



intellegens

The modern day blacksmith

Gareth Conduit

Intellegens machine learning for materials design



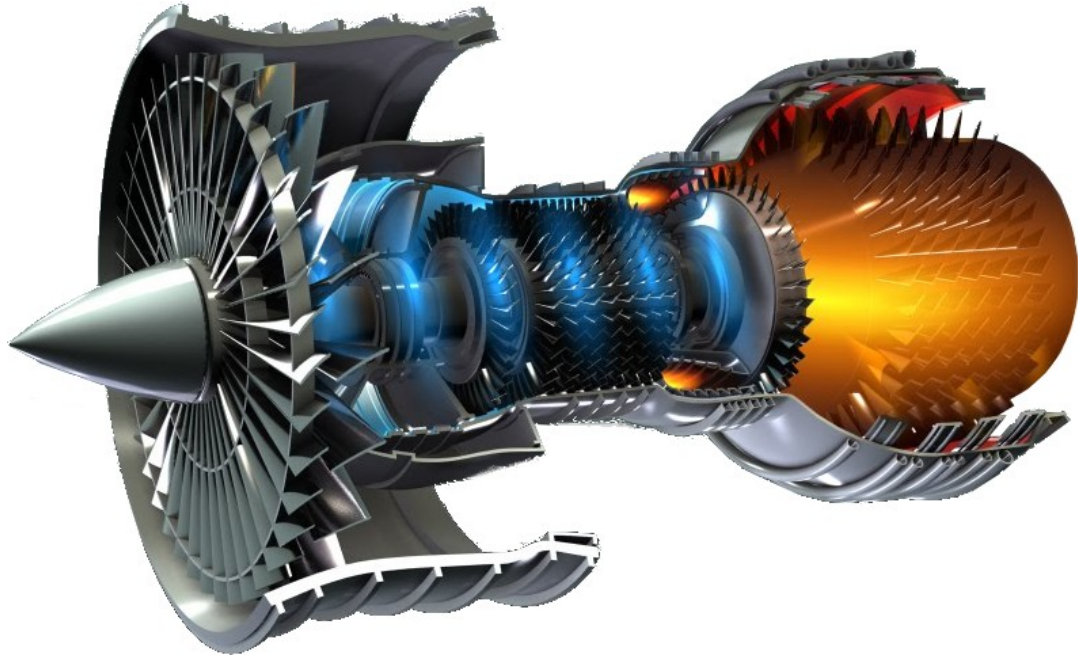
Alchemite™ developed at **University of Cambridge** & **Intellegens**

Design materials for **multiple target properties**

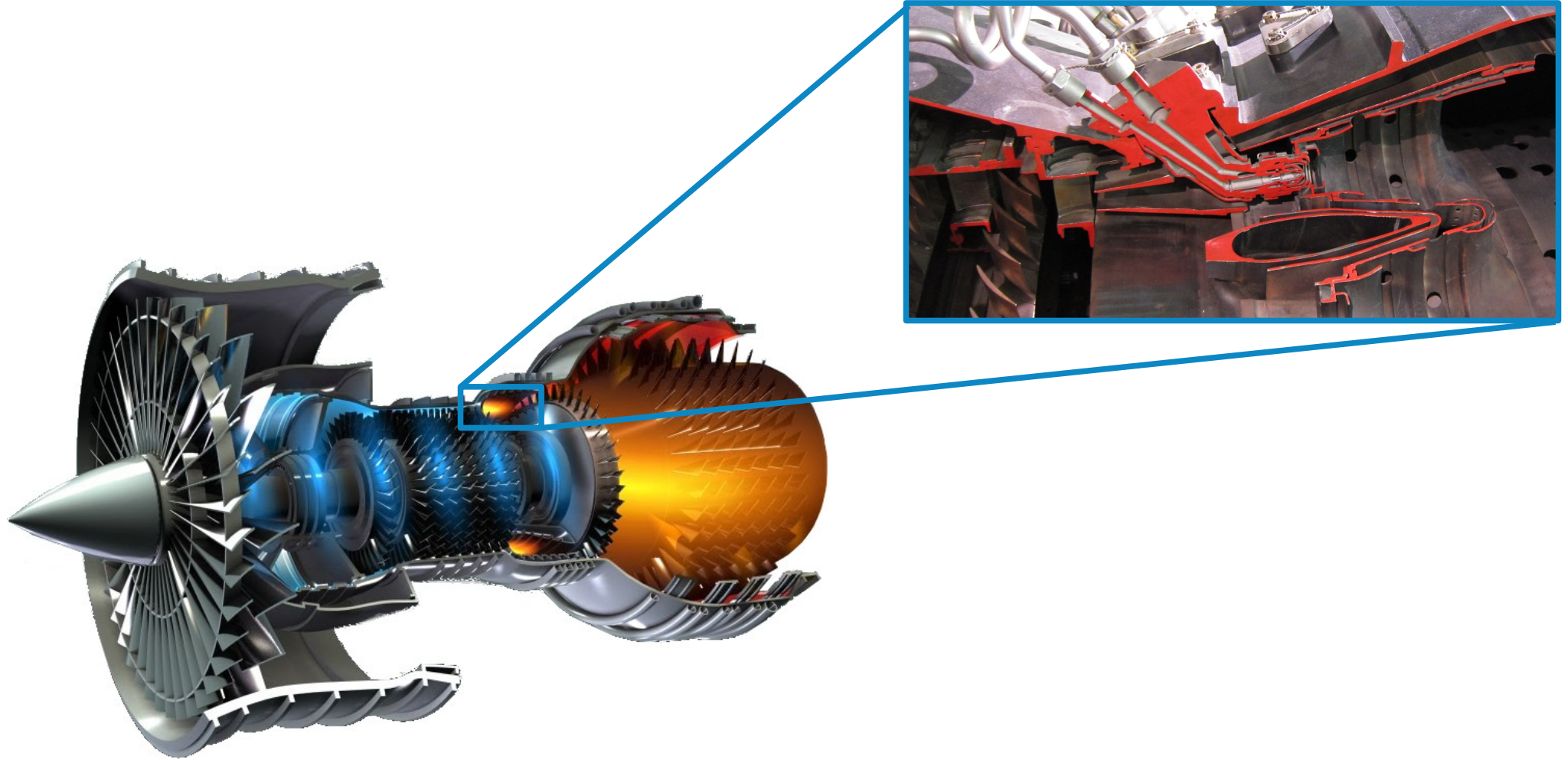
Merge simulations, physical laws, and experimental data to exploit all available information

Accelerate materials design at **reduced cost**

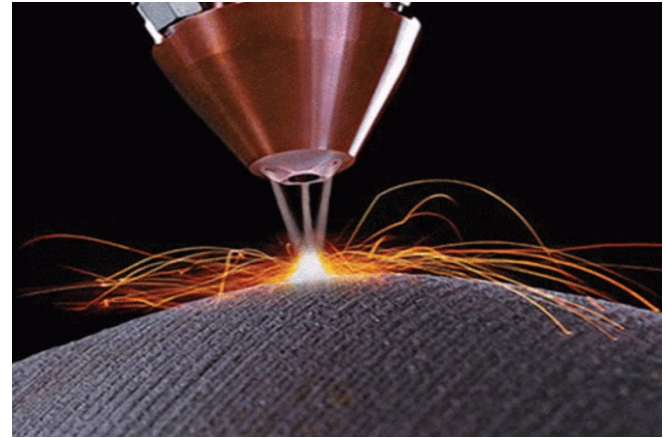
Schematic of a jet engine



Combustor in a jet engine



Direct laser deposition requires new alloys

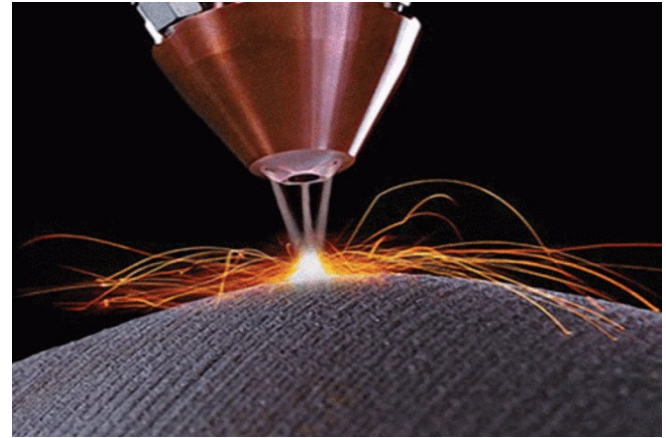


Laser

Plenty of data available for weldability

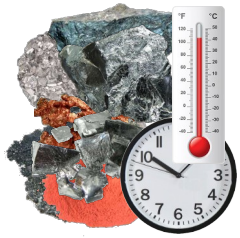


Electricity



Laser

First predict weldability

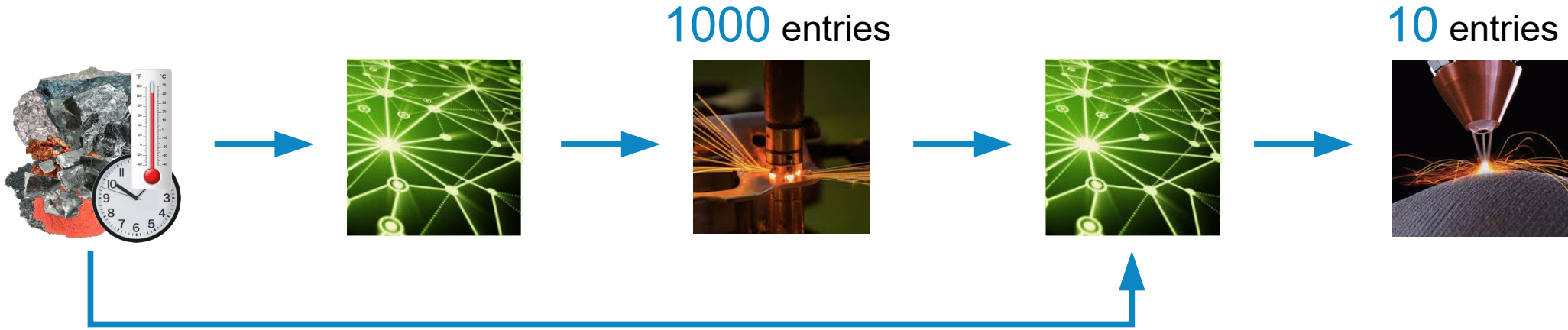


1000 entries



Use 1000 weldability entries to model complex composition → weldability

Use weldability to predict defects formed



Use **1000** weldability entries to model complex composition → weldability

10 defects entries capture the simple weldability → defect relationship

Two **interpolations** give composition → defects **extrapolation**

Target properties



Elemental cost $< 25 \text{ \$kg}^{-1}$

Density $< 8500 \text{ kgm}^{-3}$

γ' content $< 25 \text{ wt}\%$

Oxidation resistance $< 0.3 \text{ mgcm}^{-2}$

Defects $< 0.15\% \text{ defects}$

Phase stability $> 99.0 \text{ wt}\%$

γ' solvus $> 1000^\circ\text{C}$

Thermal resistance $> 0.04 \text{ K}\Omega^{-1}\text{m}^{-3}$

Yield stress at 900°C $> 200 \text{ MPa}$

Tensile strength at 900°C $> 300 \text{ MPa}$

Tensile elongation at 700°C $> 8\%$

1000hr stress rupture at 800°C $> 100 \text{ MPa}$

Fatigue life at 500 MPa , 700°C $> 10^5 \text{ cycles}$

Composition



Cr 19%



Co 4%



Mo 4.9%



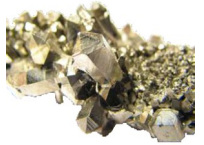
W 1.2%



Zr 0.05%



Nb 3%



Al 2.9%



C 0.04%



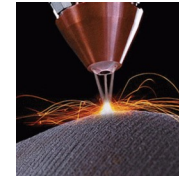
B 0.01%



Ni



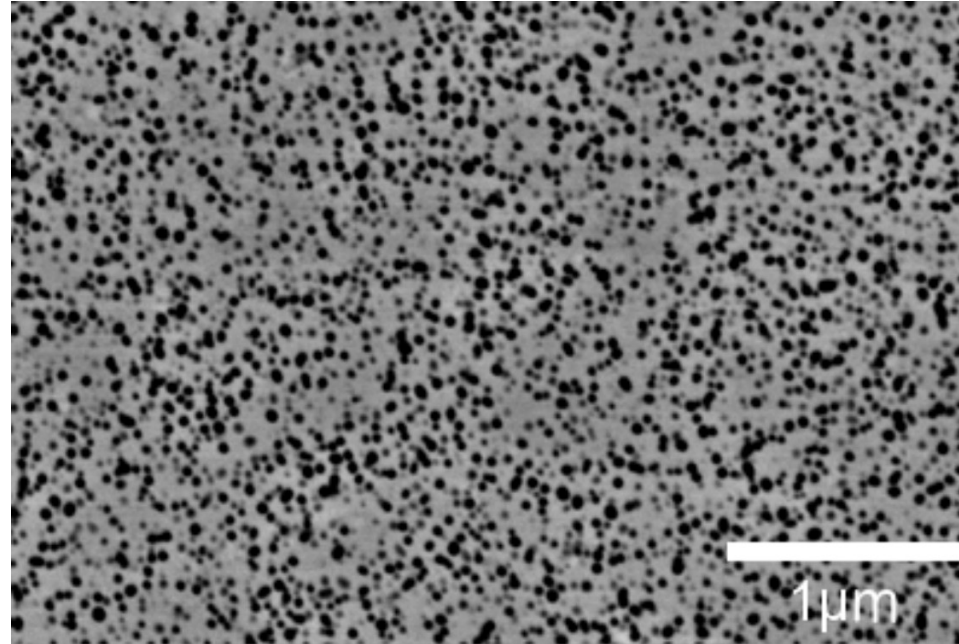
Expose 0.8



T_{HT} 1300°C

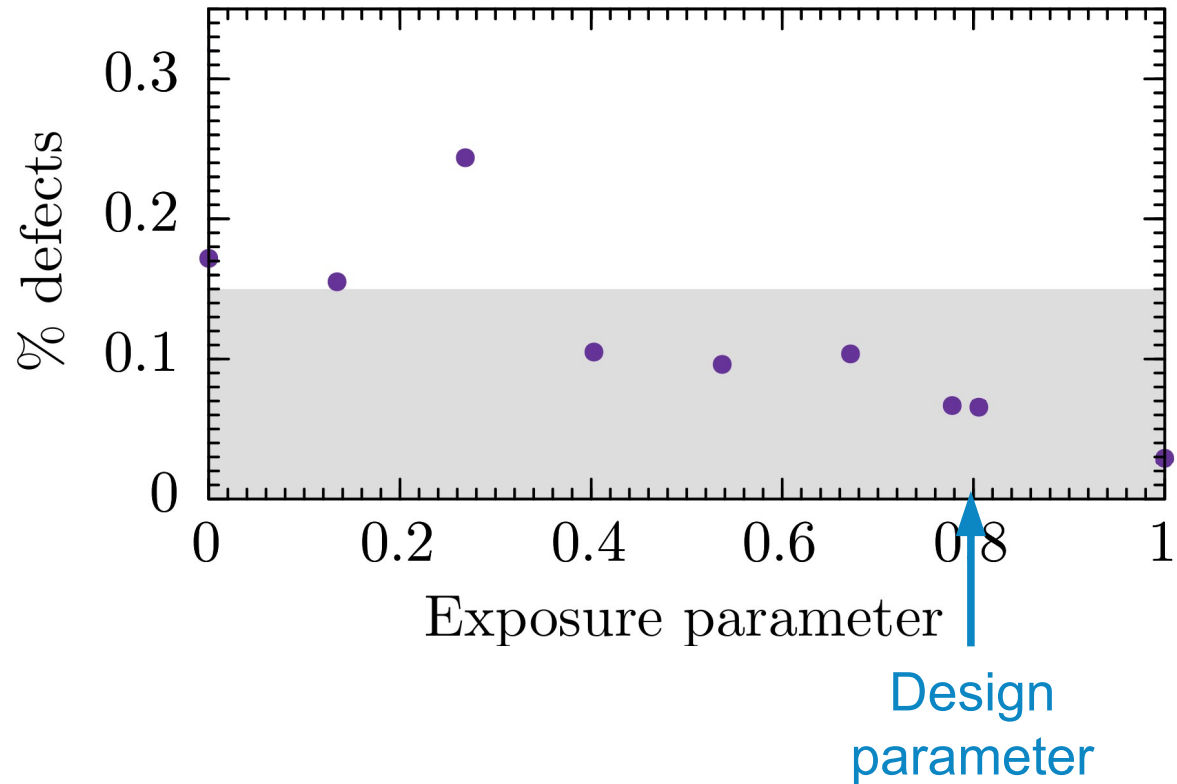


Microstructure

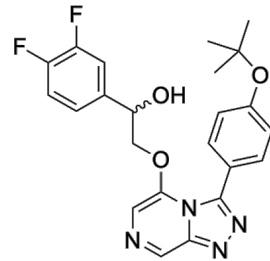
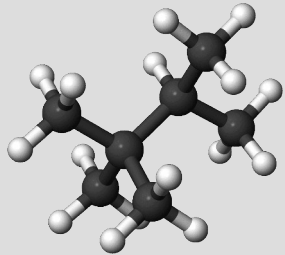
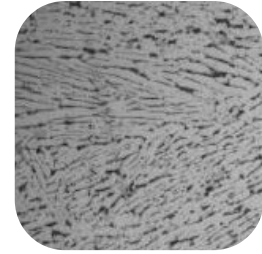
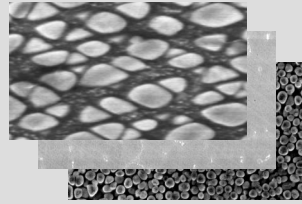
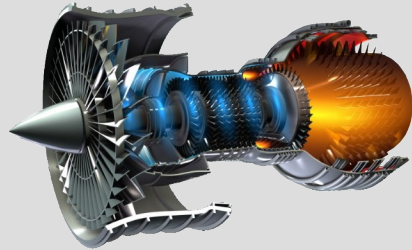


Probabilistic neural network identification
of an alloy for direct laser deposition
Materials & Design 168, 107644 (2019)

Testing the defect density



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Materials & Design 168, 107644 (2019)



e-therapeutics

AstraZeneca



Summary



Alchemite™ merges different experimental quantities and computer simulations into a **holistic** design tool

Accelerate materials design at **reduced cost**

Designed and experimentally verified **direct laser deposition** alloy, and many other experimentally verified **materials** and **drugs**

Alchemite™ taken to market by **Intellegens**