The modern day blacksmith

Gareth Conduit

Alchemite™, a unique neural network algorithm to

Train from sparse datasets

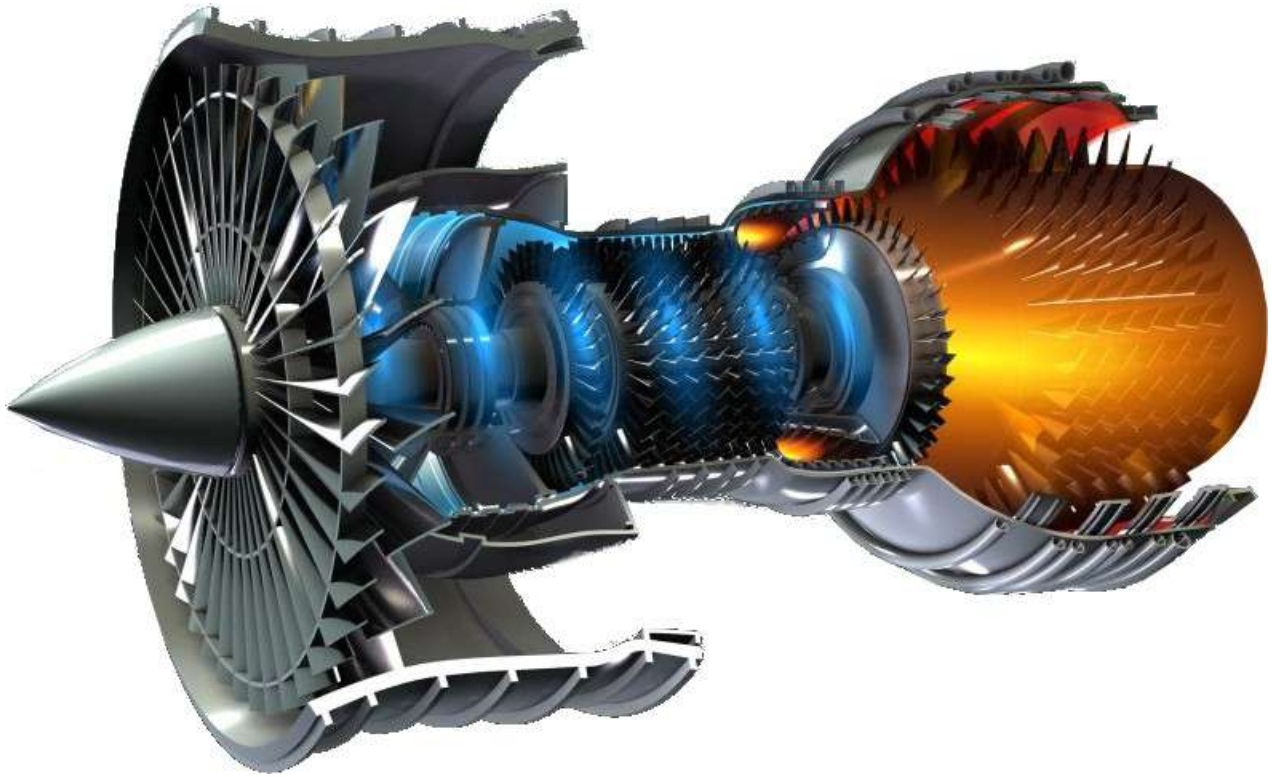
Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

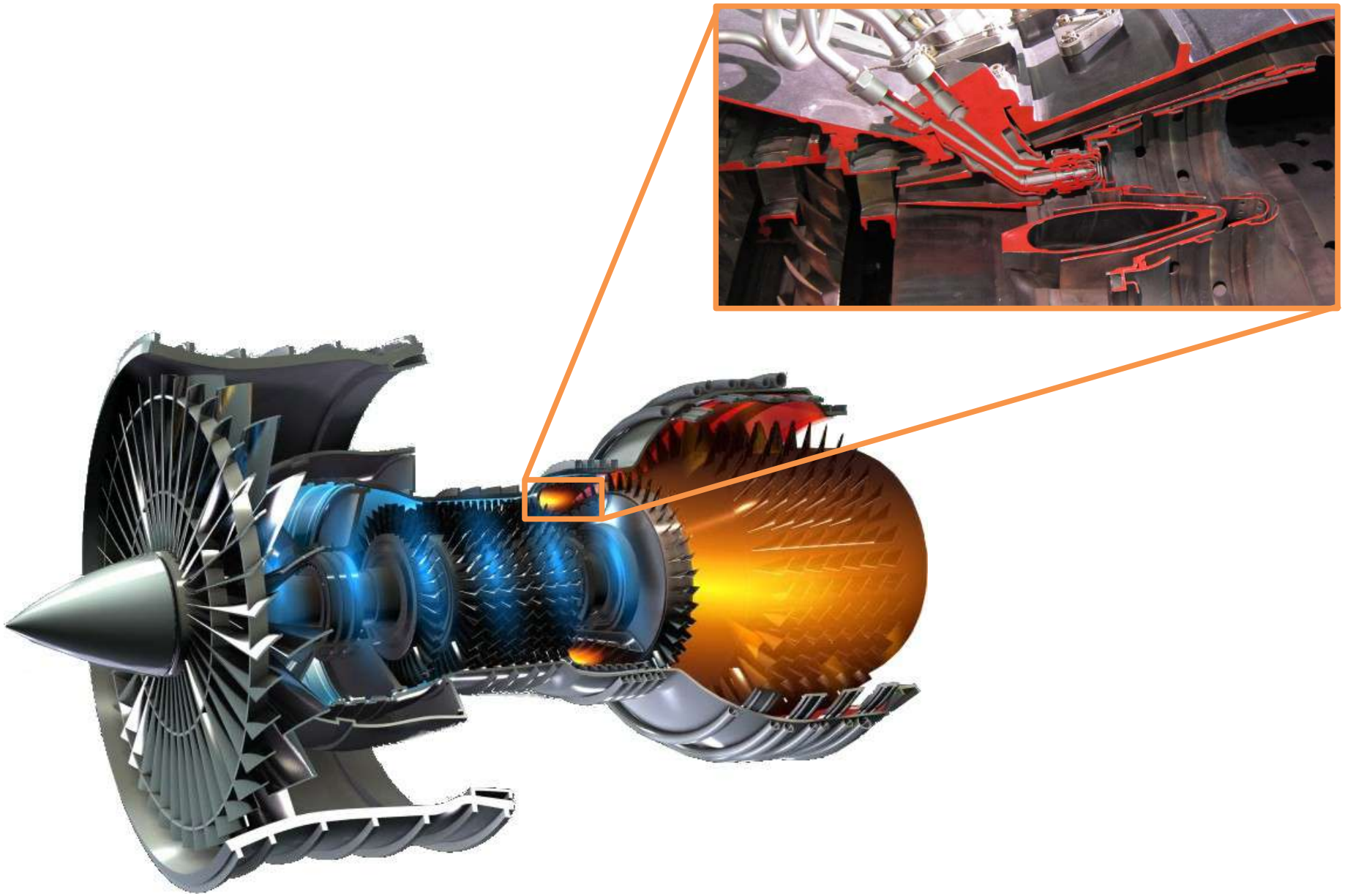
Accelerate materials and drugs discovery

Generic with proven applications in materials discovery and drug design

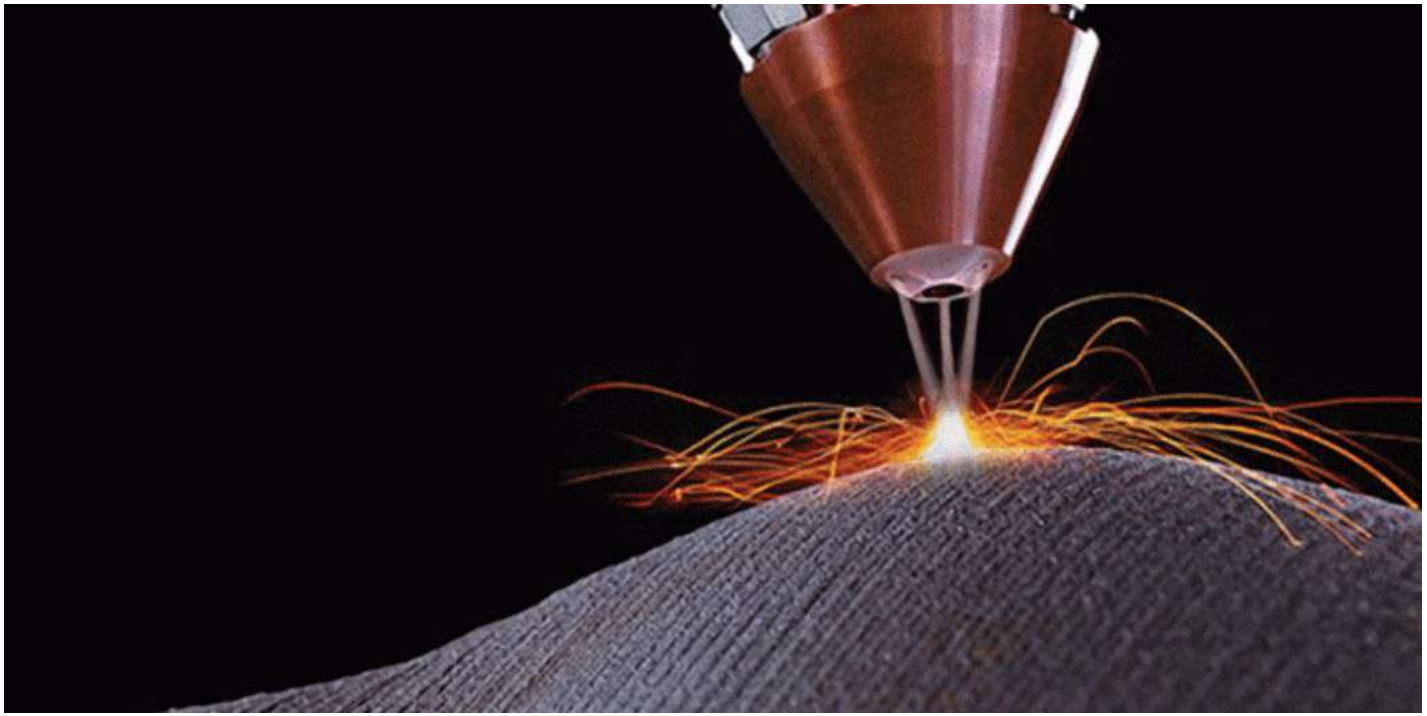
Problem statement: materials for a jet engine



Combustor in a jet engine



Direct laser deposition requires new alloys

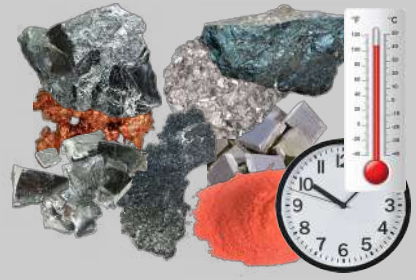


Target properties

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

Neural networks for materials design

Composition



Properties

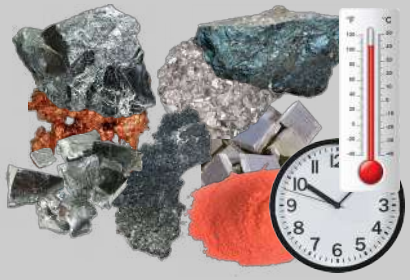
Process

Fatigue

Welding

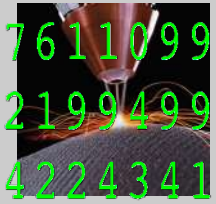
Neural networks for materials design

Composition



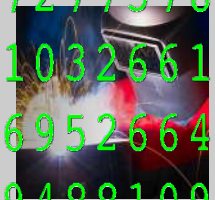
Properties

Process



Fatigue

Welding



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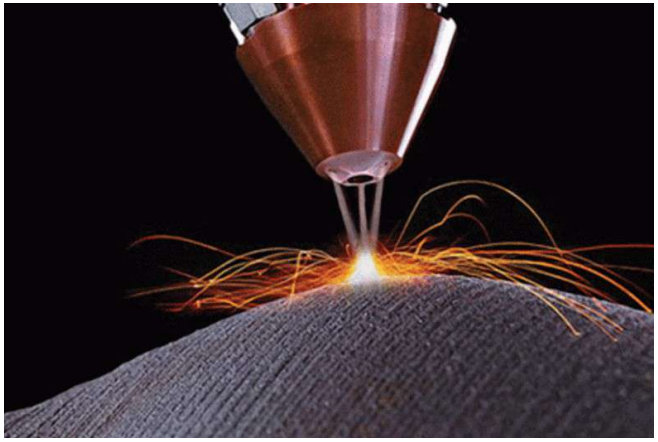

Laser

Electricity

Neural networks for materials design

Composition

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Process

Fatigue

Welding

Neural networks for materials design

Composition

Properties

Process

Fatigue

Welding

Composition

Properties

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Composition

Cr: 19%

Co: 4%

Mo: 4.9%

W: 1.2%

Zr: 0.05%

Nb: 3%

Al: 2.9%

C: 0.04%

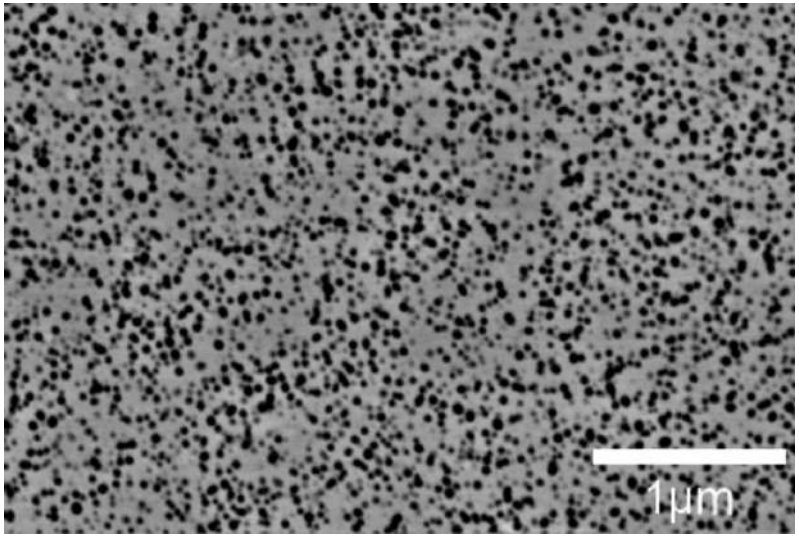
B: 0.01%

Ni

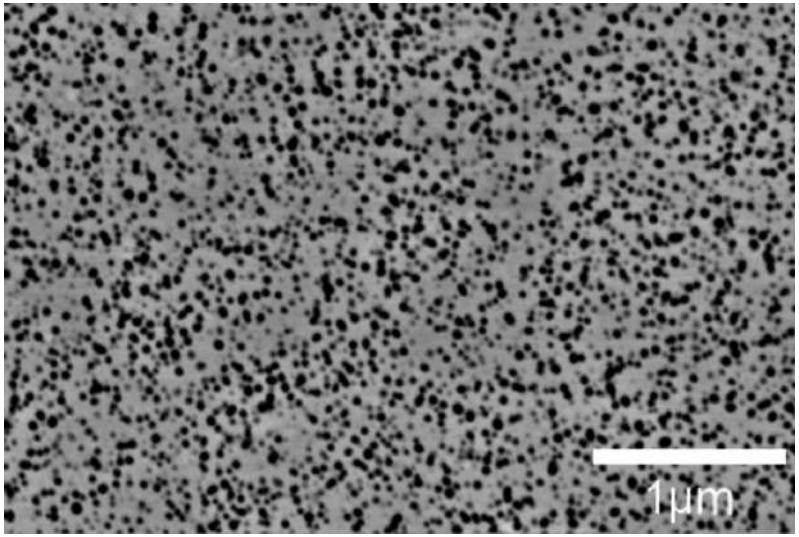
Expose 0.8

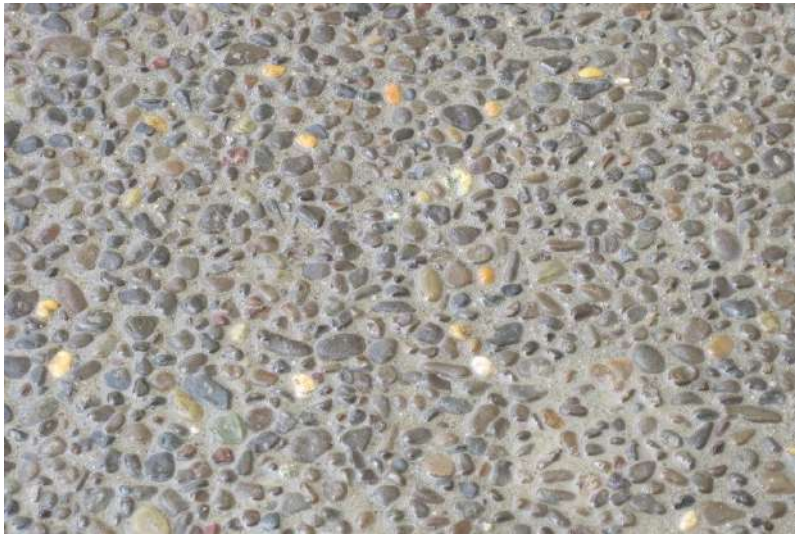
T_{HT} 1300ºC

Microstructure

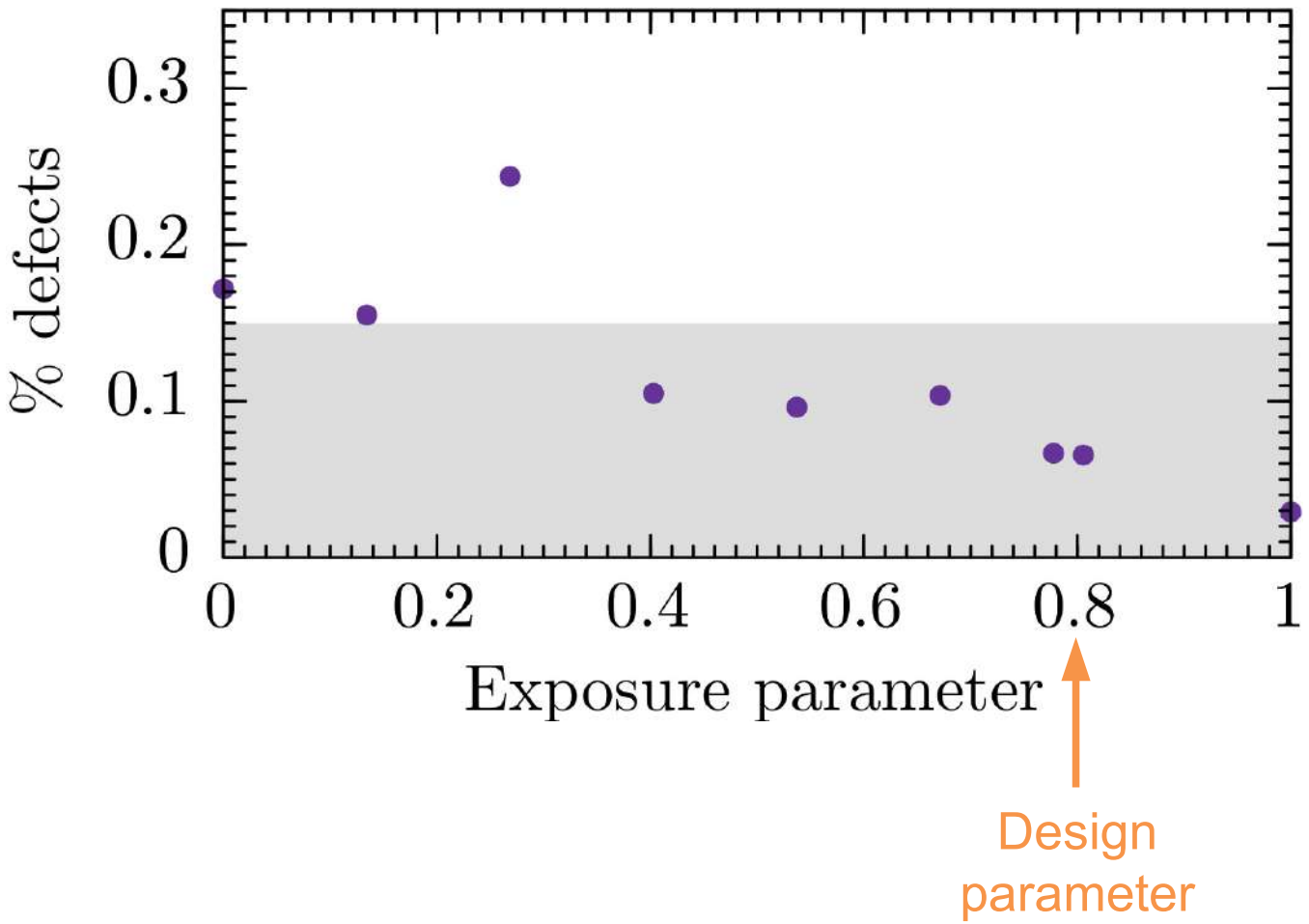


Strength comes from texture like concrete

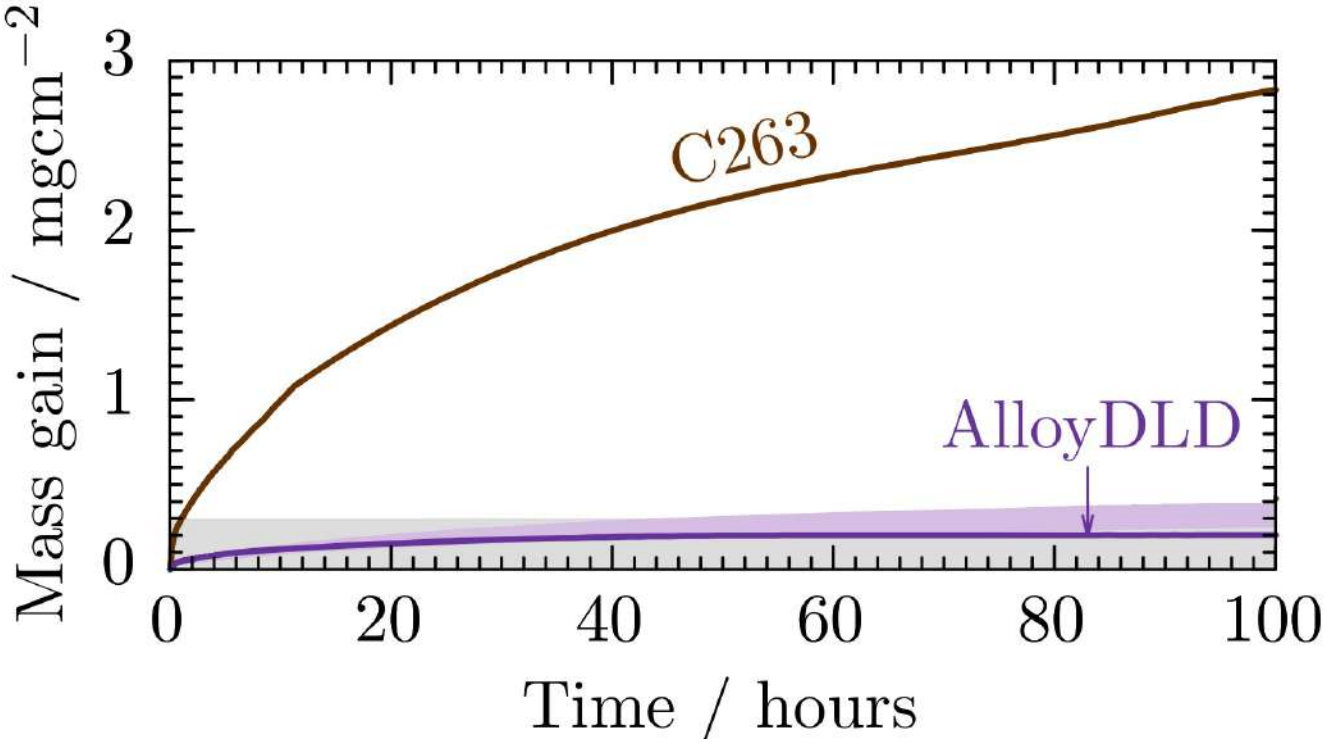




Testing the processability: horizontal printing



Testing the oxidation resistance



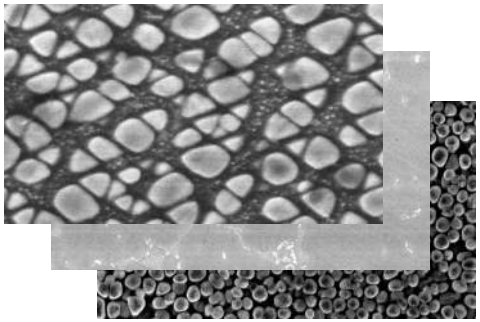
Printing components for an engine

Materials Solutions

ROLLS ROYCE

Materials designed

Nickel and molybdenum



Experiment and DFT for batteries

Steel for welding

Founding of Intellegens

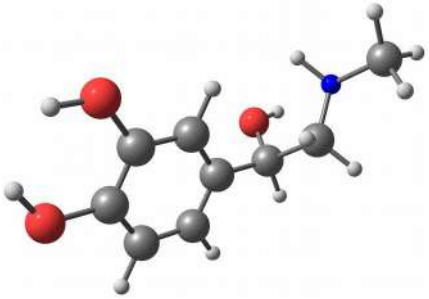
Successful projects as academic, co-founded Intellegens alongside software engineer Ben Pellegrini

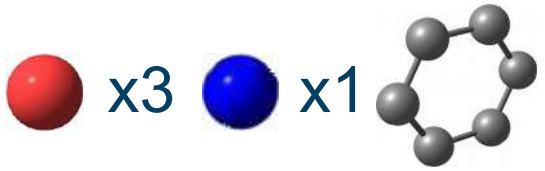
InnovateUK enabled first stage of productization

Support from angel Graham Snudden and University of Cambridge

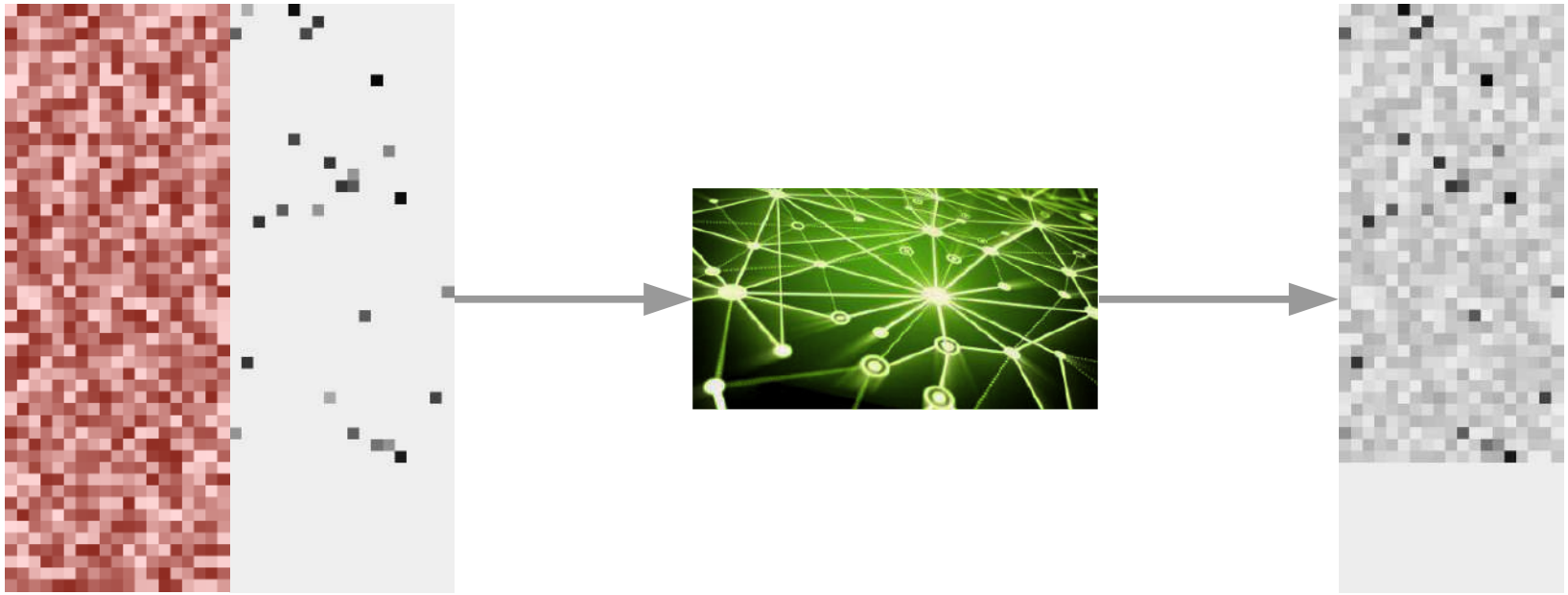
Offer advanced machine learning, first perform consultancy project, then move to product

Quantitative structure-activity relationships





Molecular weight=183 Da



e-therapeutics

Takeda

Roadmap to productization

Reseller agreement with drug discovery software company Optibrium

Machine learning tool embedded into next generation of Optibrium software for release in October 2020

InnovateUK award enables collaboration with Medicine Discovery Catapult

Summary

Platform: unique ability to merge different experimental quantities and computer simulations into a holistic design tool

Experience: perform consultancy projects to hone approach and gain reputation: alloy for direct laser deposition and complete 10^{11} drug database entires

Business: development of product with Optibrium

Intellegens

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