



Machine learning for the design of
materials, chemicals, and drugs

About

University of Cambridge spin out

Machine learning software to aid experimental design

Merge and aggregate data

Predictive models **reduce costs** and **accelerate discovery**
process

Traditional experimental design

Process is **expert driven**, subjective, and **iterative** through trial and improvement

Process takes ~20 years and specialist alloys cost >\$10m to develop, drugs cost >\$1bn

Alchemite™ machine learning

Standard algorithms need **all** inputs to calculate outputs

Typical experimental data is 0.05% complete

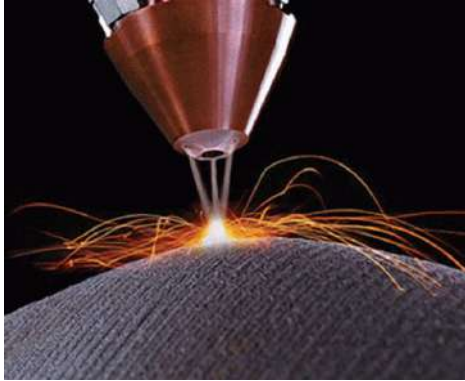
Alchemite™ predicts from **available** inputs

Optimized design process

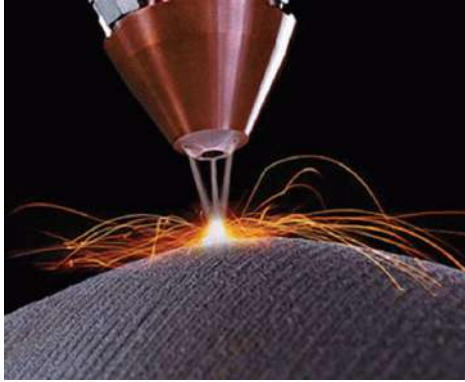
Reduce costs - 90% reduction in experiments and fewer measurements for expensive quantities

Accelerate discovery and validation to 2 years

Case study: alloy for direct laser deposition



Direct laser deposition is similar to welding

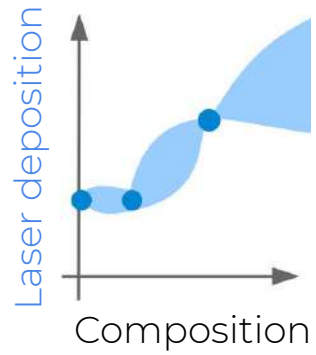


Direct laser
deposition

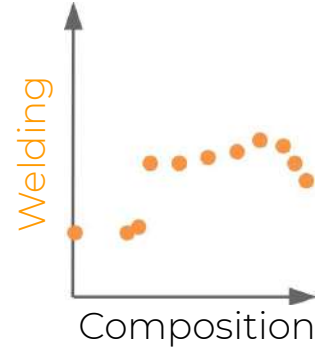
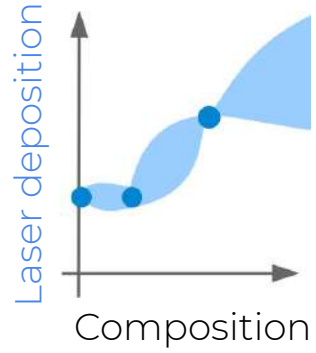


Welding

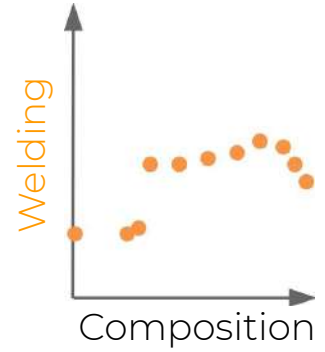
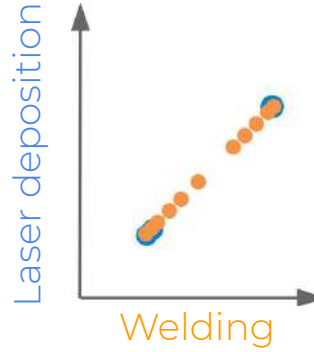
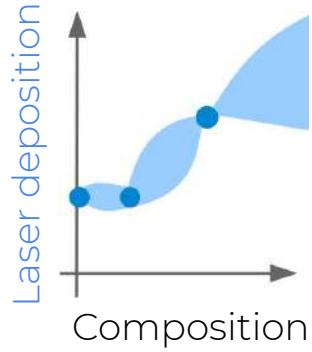
Lack of data for laser deposition



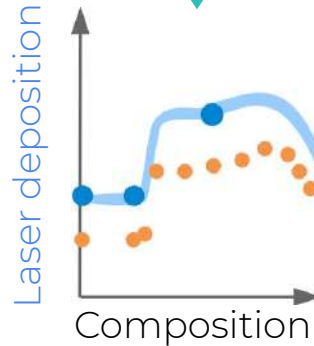
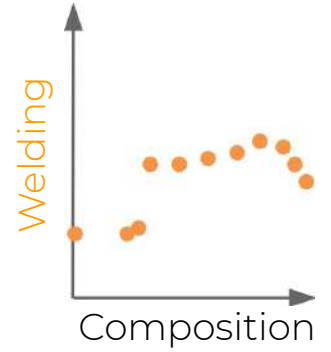
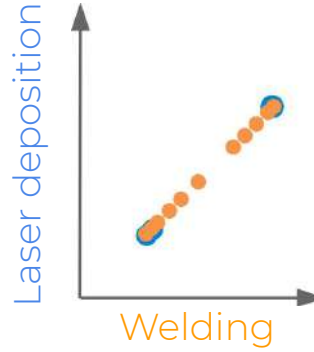
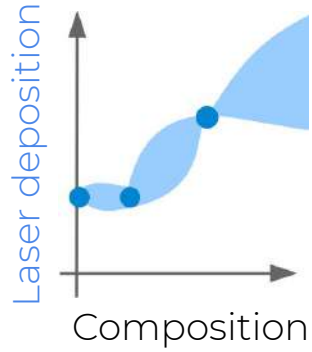
Large amount of welding data



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



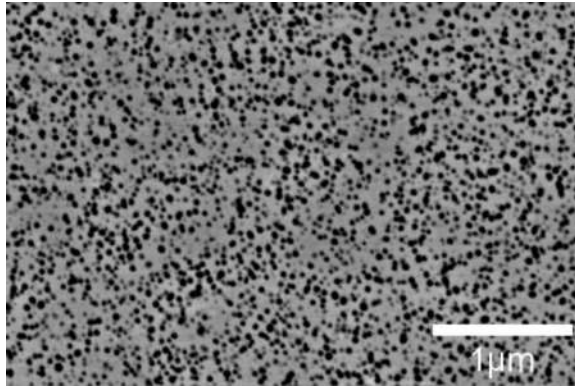
Exposure 0.8



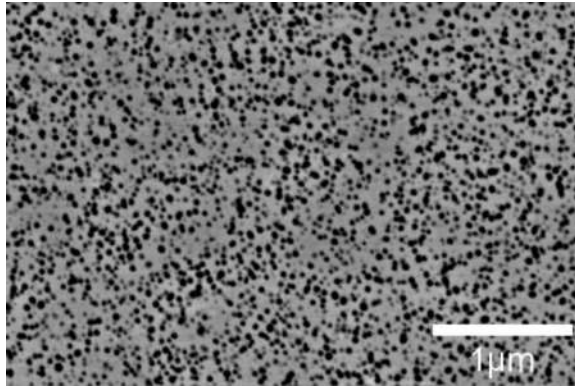
T_{HT} 1230°C



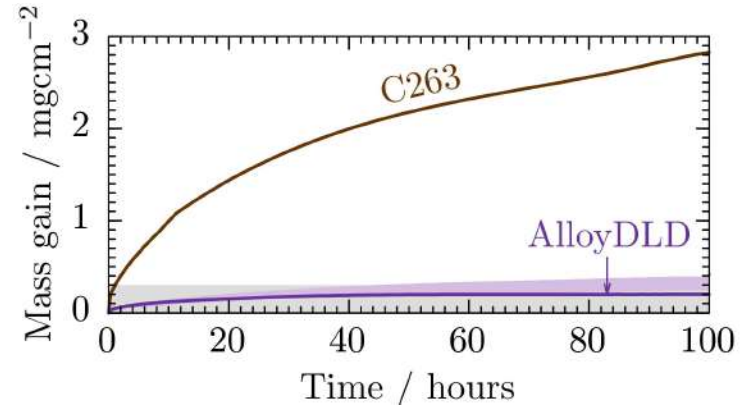
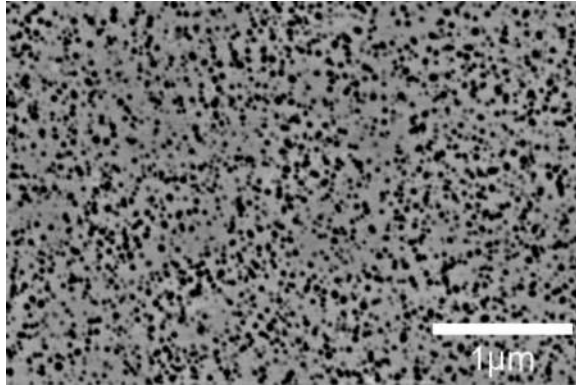
Experimental validation



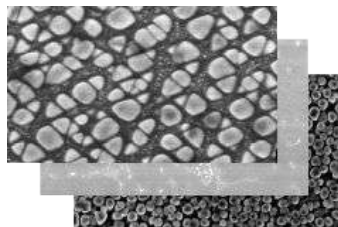
Experimental validation



Experimental validation



Further materials and drug design



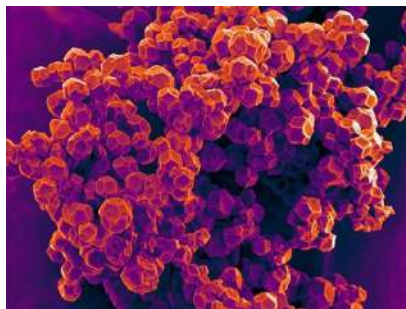
Nickel & moly alloys



Batteries



Steels of welding



Metal-organic framework

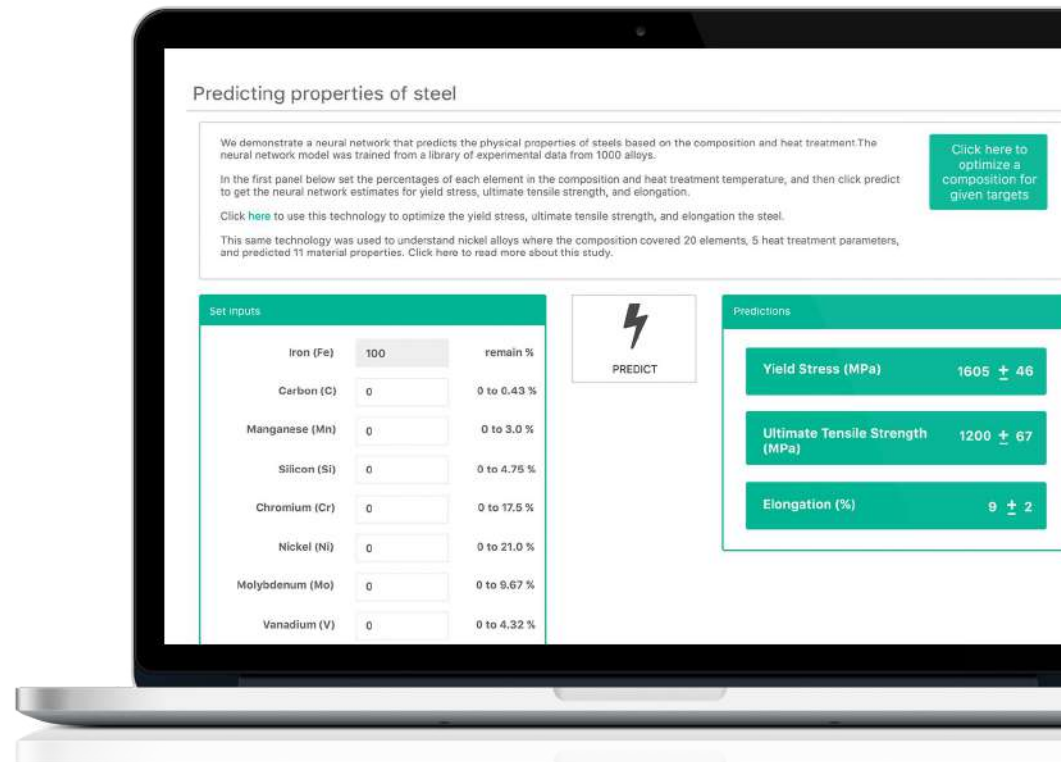
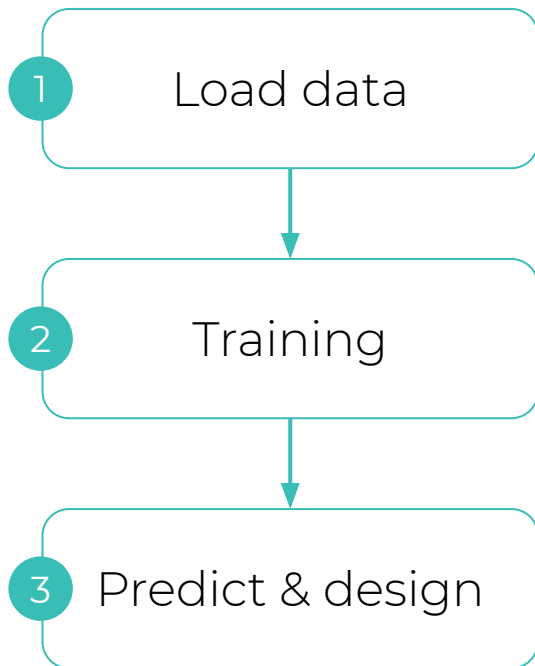


Lubricants



Drug design

Future opportunities: Integrated software

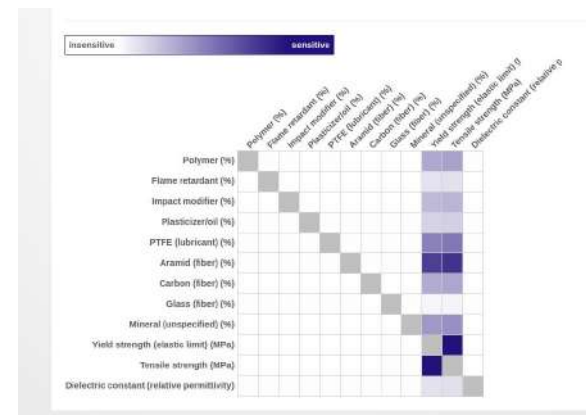
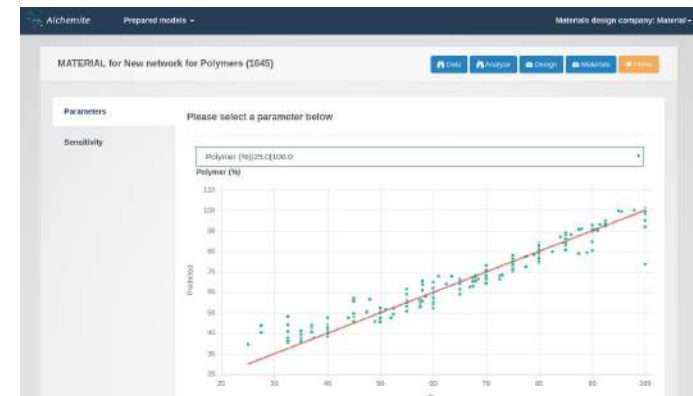


Manage and analyse models

Alchemite Prepared models Materials design company: Material

Dashboard Project settings Create a new model

Status	Name	Raw data	Accuracy	Train time	
✓	Model for hardness_loss_v2.csv: 574 hardness_loss_v2.csv	67 rows, 10 cols	78% <div style="width: 78%;"></div>	43.63	Data Analyse Design Materials ⌵
✓	Model for Titanium_set4.csv: 470 Titanium_set4.csv	52 rows, 24 cols	71% <div style="width: 71%;"></div>	5.26	Data Analyse Design Materials ⌵
✓	New network for Polymers Polymer_sample.csv	885 rows, 12 cols	66% <div style="width: 66%;"></div>	389.28	Data Analyse Design Materials ⌵



Design, analyse, and share new materials

Materials design company: Material

MATERIAL for Model for hardness_loss_v2.csv: 574 (2038)

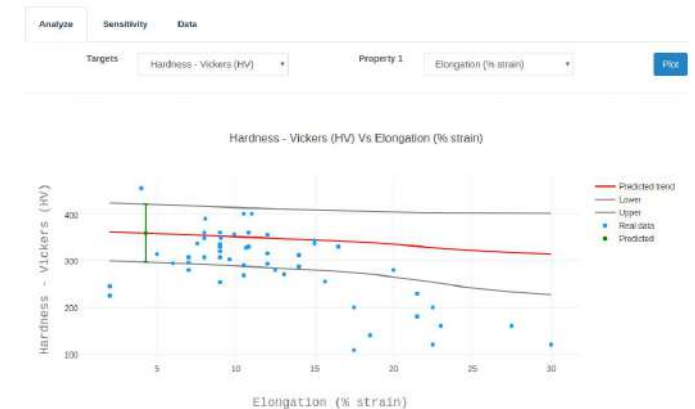
Data Analyze Design Materials Home

Design Material

Please use the form below to add desired targets variables, other variables will be optimised

Design globally or locally

Type	Name	Value	Target	Designed values	Uncertainty
	C (0.0 - 5.91)	0.035	Target: Above		
	Mn (0.0 - 15.58)	0.88	Target: Exact		
	Si (0.0 - 2.07)	0.43	Design start		
	Cr (0.0 - 32.6)	1.6	Design start		
	Mo (0.0 - 6.3)	0.37	Design start		
	V (0.0 - 1.25)	0.0	Design start		
	Nb (0.0 - 6.46)	0.0	Design start		



Summary of future opportunities of Alchemite™

Seek applications of Alchemite™ full stack solution to **merge** sparse data

Designed and **experimentally verified** alloy for direct laser deposition, and other alloys and drugs

Contact

ben@intellegens.ai

Website

<https://intellegens.ai>

Demo

https://app.intellegens.ai/steel_optimise

Papers

<https://www.intellegens.ai/paper.html>