Intellegens

UNIVERSITY OF CAMBRIDGE

# The modern-day blacksmith

Gareth Conduit

# About

Machine learning software to aid experimental design

Merge and aggregate all sources of data: experimental, computational, and analytical

Predictive models reduce costs and accelerate discovery process

# Traditional experimental design

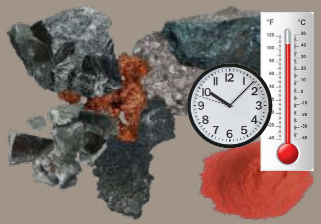
Process is expert driven, subjective, and iterative through trial and improvement

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

# Standard machine learning

Standard algorithms exploit composition-property correlations

Composition



Properties

# Alchemite™ machine learning on sparse data

Standard algorithms exploit composition-property correlations

Alchemite™ predicts from available inputs: property-property correlations and computer simulations

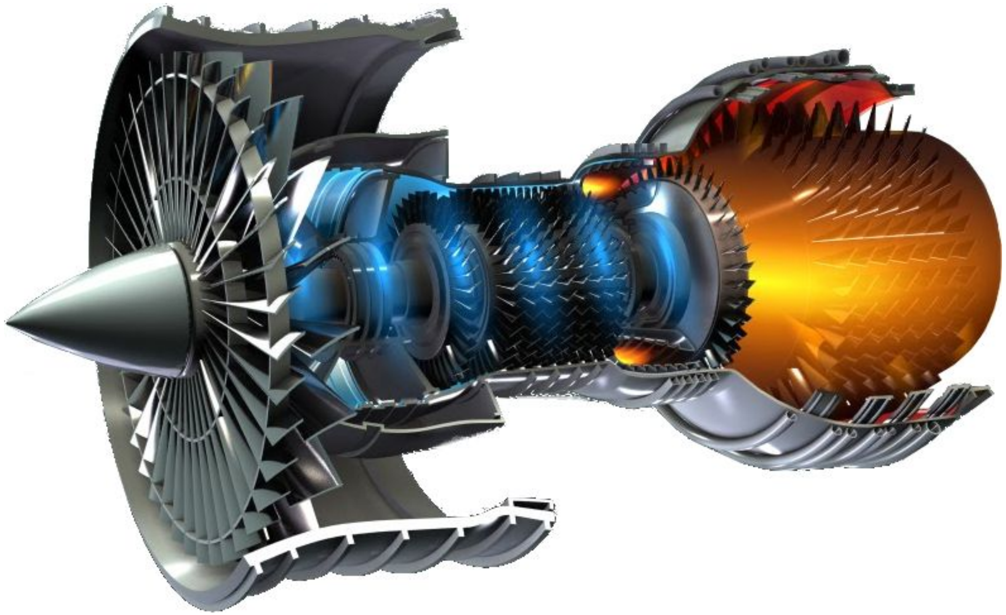
Typical experimental data is 0.2% complete so algorithm must handle missing data

# Optimized design process

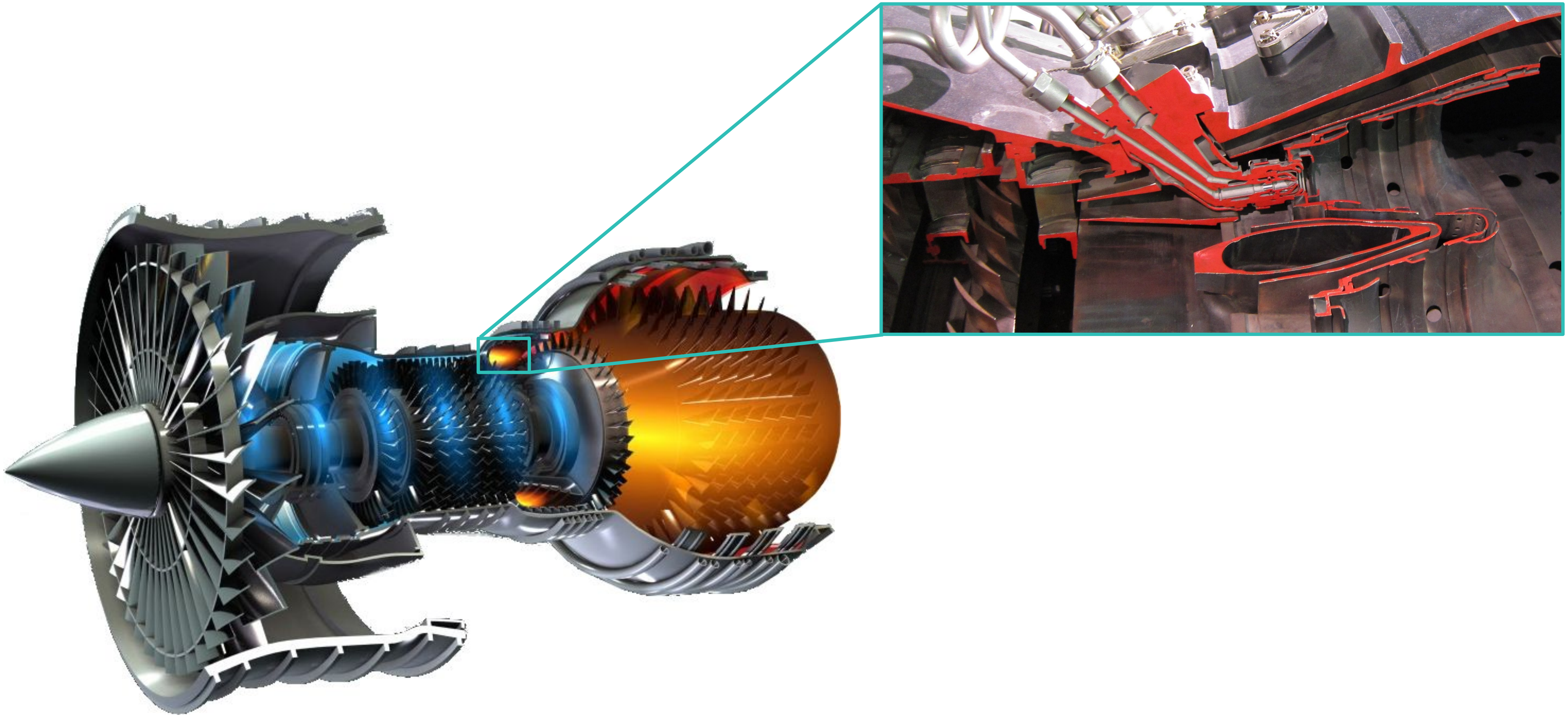
Reduce costs - 90% reduction in experiments and fewer measurements for expensive quantities

Accelerate discovery and validation to 2 years

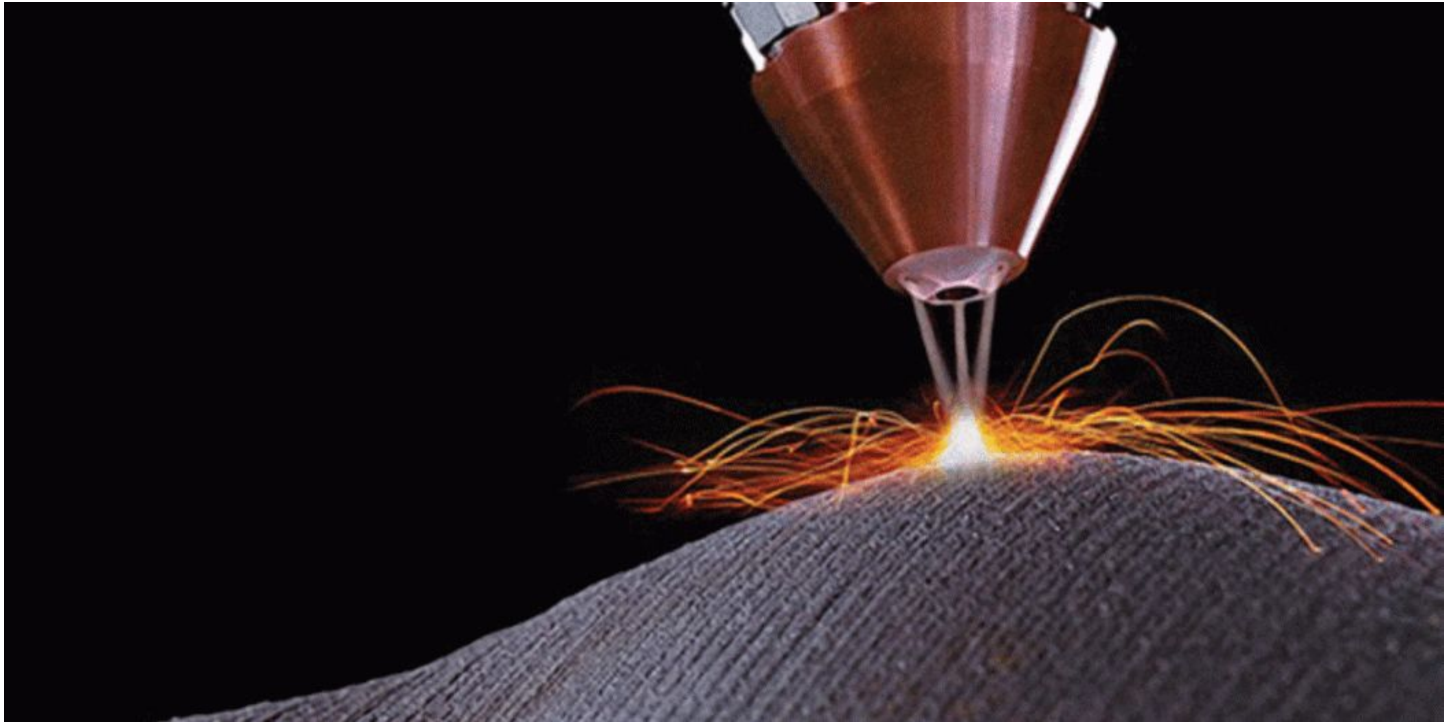
# Schematic of a jet engine



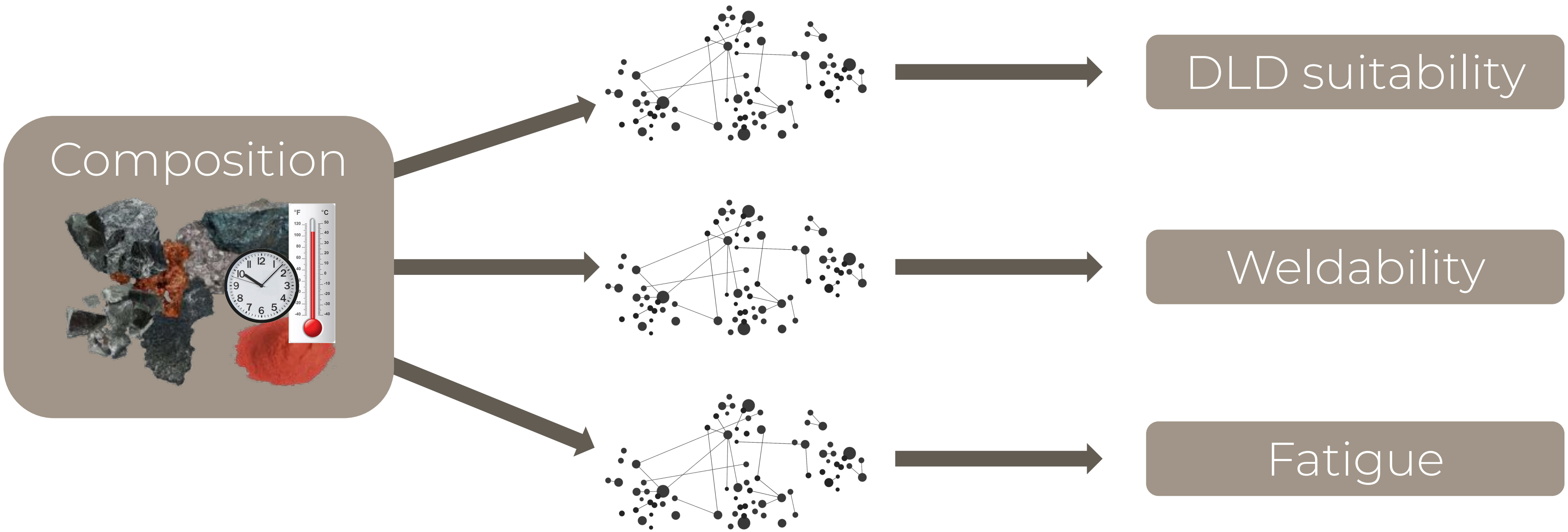
# Combustor in a jet engine



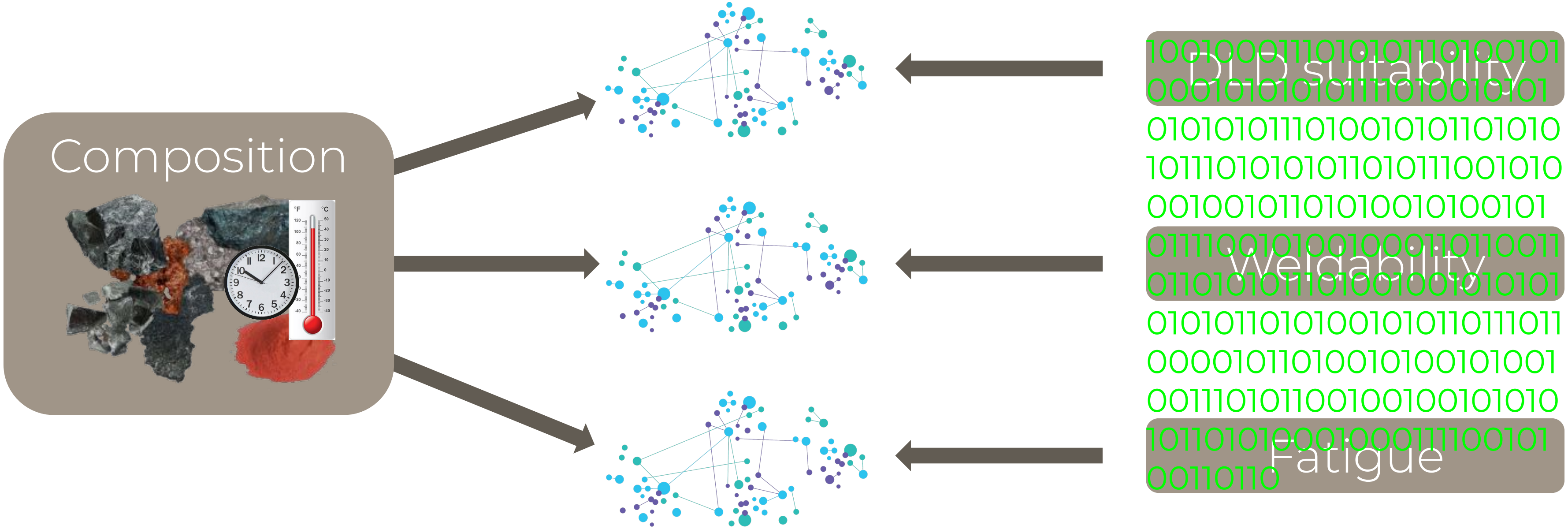
# Direct laser deposition requires new alloys



# Black box for materials design



# Train from existing data



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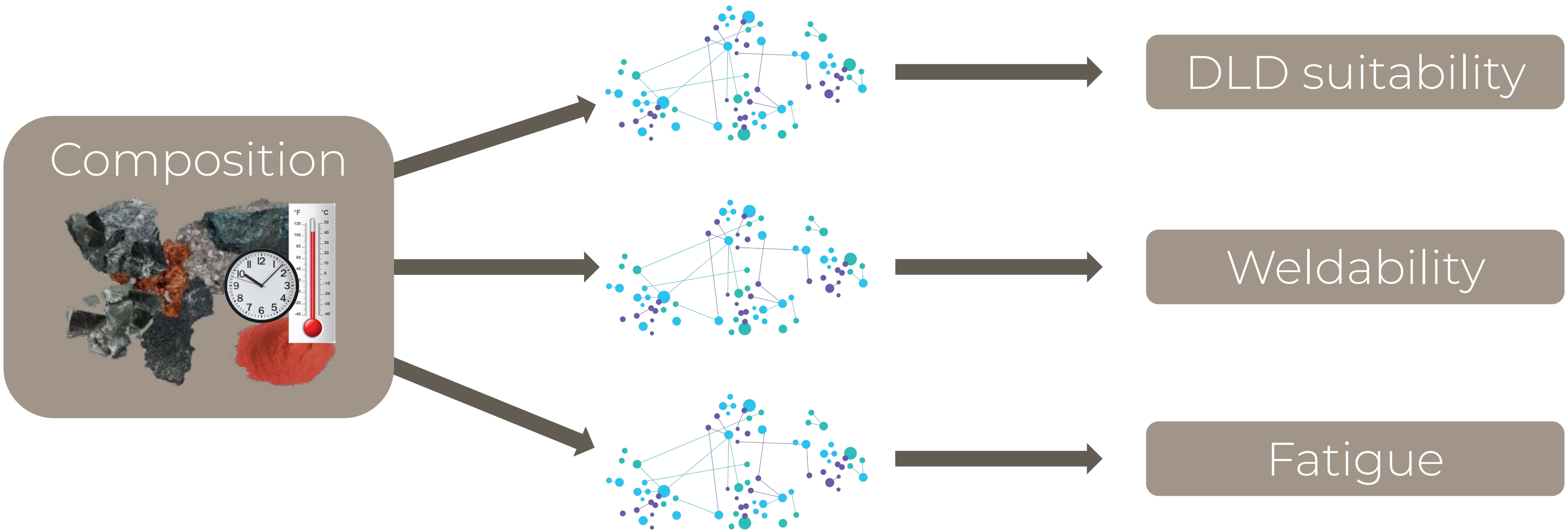
# Predict to design new materials



# Little data to discover new materials

Only 10 results available for suitability for direct laser deposition

Simplest possible machine learning model is a straight line

$y = mx + c$

# Little data to discover new materials

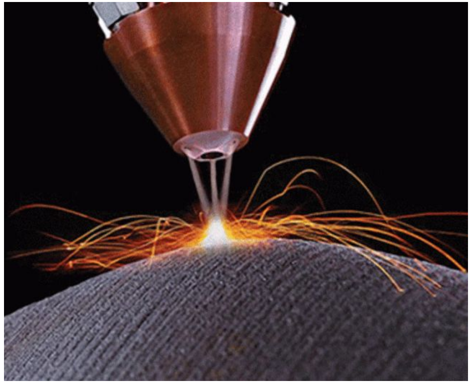
Only 10 results available for suitability for direct laser deposition

Simplest possible machine learning model is a hyperplane

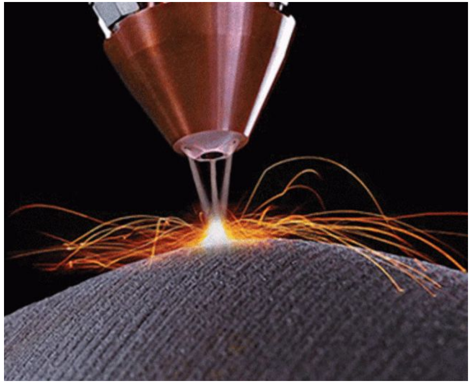
$$y = m_1x_1 + m_2x_2 + m_3x_3 + \dots + m_{30}x_{30} + c$$

Mathematical impossibility to fit 31 variables with 10 pieces of data

# Case study: alloy for direct laser deposition



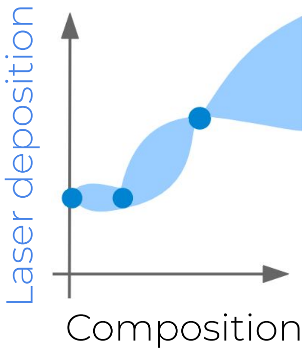
# Direct laser deposition is similar to welding



Direct laser deposition

Welding

# Lack of data for laser deposition



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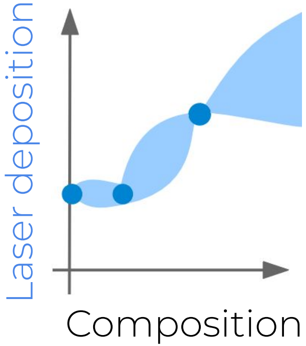
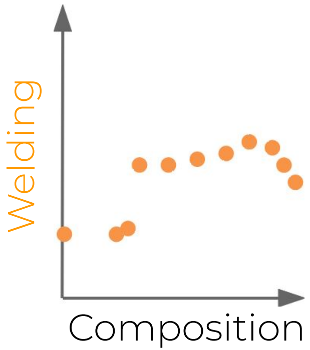
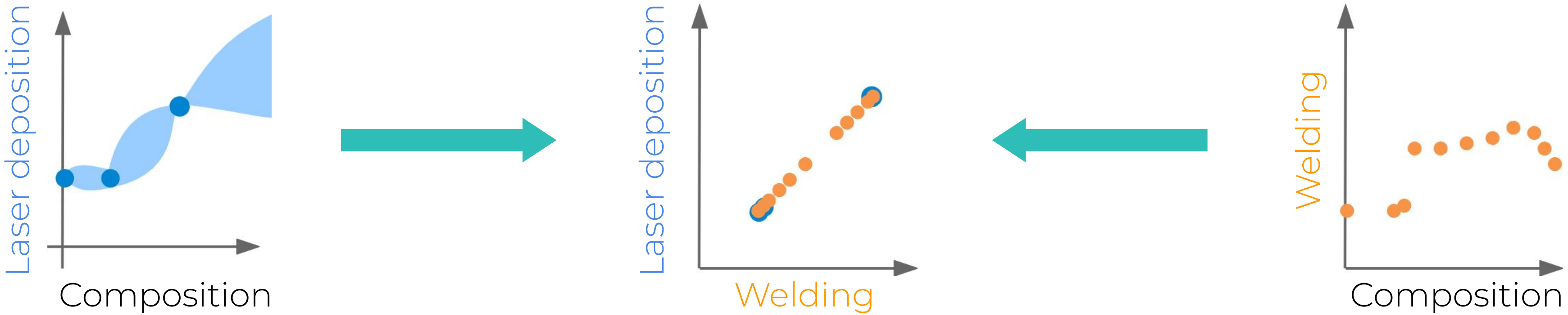
# Large amount of welding data

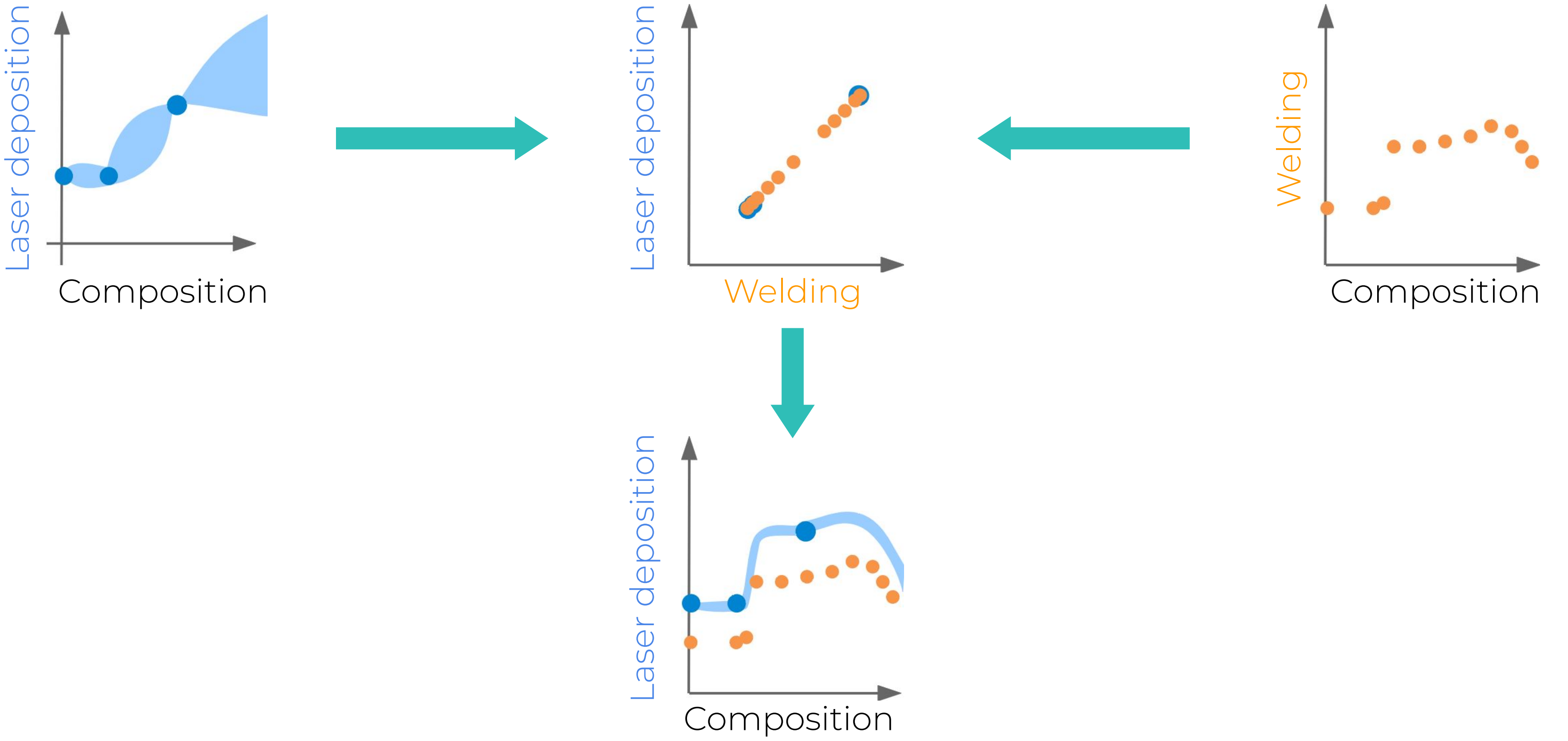


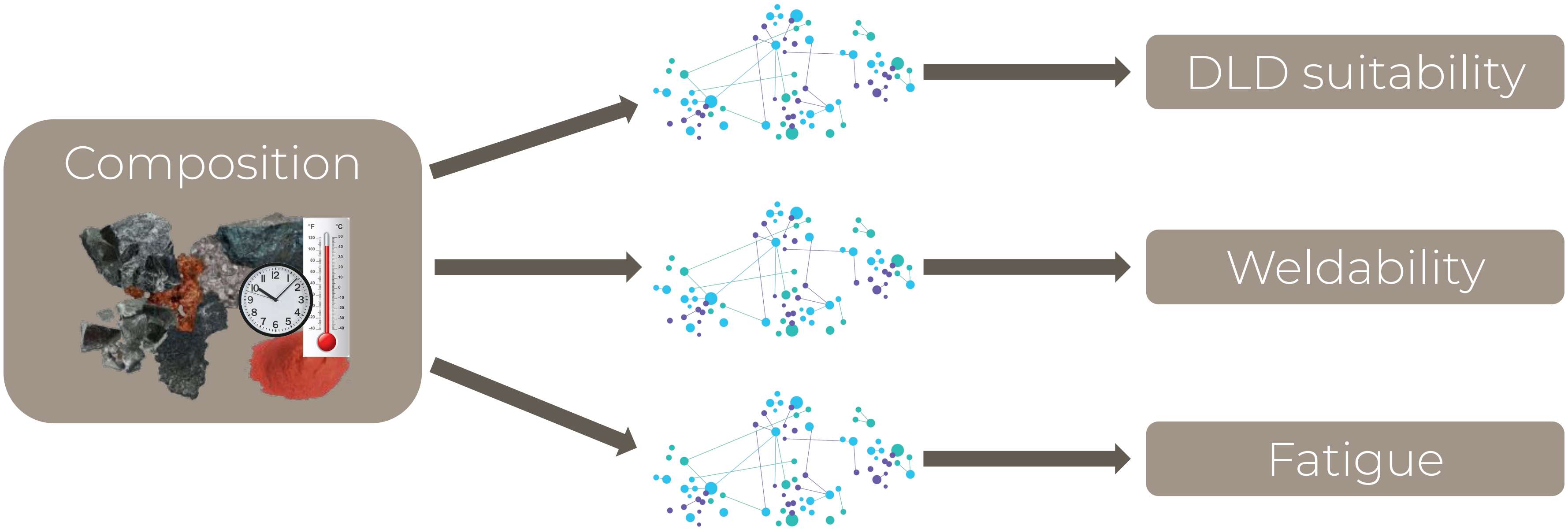
# Simple welding-deposition relationship



# Welding data guides extrapolation

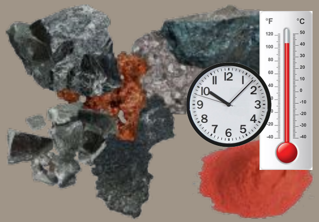


# Standard machine learning



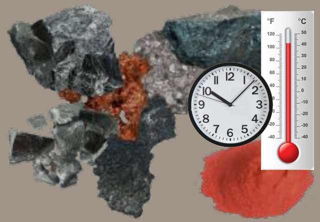
# Holistic machine learning for materials design

Composition



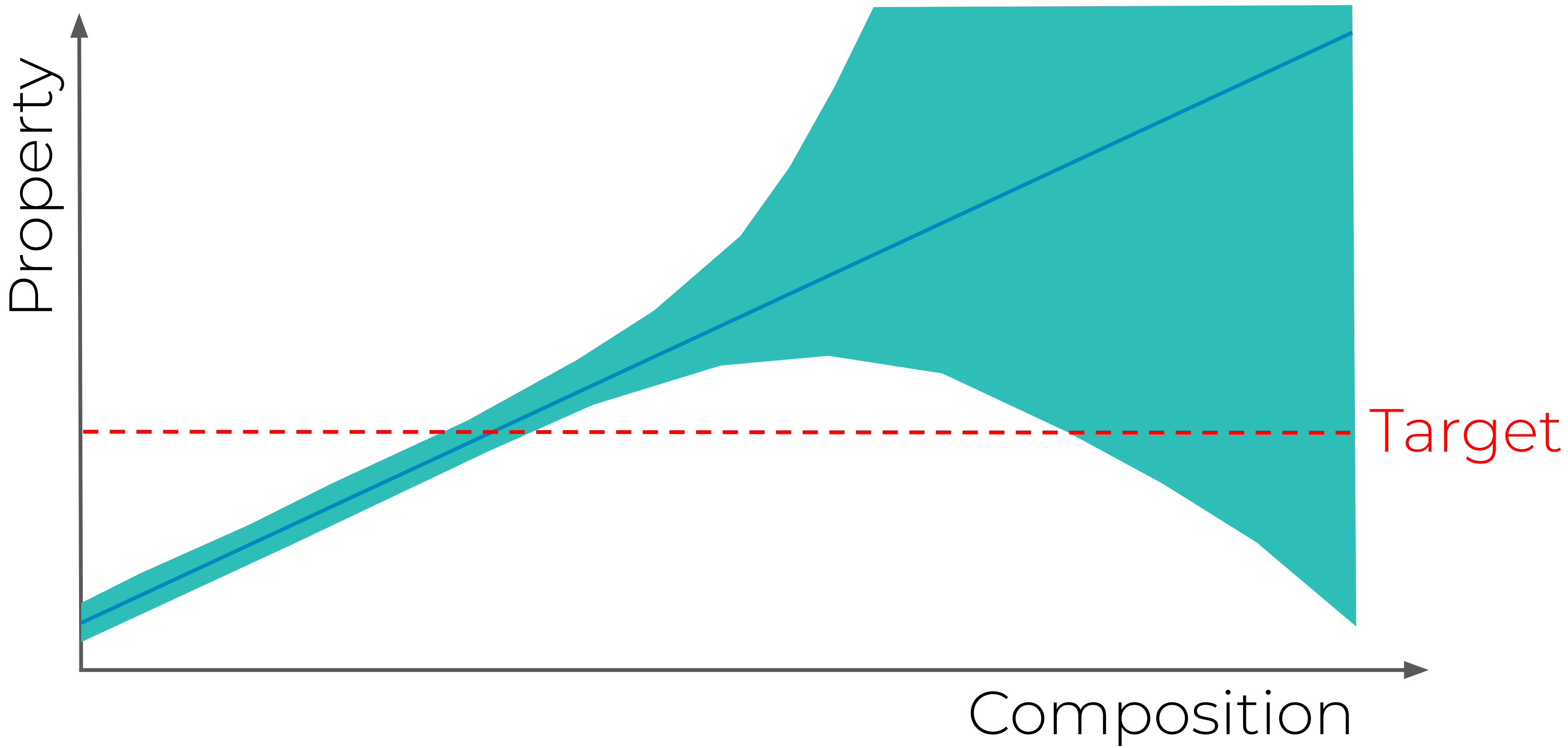
DLD suitability
Weldability
Fatigue

Composition



DLD suitability
Weldability
Fatigue

# Maximize likelihood of alloy exceeding targets



# Targets for direct laser deposition alloy

| | |
|---|---|
| Elemental cost | < 25 $\$kg^{-1}$ |
| Density | < 8500 $kgm^{-3}$ |
| γ' content | < 25 wt% |
| Oxidation resistance | < 0.3 $mgcm^{-2}$ |
| DLD suitability | < 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%

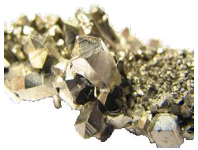
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



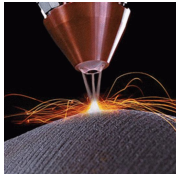
Al 2.9%

C 0.04%

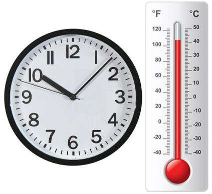
B 0.01%

Ni balance

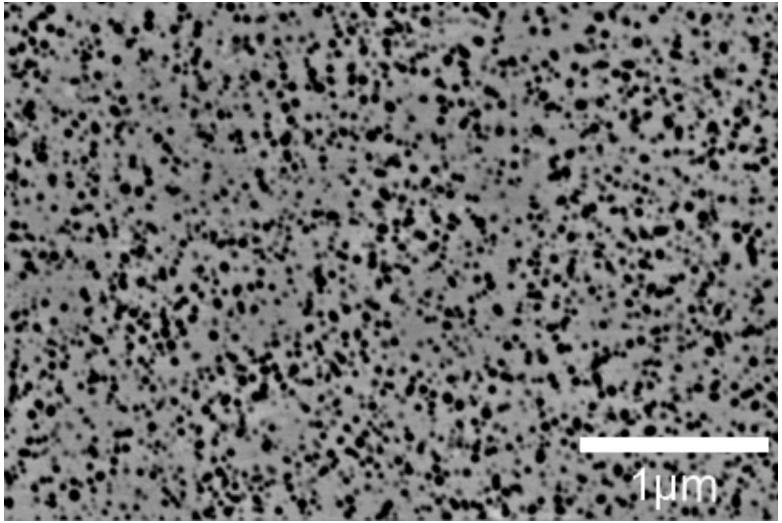
Expose 0.8



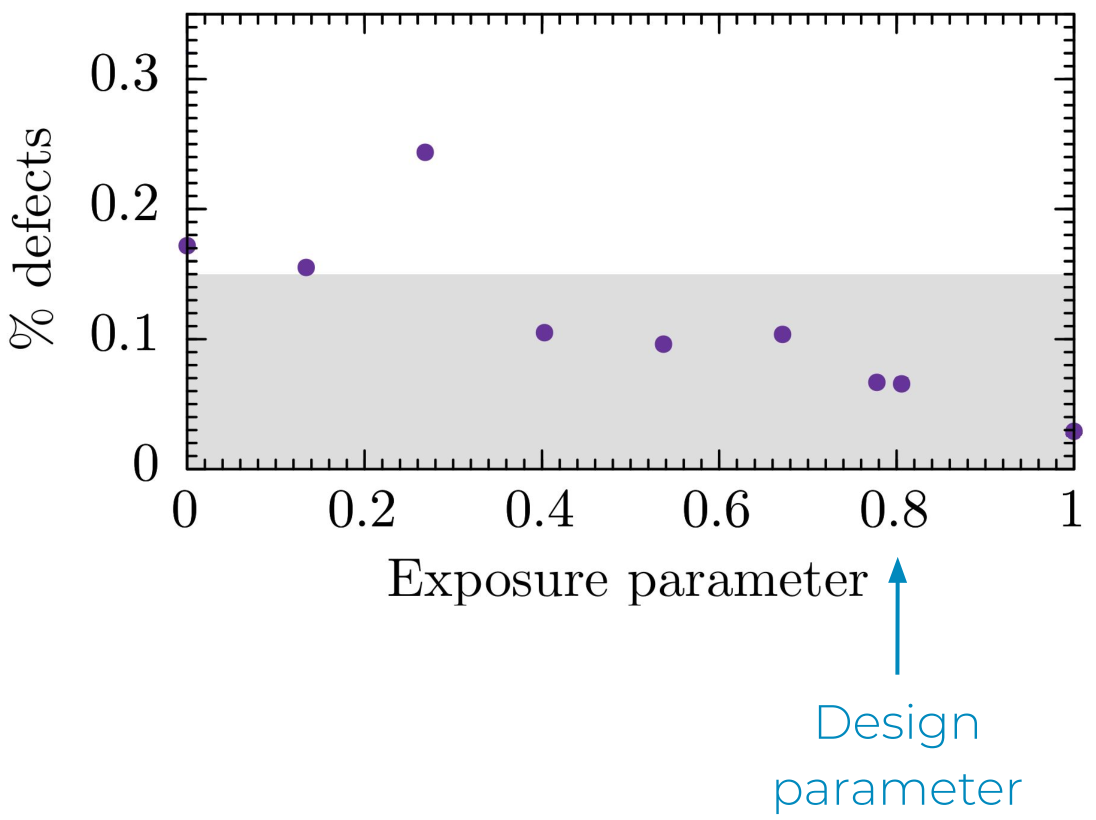
$T_{HT}$ 1230°C



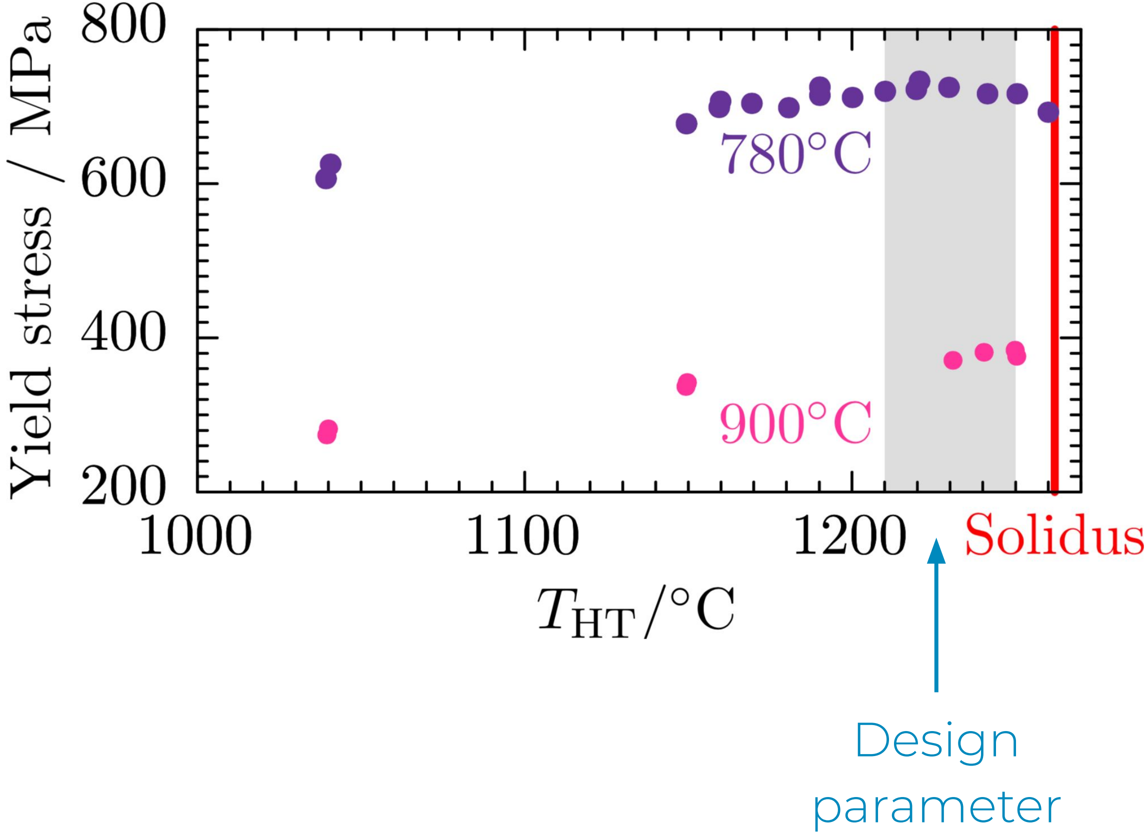
# Experimental validation: microscope



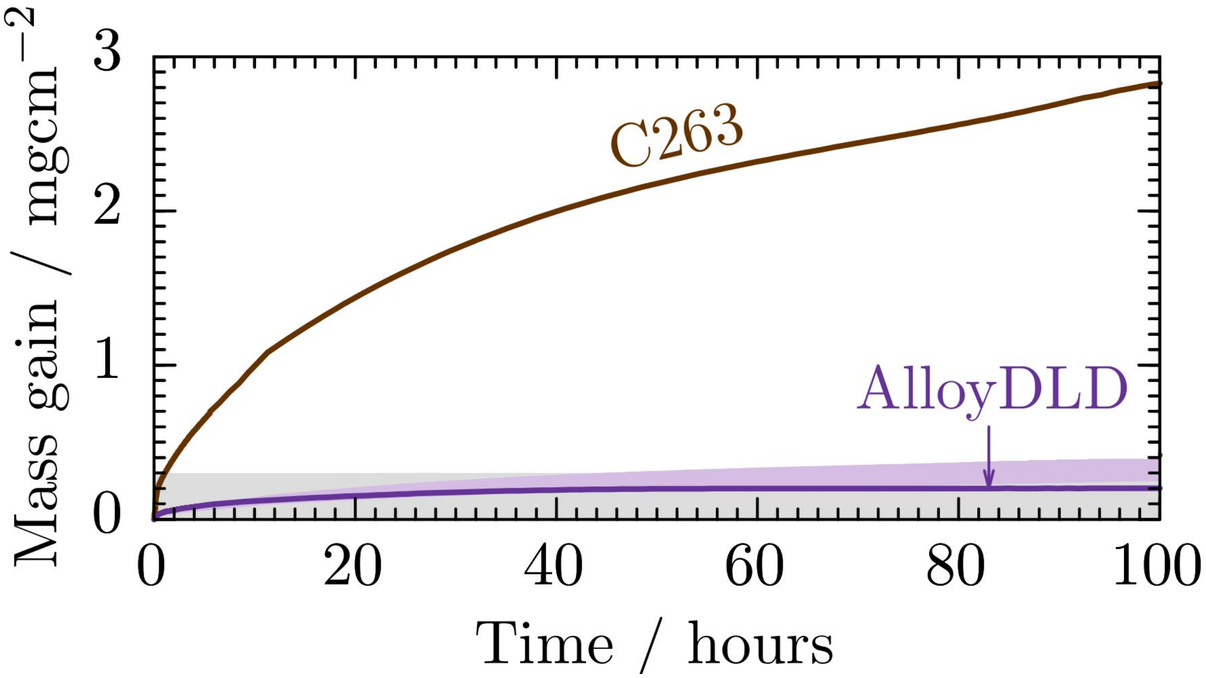
# Experimental validation: defects



# Experimental validation: yield stress



# Experimental validation: oxidation resistance

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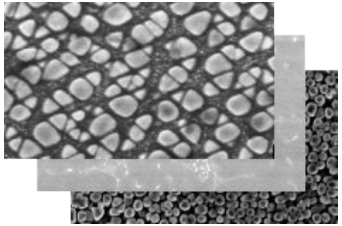
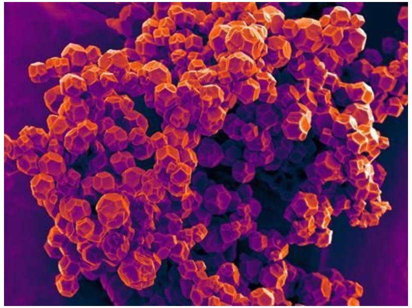
# Further materials design



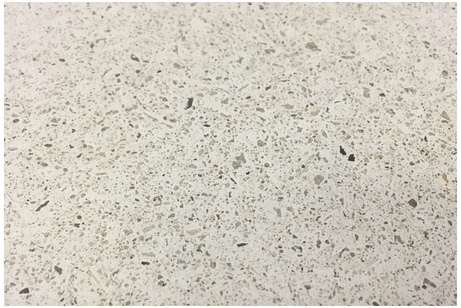
Nickel & moly alloys


Batteries

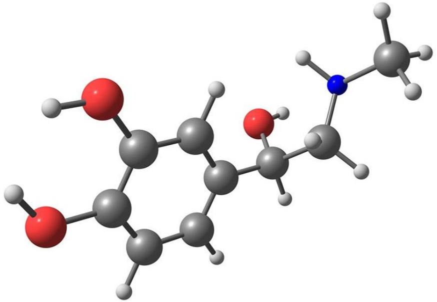
Steels of welding



Metal-organic framework



Concrete



Pharmaceutical

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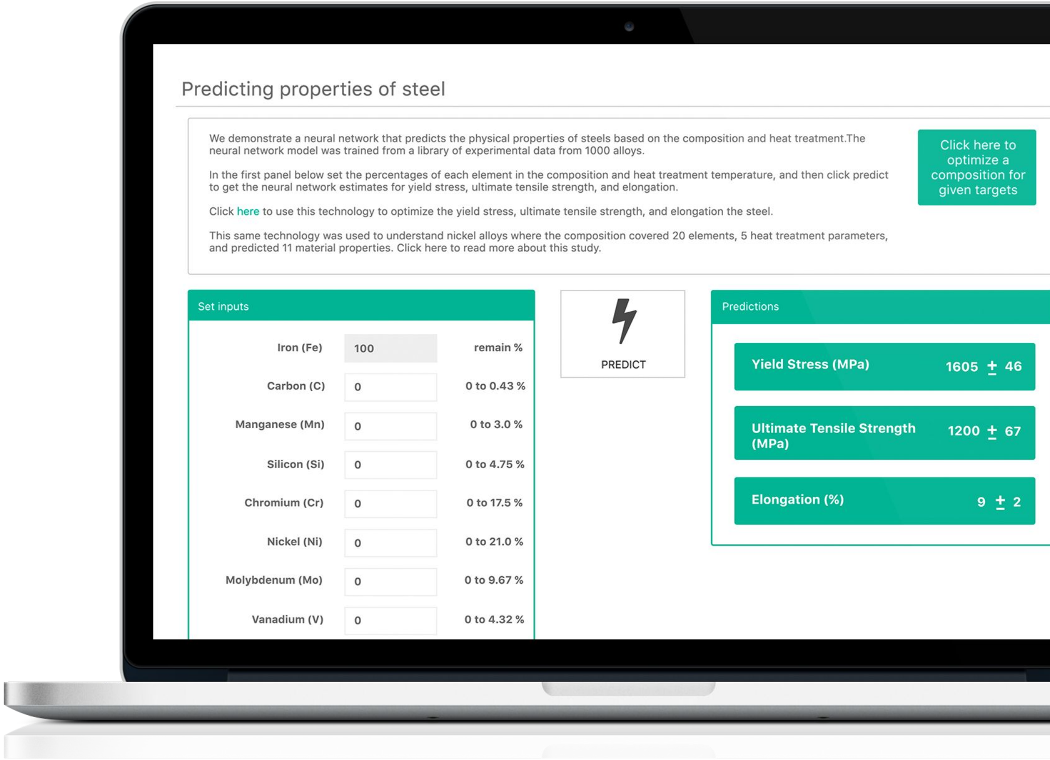
# Future opportunities: Integrated software

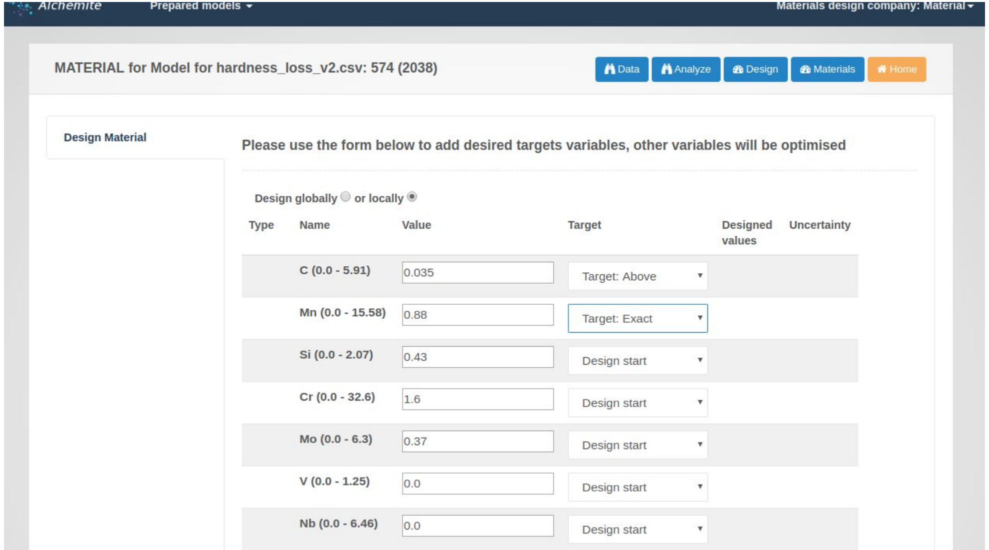
1 Load data

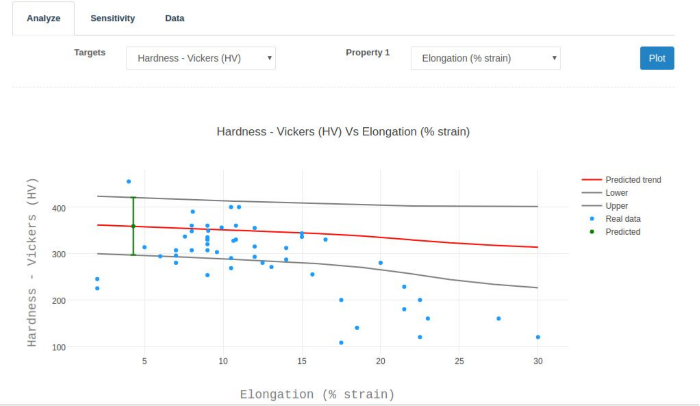
2 Training

3 Design

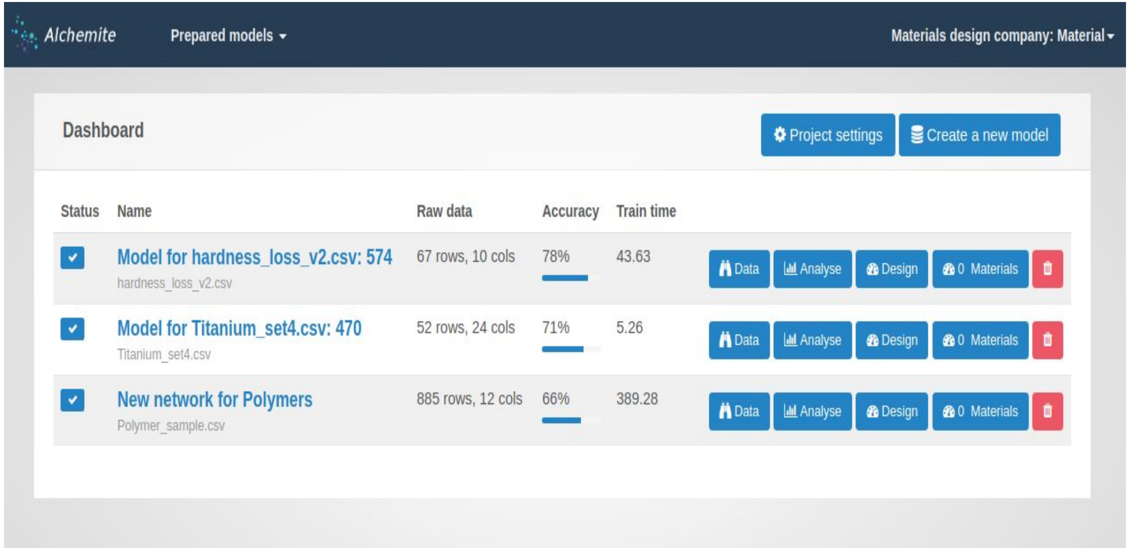


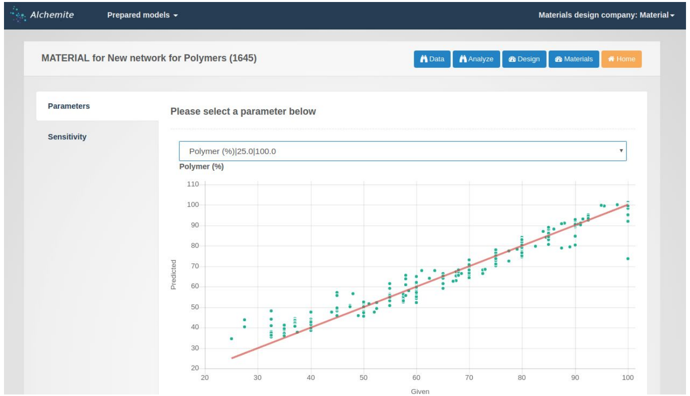
# Design and interrogate new materials

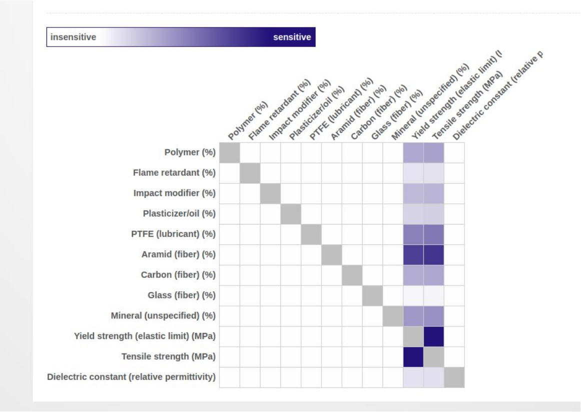


# Manage and share models

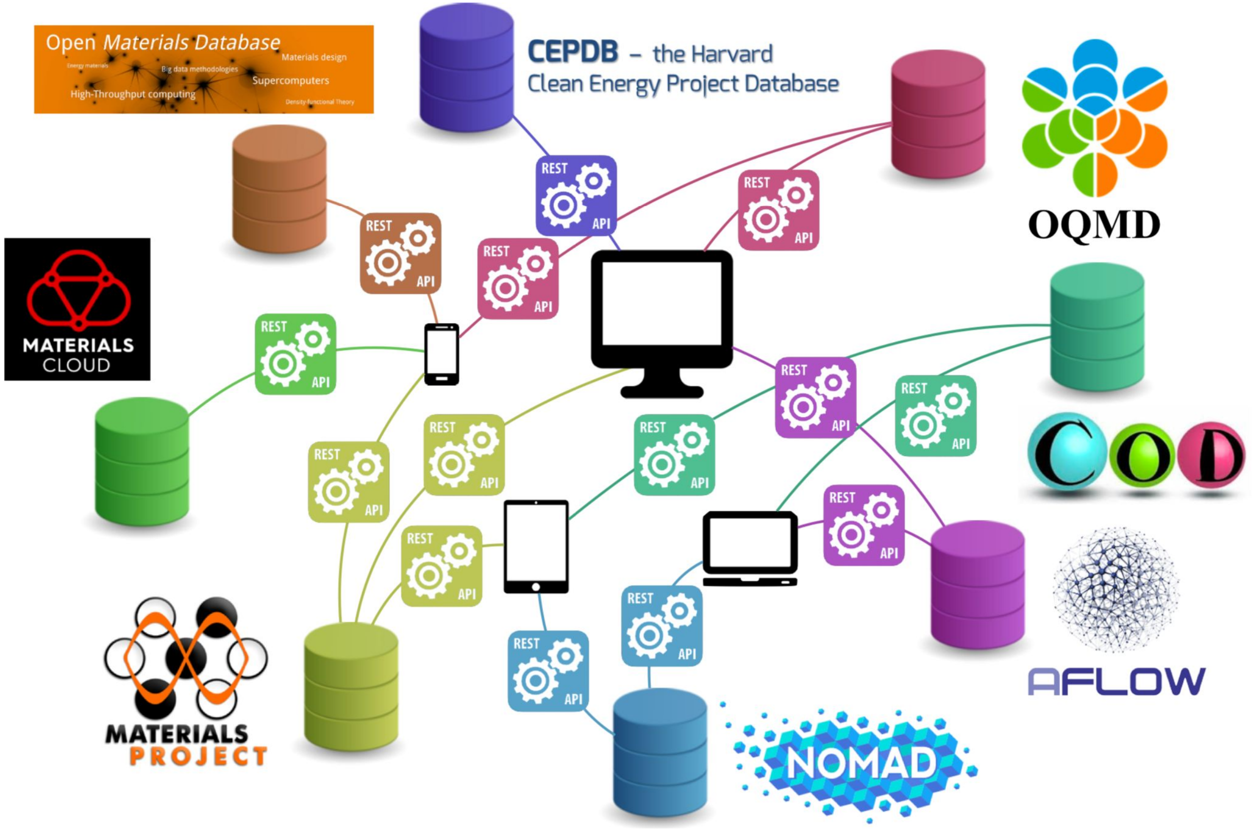


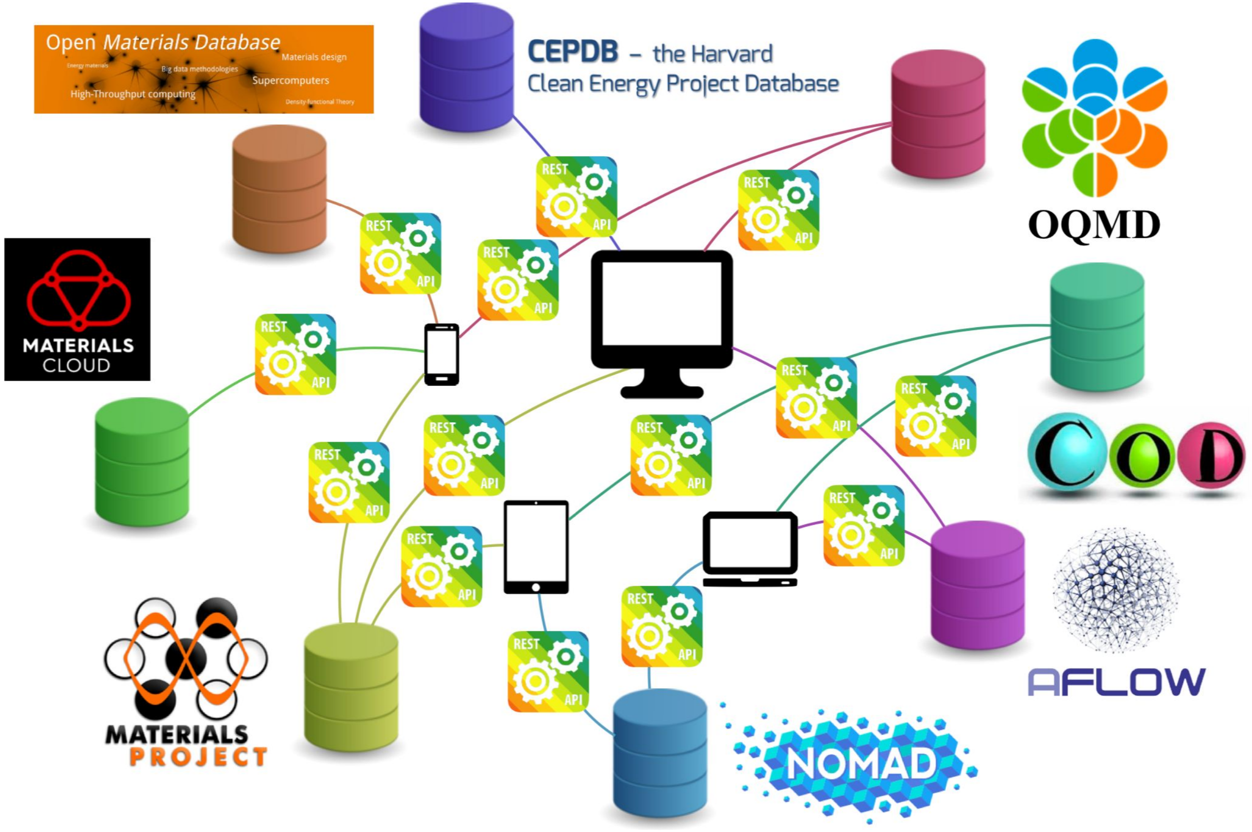



# Zoo of materials databases

# Labor intensive to harvest data



# Universal API would ease access



# OPTiMaDe

Open Databases Integration for Materials Design

A RESTful API to access leading electronic structure materials databases

Supported by CECAM to now extend to molecular dynamics and bio-simulations

http://www.optimade.org/

# Machine learning for materials design

Merge sparse databases to deliver deep insights into new materials

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