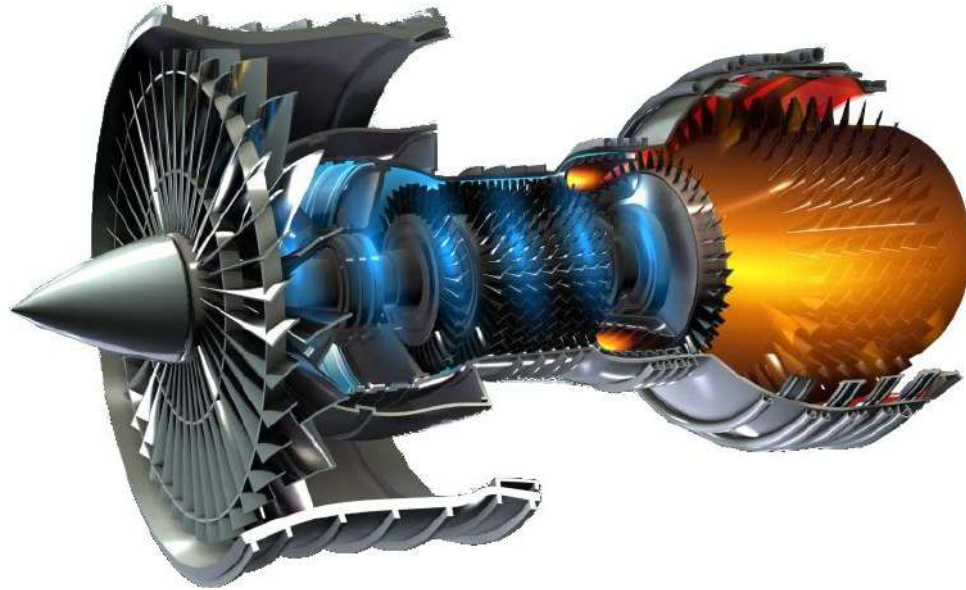
Machine learning software to aid experimental design
developed at University of Cambridge

Alchemite™ predicts from **available** inputs

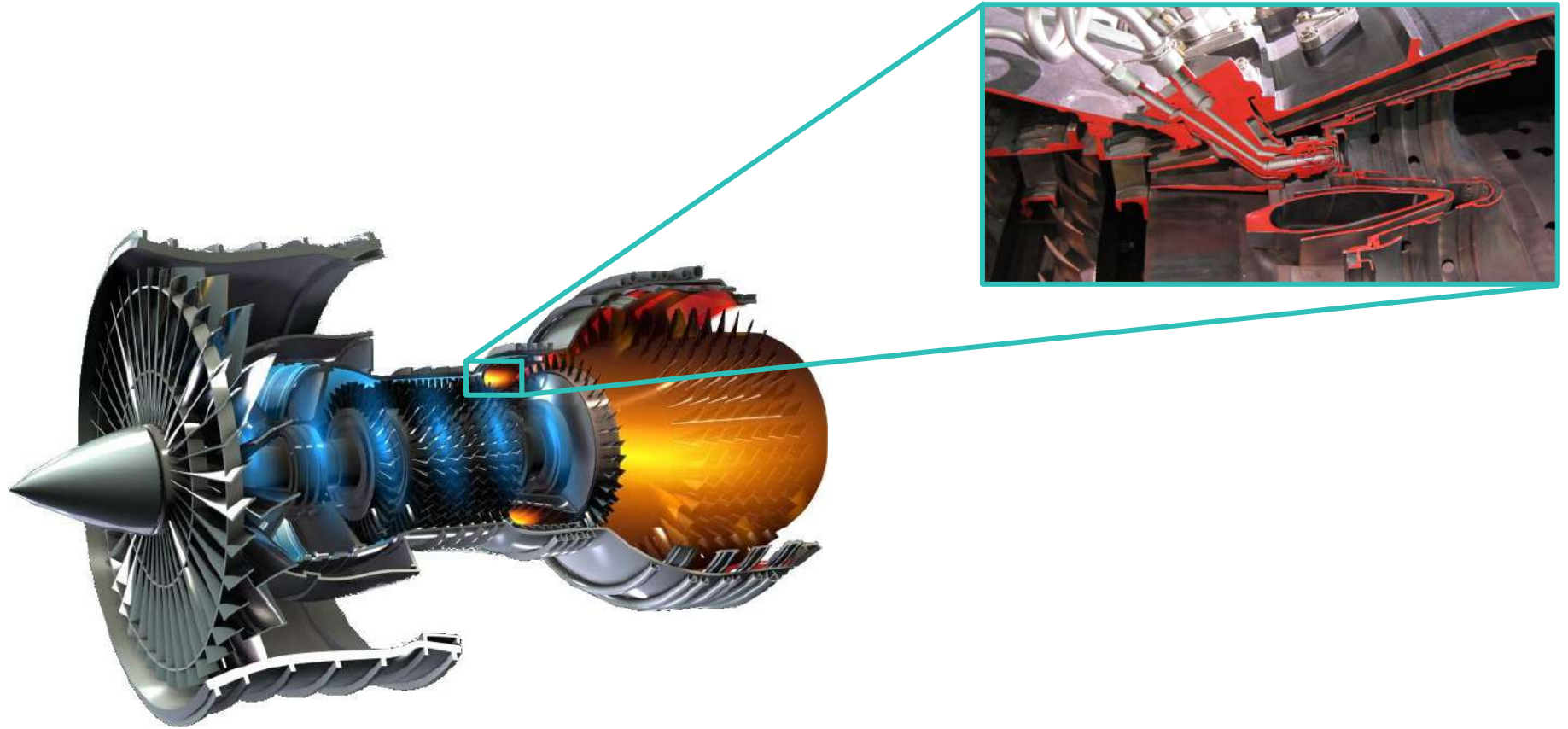
Reduce costs - 90% reduction in experiments and fewer
measurements for expensive quantities

Accelerate discovery and validation to 2 years

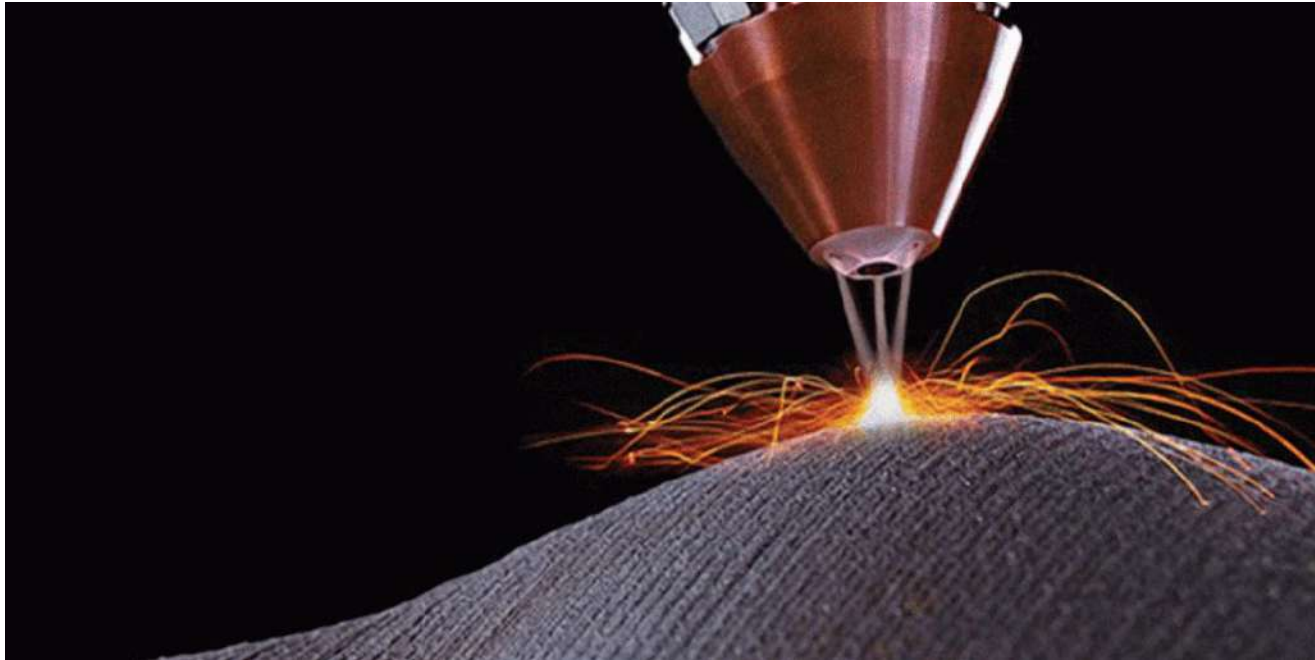
Case study: alloy for direct laser deposition



Case study: additive manufacturing



Additive manufacturing requires new alloys



Machine learning



Processability



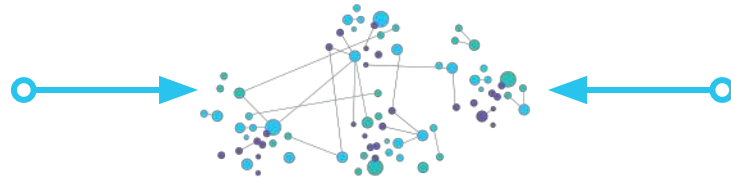
Fatigue life



Cost



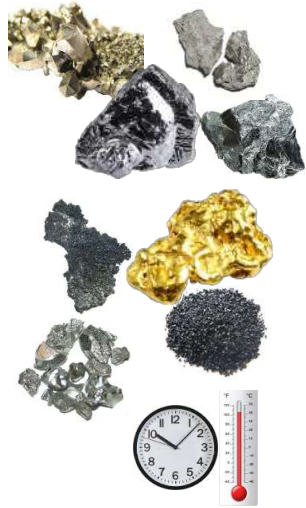
Machine learning



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Fatigue life
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Machine learning



Processability



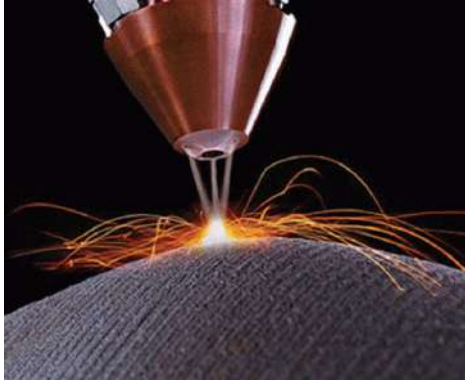
Fatigue life



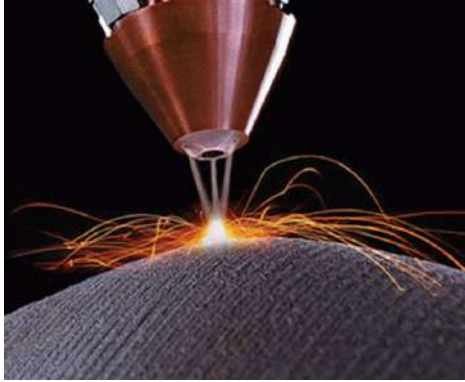
Cost



Case study: alloy for direct laser deposition



Direct laser deposition is similar to welding

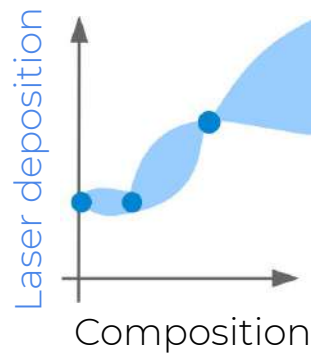


Direct laser
deposition

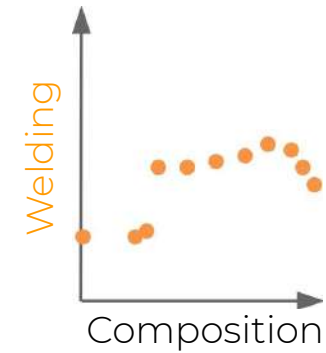
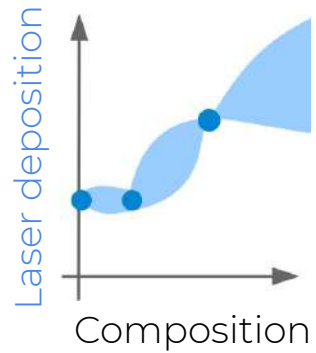


Welding

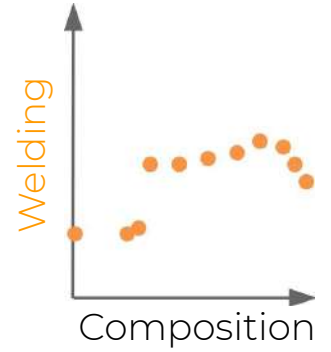
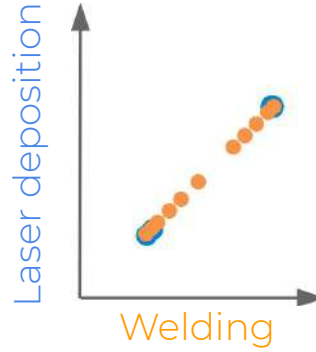
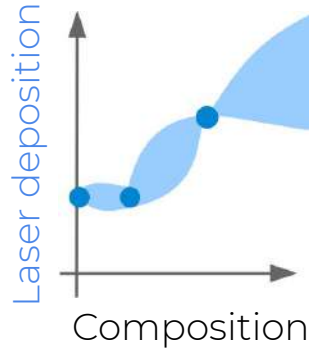
Lack of data for laser deposition



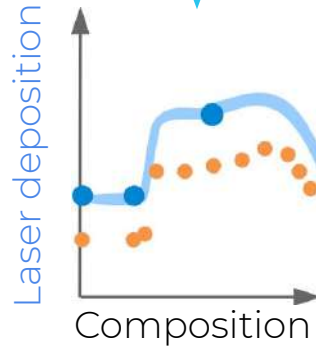
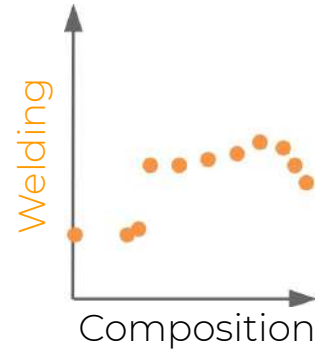
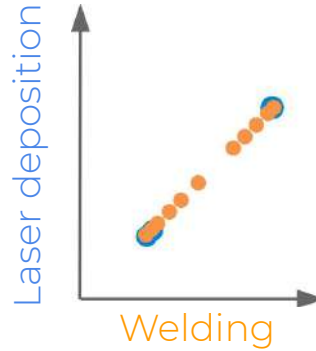
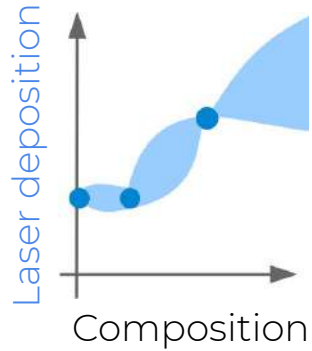
Large amount of welding data



Simple welding-deposition relationship



Welding data guides extrapolation



Targets for direct laser deposition alloy

Elemental cost	< 25 \$kg ⁻¹
Density	< 8500 kgm ⁻³
γ' content	< 25 wt%
Oxidation resistance	< 0.3 mgcm ⁻²
Processability	< 0.15% defects
Phase stability	> 99.0 wt%
γ' solvus	> 1000 °C
Thermal resistance	> 0.04 K Ω^{-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 of alloy for direct laser deposition

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 balance



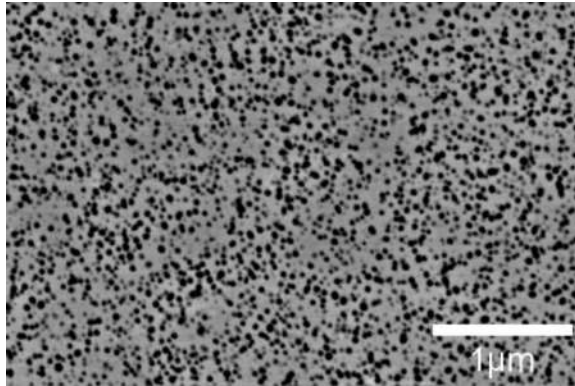
Exposure 0.8



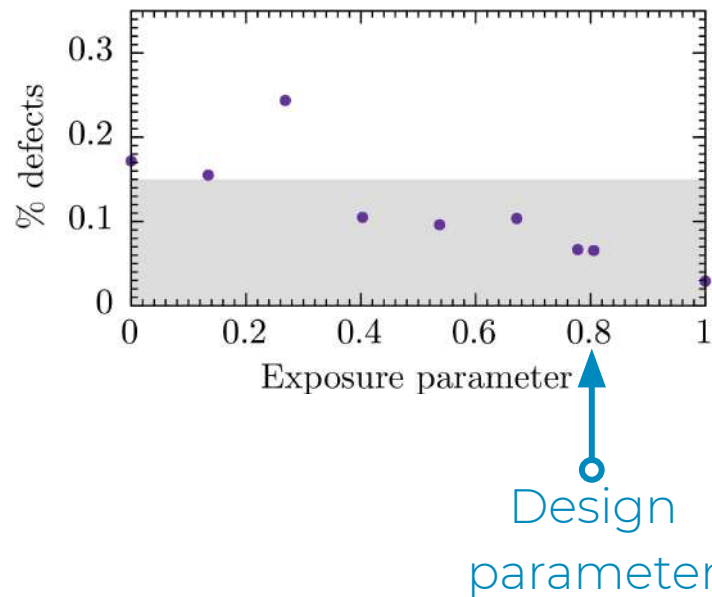
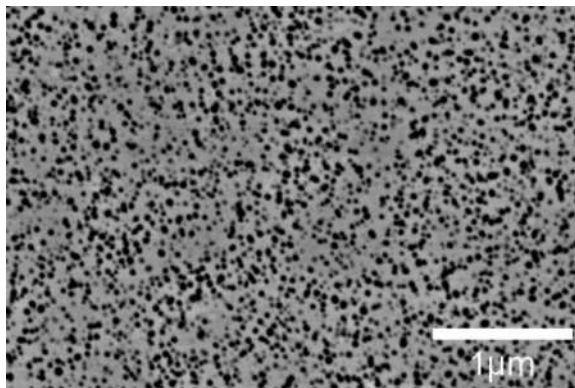
T_{HT} 1230°C



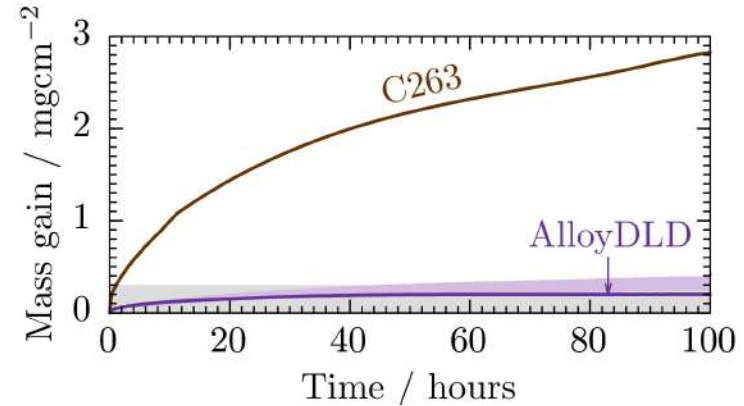
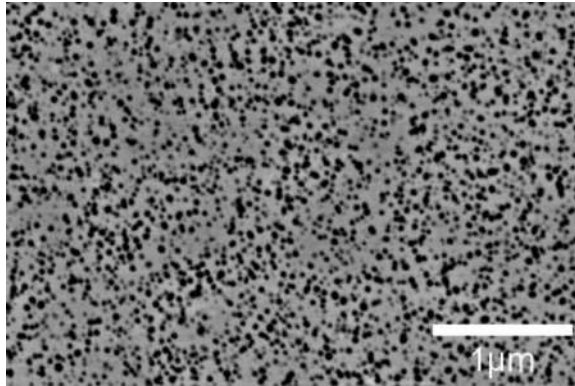
Experimental validation: microstructure



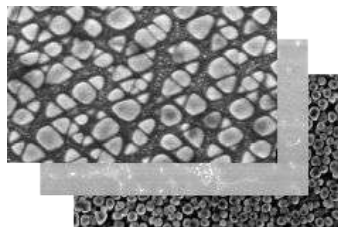
Experimental validation: defects



Experimental validation: oxidation resistance



Further materials and drug design



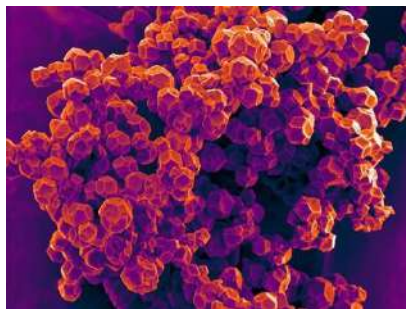
Nickel & moly alloys



Batteries



Steels for welding



Metal-organic framework

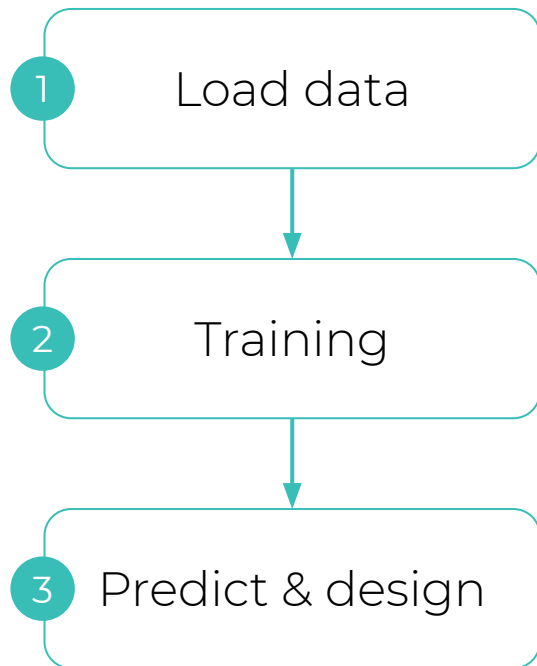


Concrete



Drug design

Future opportunities: Integrated software



Predicting properties of steel

We demonstrate a neural network that predicts the physical properties of steels based on the composition and heat treatment. The neural network model was trained from a library of experimental data from 1000 alloys.

In the first panel below set the percentages of each element in the composition and heat treatment temperature, and then click predict to get the neural network estimates for yield stress, ultimate tensile strength, and elongation.

Click [here](#) to use this technology to optimize the yield stress, ultimate tensile strength, and elongation of the steel.

This same technology was used to understand nickel alloys where the composition covered 20 elements, 5 heat treatment parameters, and predicted 11 material properties. Click [here](#) to read more about this study.

Click here to optimize a composition for given targets

Set inputs		
Iron (Fe)	100	remain %
Carbon (C)	0	0 to 0.43 %
Manganese (Mn)	0	0 to 3.0 %
Silicon (Si)	0	0 to 4.75 %
Chromium (Cr)	0	0 to 17.5 %
Nickel (Ni)	0	0 to 21.0 %
Molybdenum (Mo)	0	0 to 9.67 %
Vanadium (V)	0	0 to 4.32 %

PREDICT

Predictions

Yield Stress (MPa)	1605 ± 46
Ultimate Tensile Strength (MPa)	1200 ± 67
Elongation (%)	9 ± 2

Uses of Alchemite™

Validate data

Identify outliers and impute missing data

Guide experiments

Recommend the next experiment to improve understanding

Optimise formulations

Design material that satisfies targets and understand the effect of altering each ingredient

Deployment of Alchemite™

Consulting project

One-off project to design a new material

Alchemite™ engine & analytics platform

Deploy for use by engineers & scientists



Alchemite™ engine API

Deploy AI engine via an API into current software used by organisation

Bespoke tool development

Front-end development of bespoke tools for the Alchemite™ engine

Summary of future opportunities of Alchemite™

Alchemite™, a full stack machine learning solution to **merge** sparse data

Designed and **experimentally verified** material for thermometry, and other alloys and drugs

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Demo	https://app.intellegens.ai/steel_optimise
Papers	https://www.intellegens.ai/paper.html