Intellegens

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

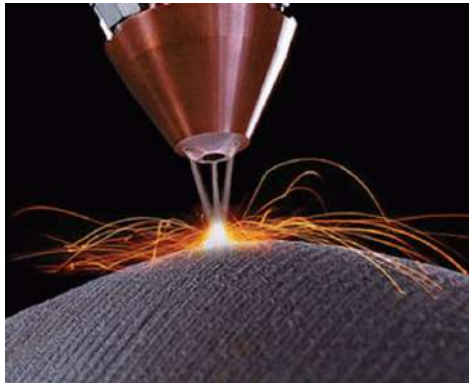
Alchemite™ predicts from available inputs

Optimized design process

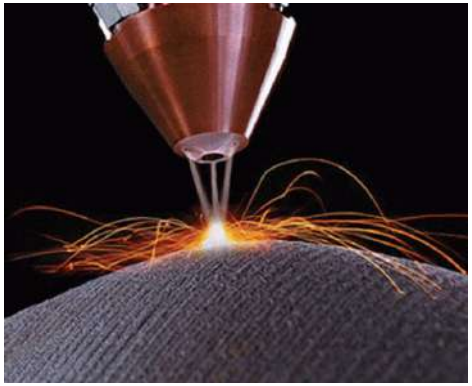
Reduce costs - 90% reduction in experiments and fewer measurements for expensive quantities

Accelerate discovery and validation to 2 years

Case study: alloy for direct laser deposition



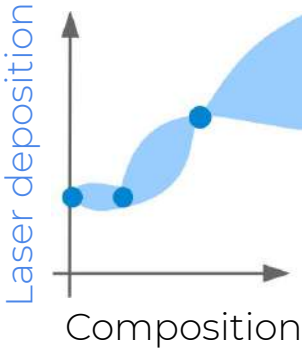
Direct laser deposition is similar to welding



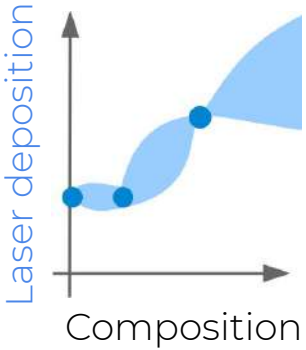
Direct laser deposition

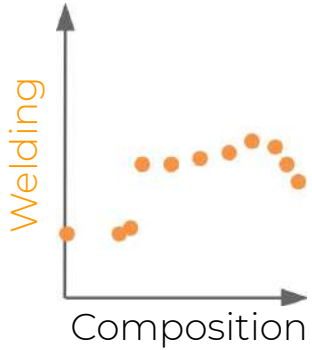
Welding

Lack of data for laser deposition

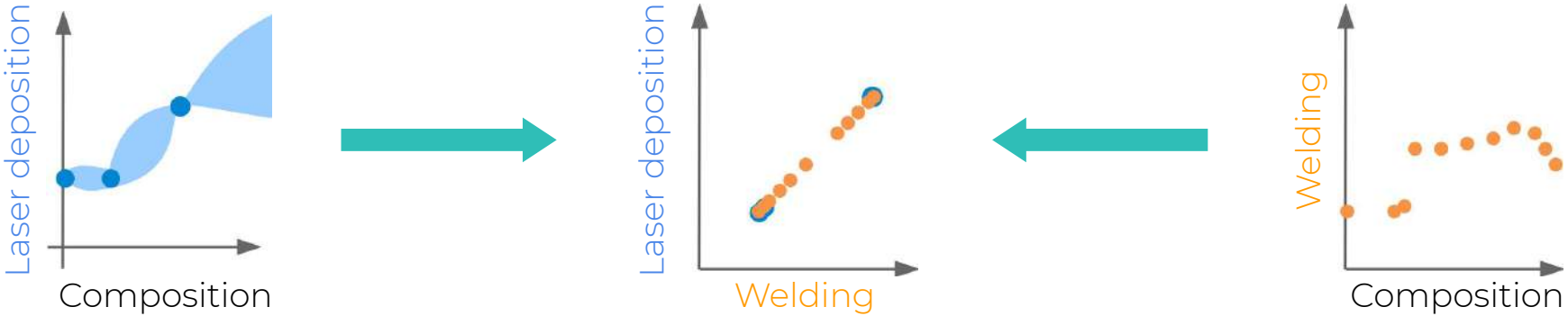


Large amount of welding data

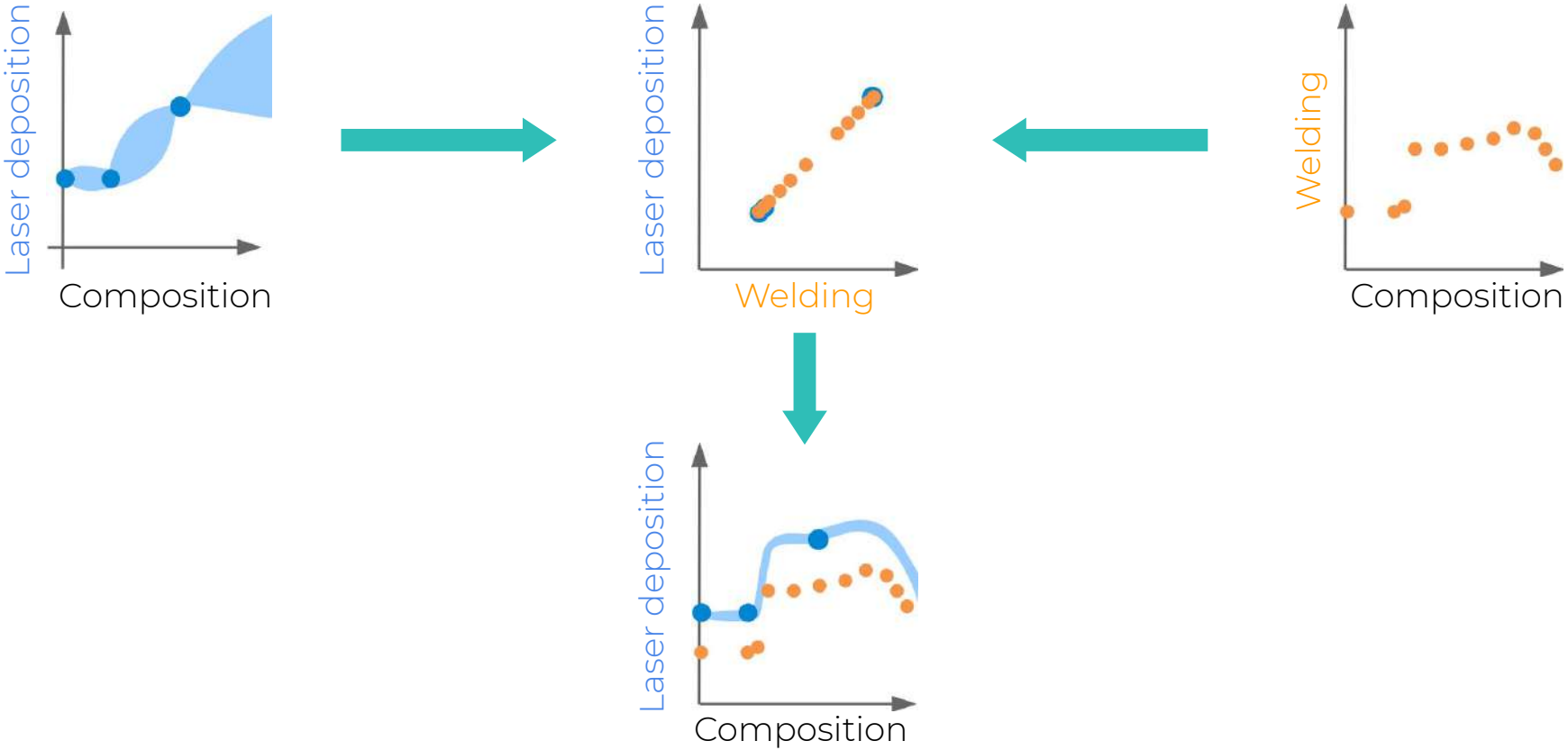




Simple welding-deposition relationship



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

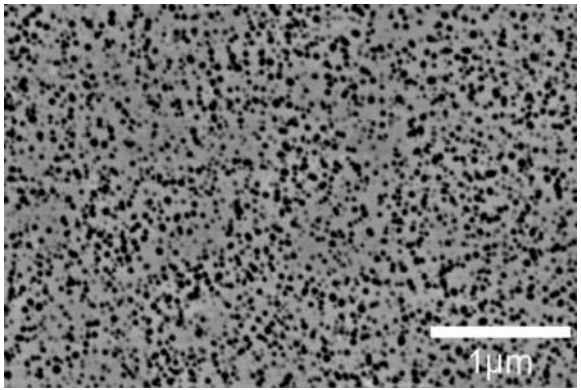
B 0.01%

Ni balance

Exposure 0.8

T_{HT} 1230°C

Experimental validation



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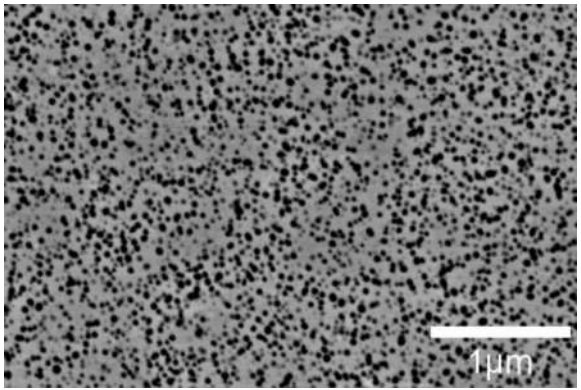
Experimental validation



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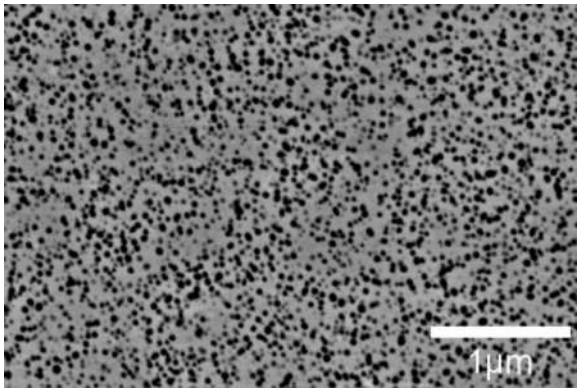
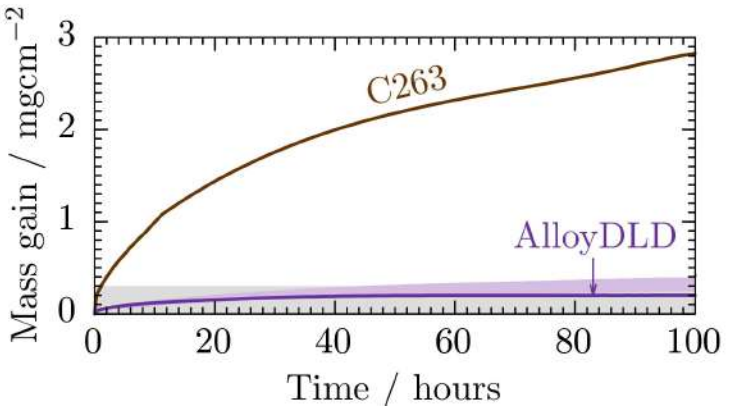
Experimental validation





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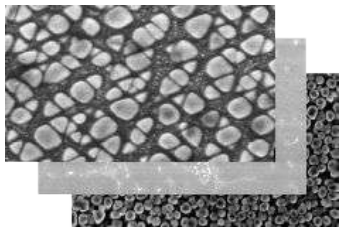
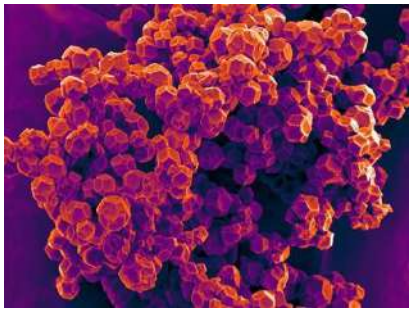
Further materials and drug design



Nickel & moly alloys

Batteries

Steels of welding



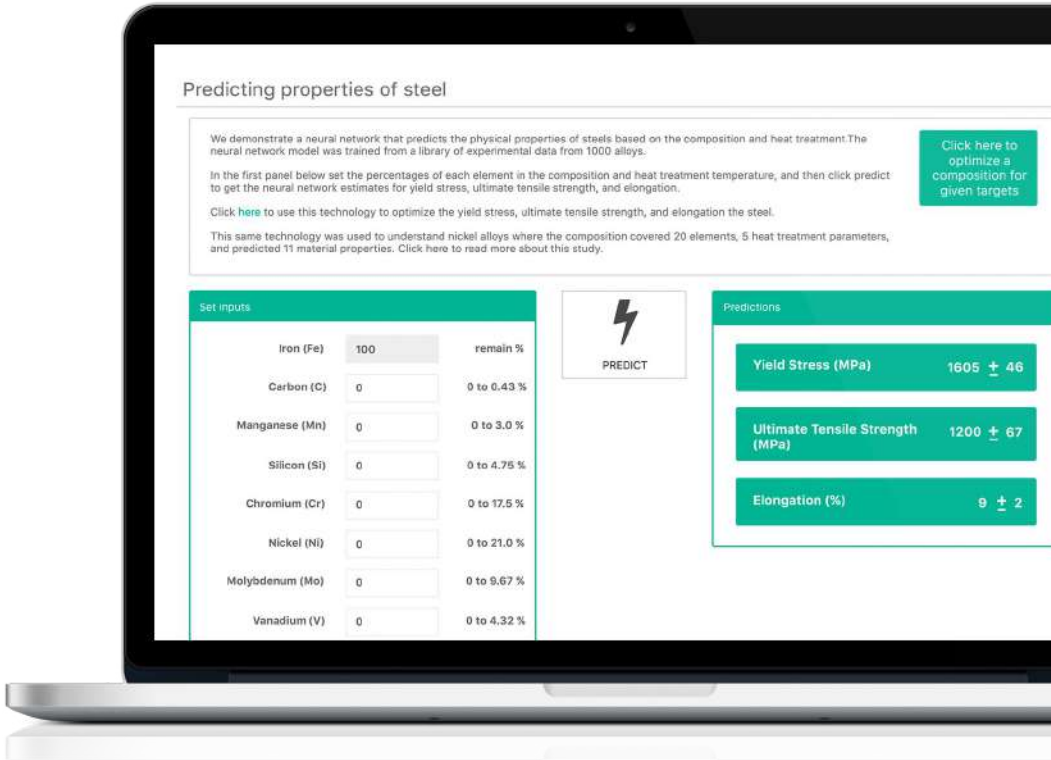
Metal-organic framework

Lubricants

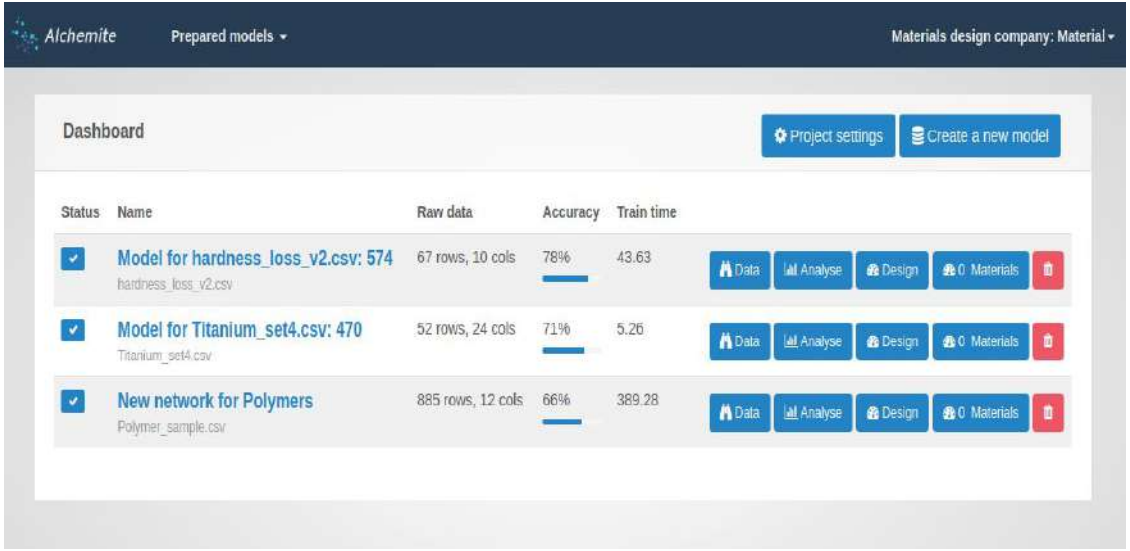
Drug design

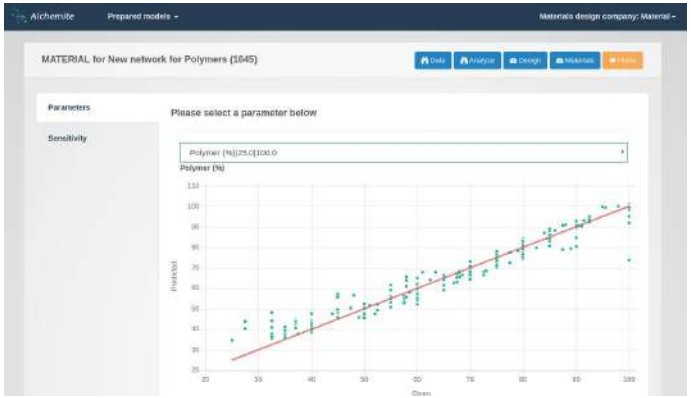
Future opportunities: Integrated software

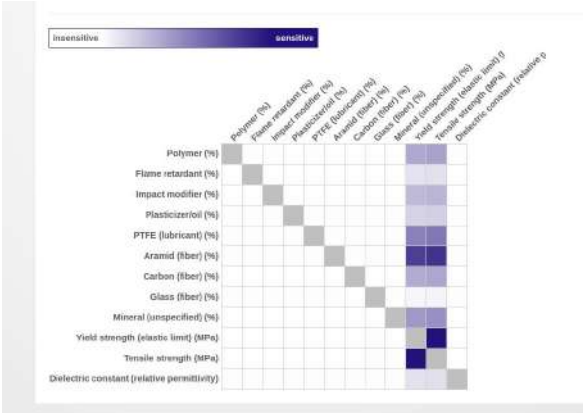
1. Load data
2. Training
3. Predict & design



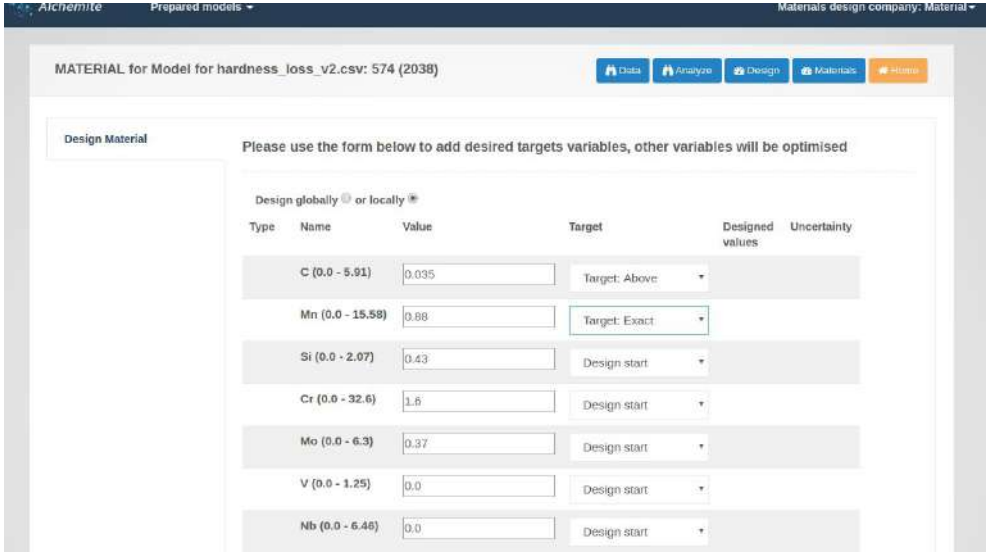
Manage and analyse models

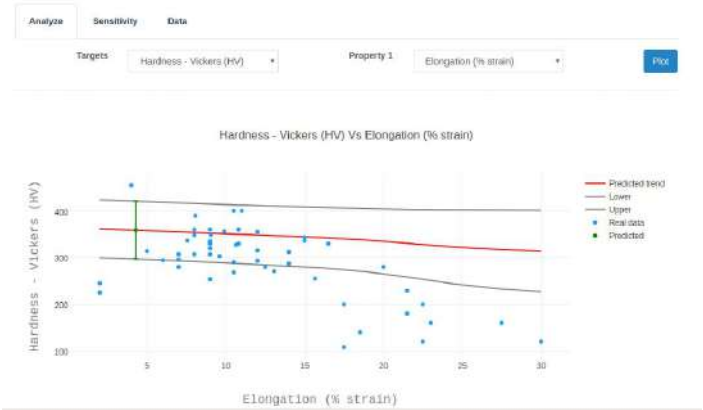






Design, analyse, and share new materials





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

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Papers	https://www.intellegens.ai/paper.html