UNIVERSITY OF CAMBRIDGE

The modern day blacksmith

Gareth Conduit

Theory of Condensed Matter group

Neural network algorithm to

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

Look forward to predict crowd behavior with Julian Hewitt

A black box

Train with complete data

Materials design

Materials design

Predict with complete data

Crystal structure

Crystal structure

Train with fragmented data

Predict with fragmented data

Materials age

1.9 million BC
Olduvai Gorge, Tanzania

Materials age

1.9 million BC
Olduvai Gorge, Tanzania

1200 BC
Britain

Materials age

1.9 million BC
Olduvai Gorge, Tanzania

1200 BC
Britain

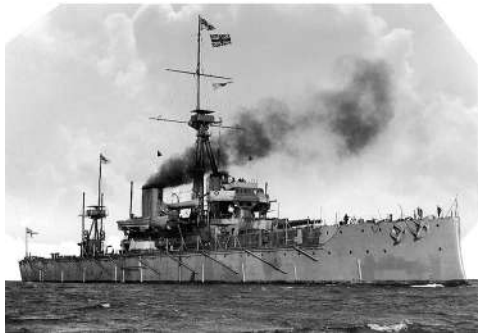
300 BC
Yorkshire

Materials age

1.9 million BC
Olduvai Gorge, Tanzania

1200 BC
Britain

300 BC
Yorkshire

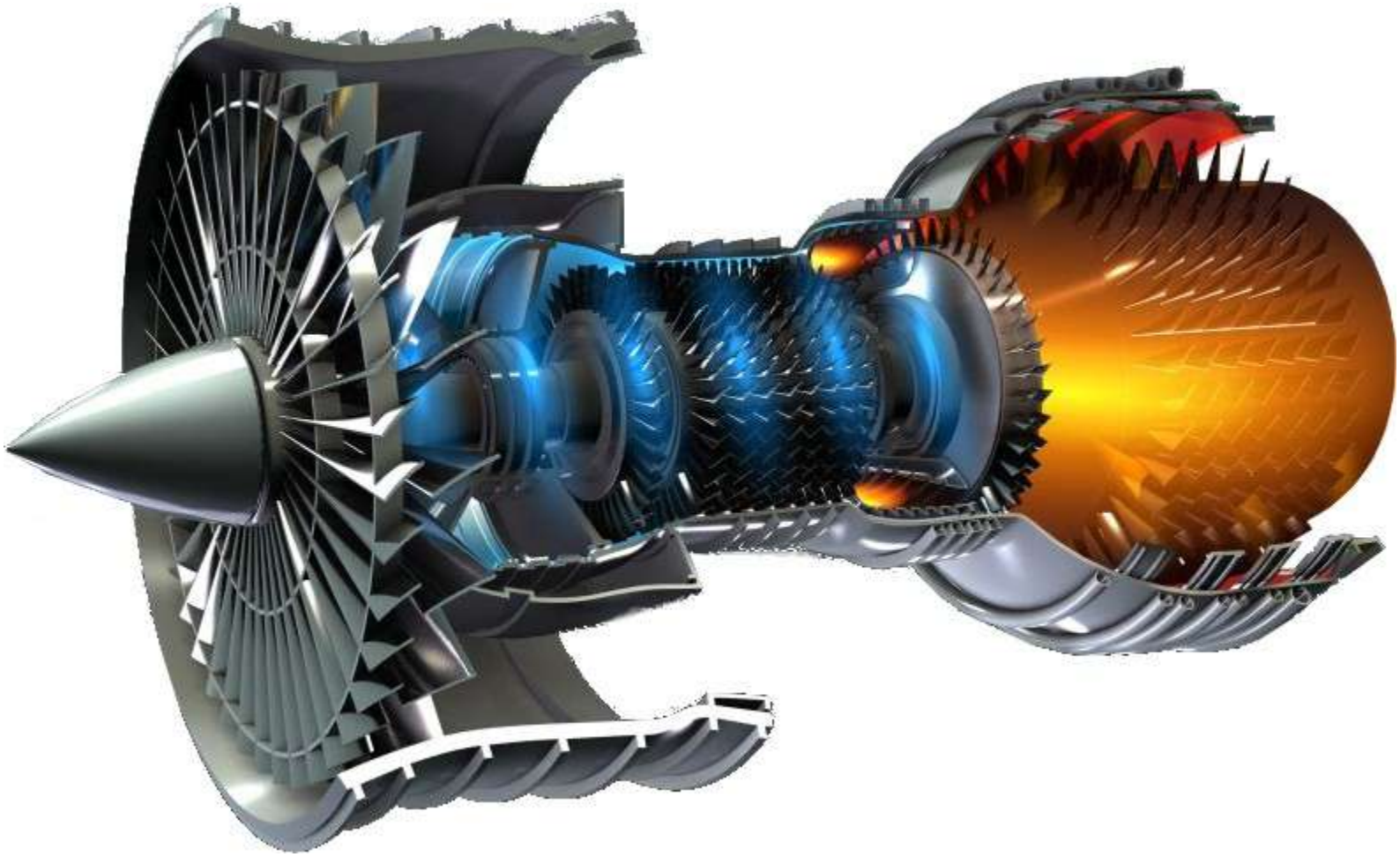


1906
Portsmouth

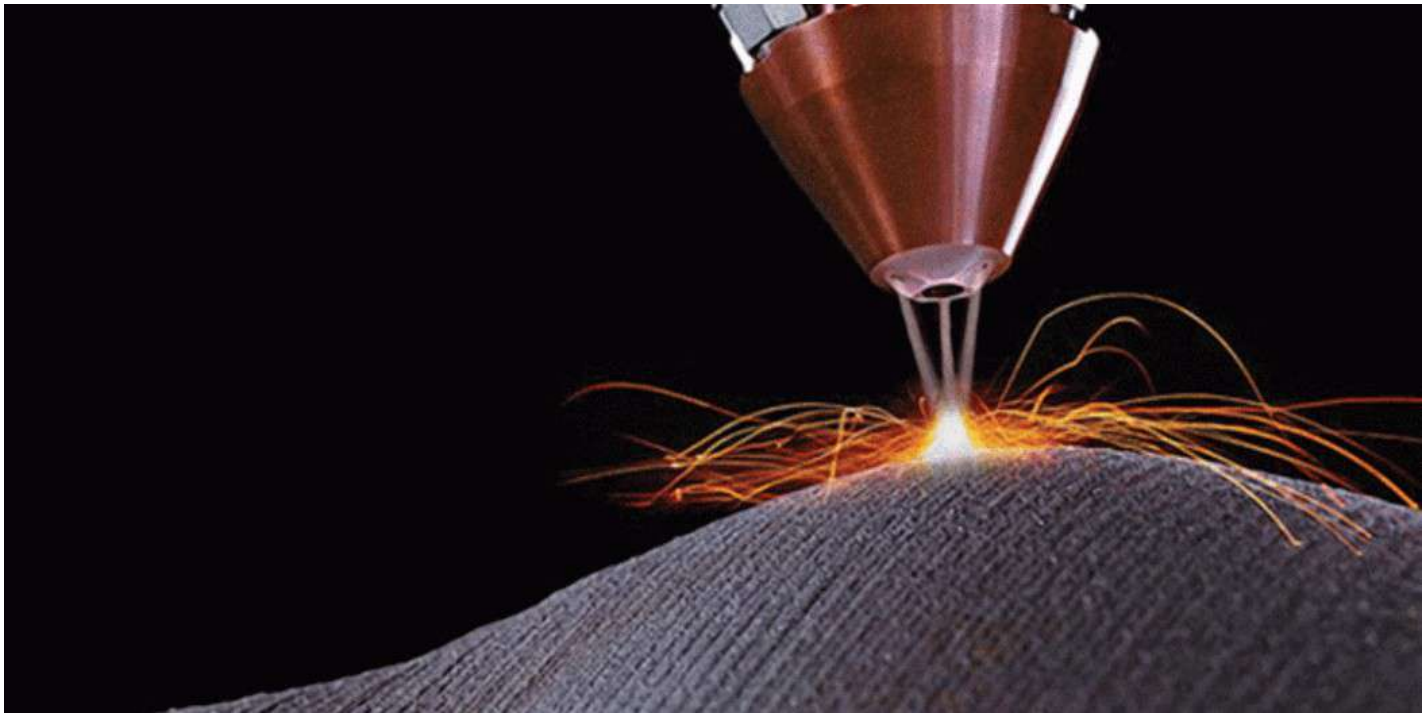
Materials: experimental interlude

Materials: experimental interlude

Schematic of a jet engine

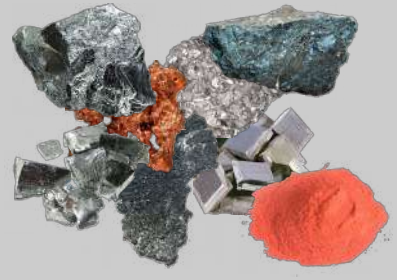


Direct laser deposition requires new alloys



Neural networks for materials design

Composition



Properties

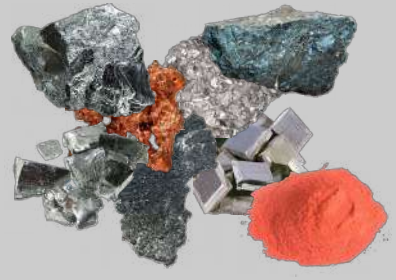
Process

Fatigue

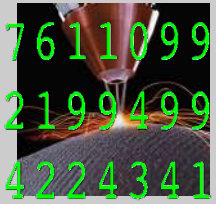
Welding

Neural networks for materials design

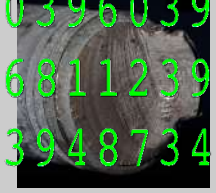
Composition



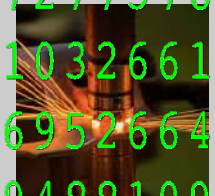
Properties



Process



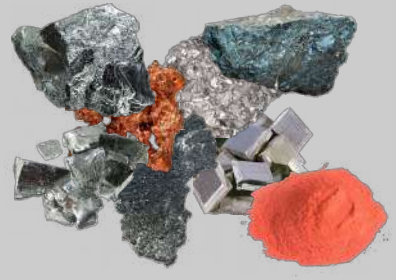
Fatigue



Welding

Neural networks for materials design

Composition



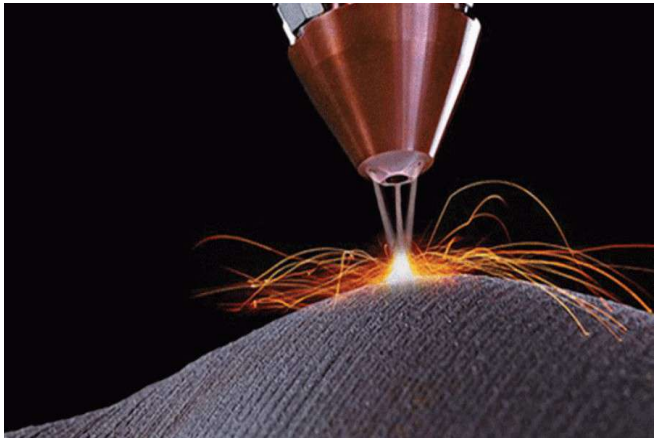
Properties

Process

Fatigue

Welding

Direct laser deposition and welding

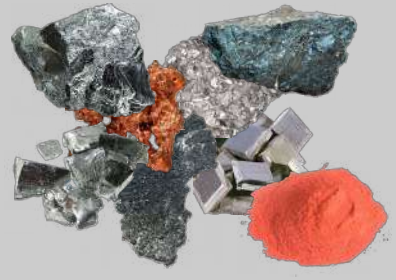


Laser

Electricity

Neural networks for materials design

Composition



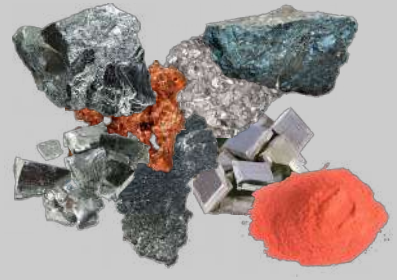
Properties

Process

Fatigue

Welding

Composition



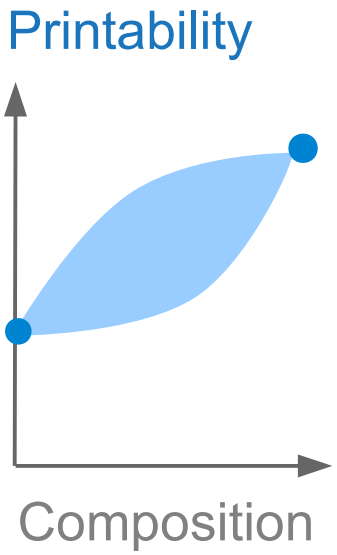
Properties

Process

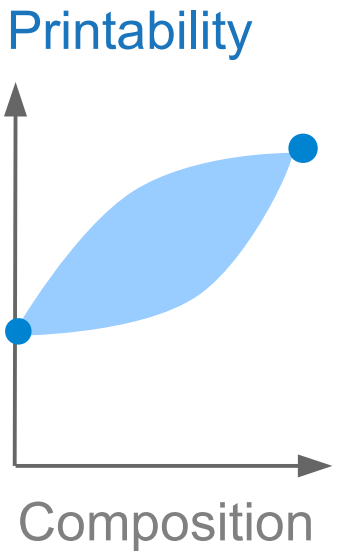
Fatigue

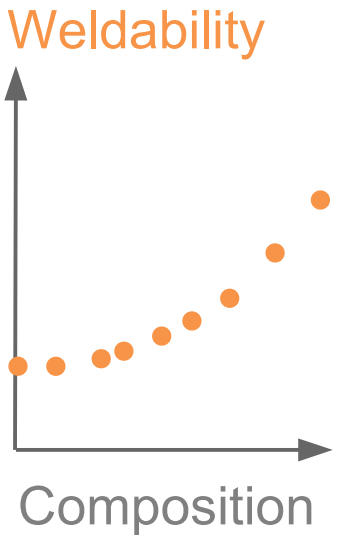
Welding

Insufficient processability results

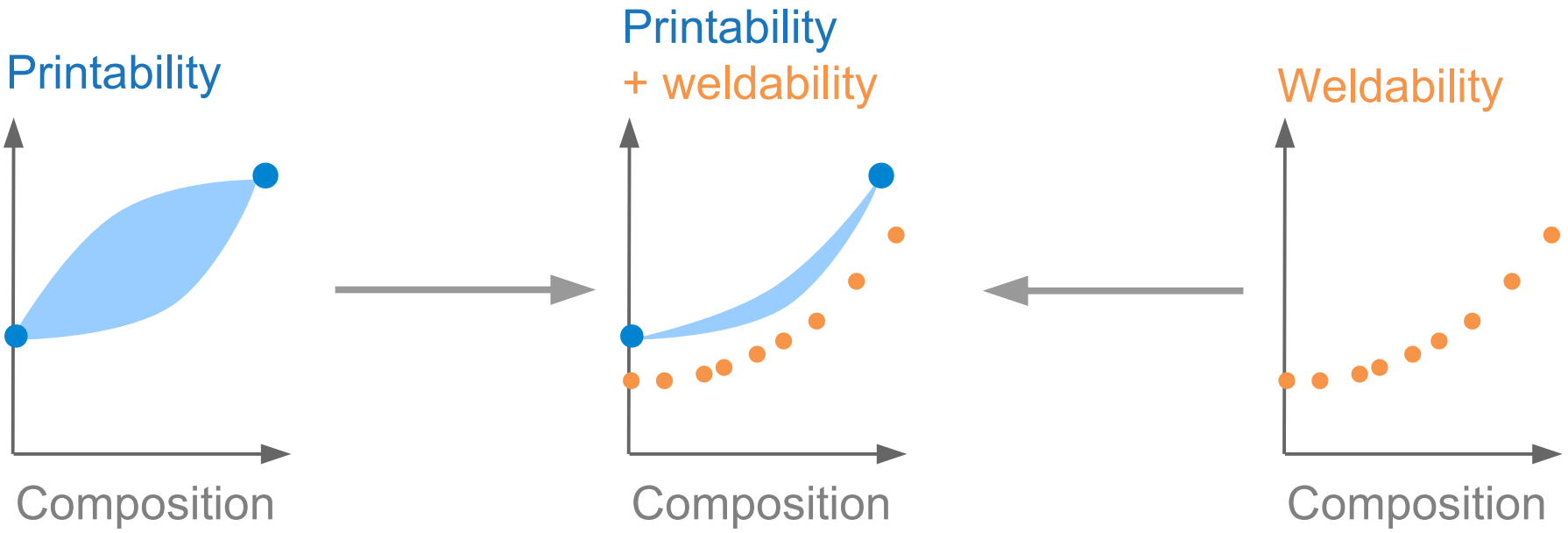


Welding is analogous to direct laser deposition





Merging properties with the neural network



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

Composition

Cr: 19%

Co: 4%

Mo: 4.9%

W: 1.2%

Zr: 0.05%

Nb: 3%

Al: 2.9%

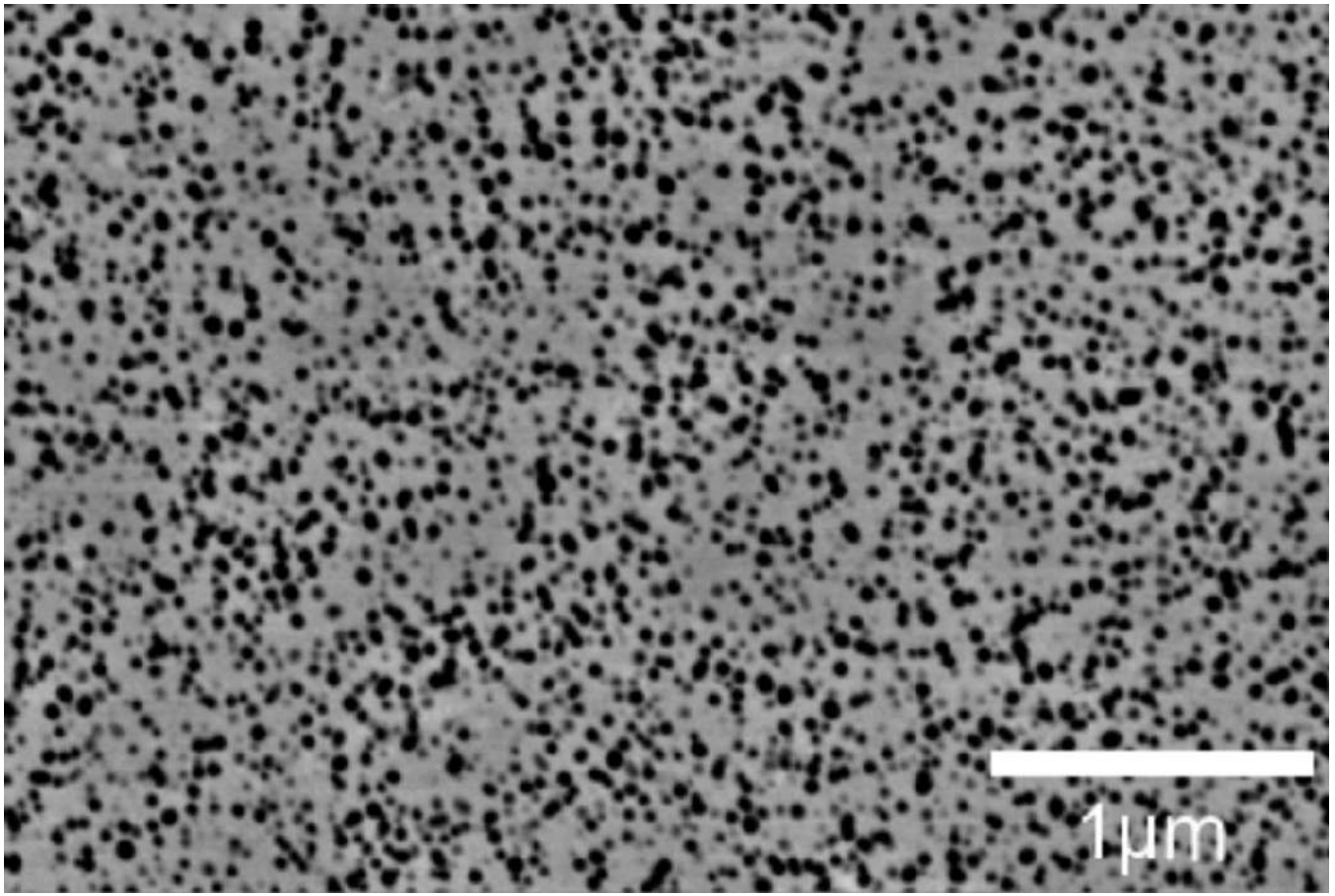
C: 0.04%

B: 0.01%

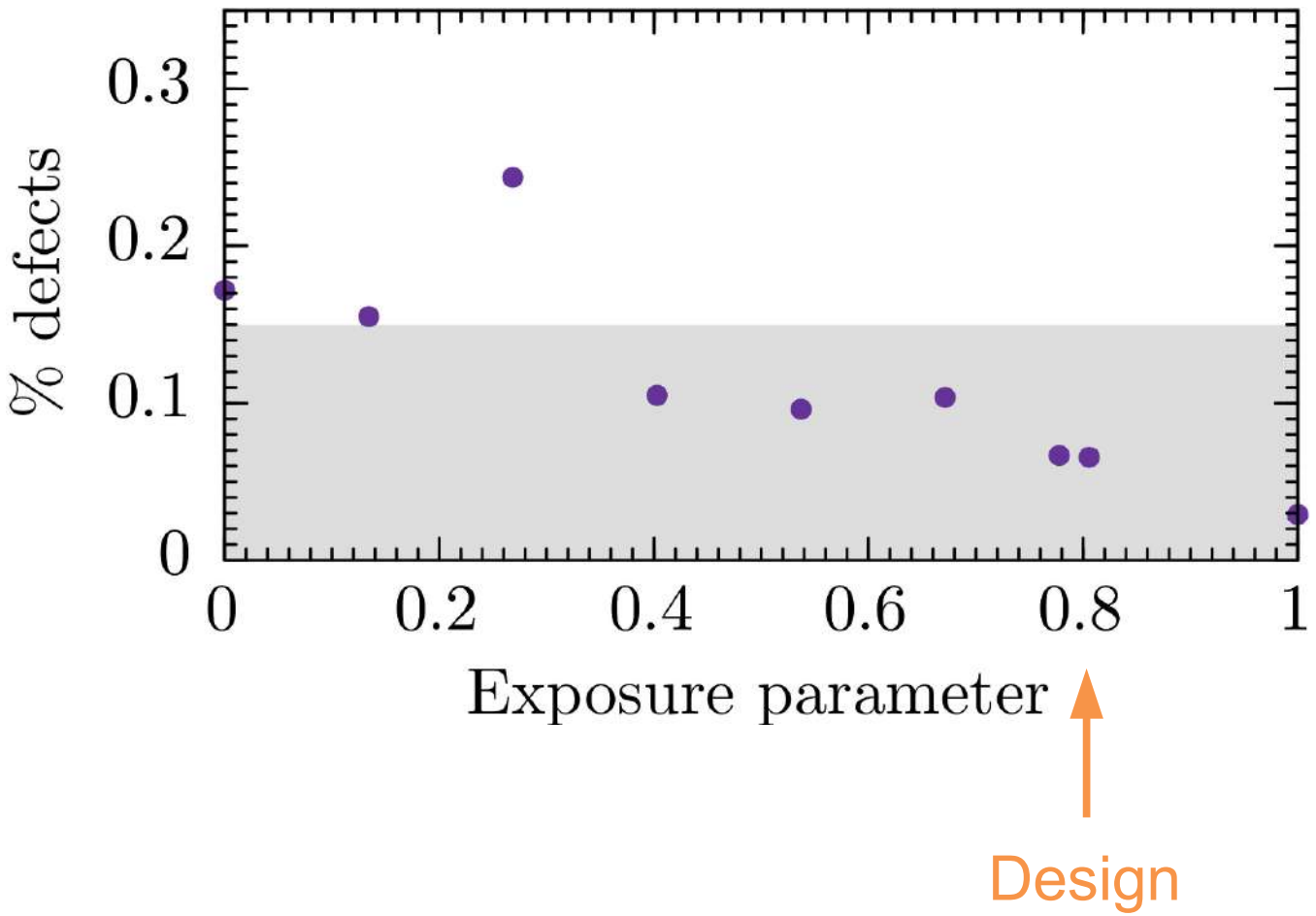
Ni

Expose 0.8

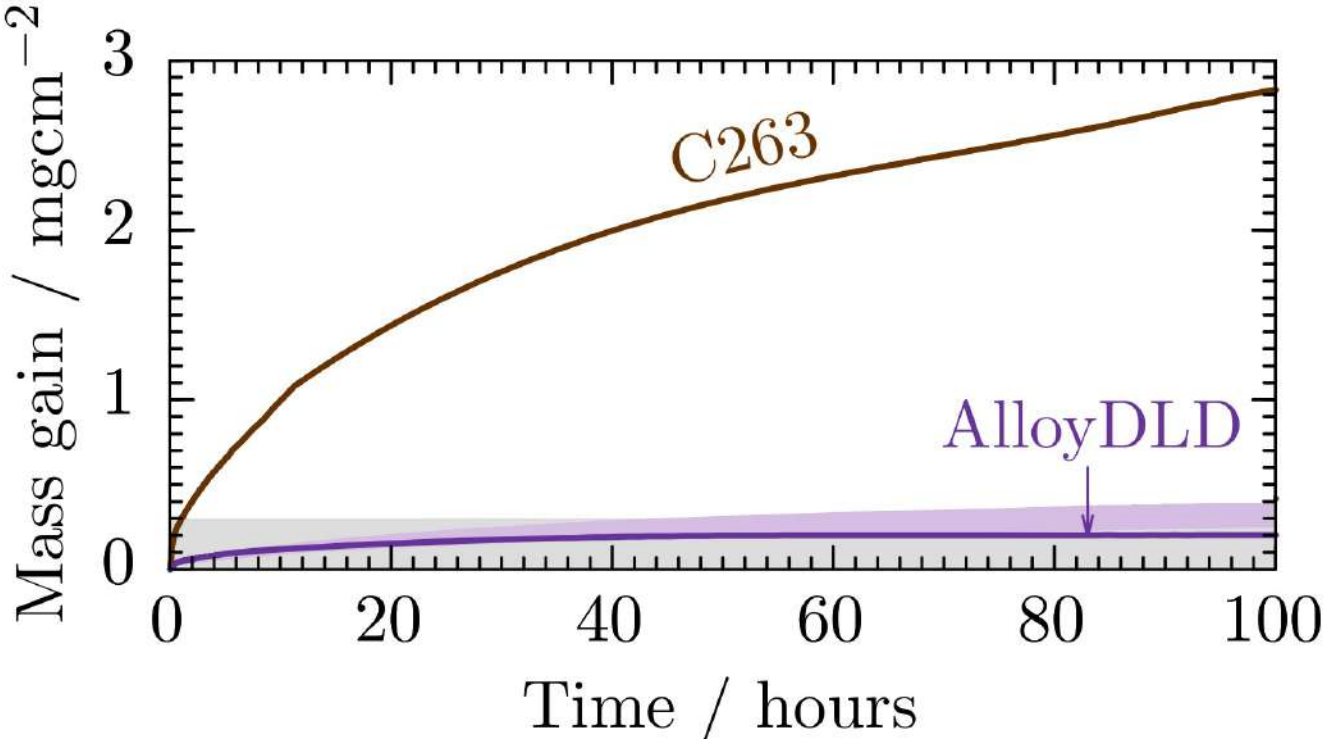
Microstructure



Testing the processability: horizontal printing



Testing the oxidation resistance



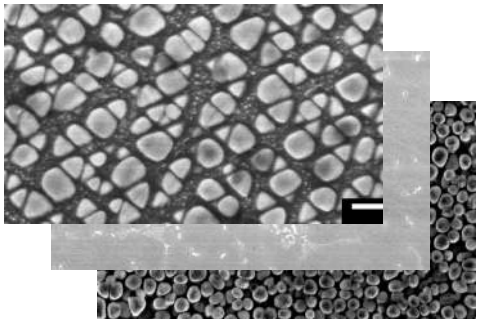
Printing a component for an engine

Materials Solutions

ROLLS ROYCE

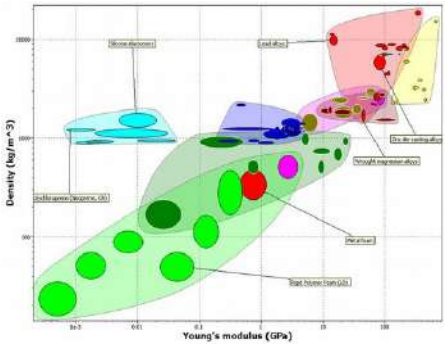
Materials designed

Nickel and molybdenum



Experiment and DFT for batteries

Identified and corrected errors in materials database



ROLLS ROYCE

SAMSUNG

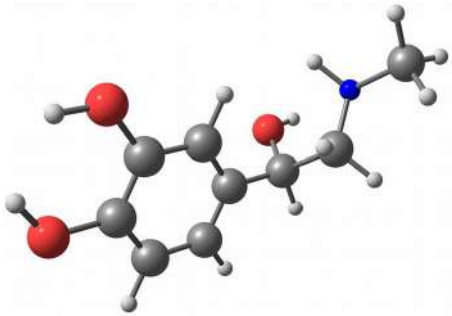
GRANTA
MATERIAL INSPIRATION

Beyond materials

Lubricants with molecular dynamics and experiments

bp

Protein prediction



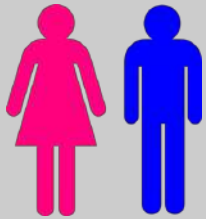
optibrium

Drug design

e-therapeutics

Understand person dynamics

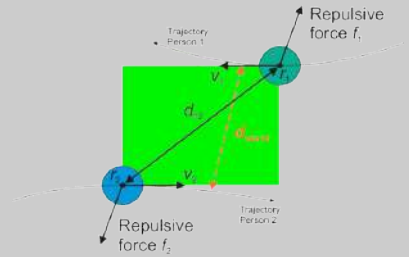
Characteristics

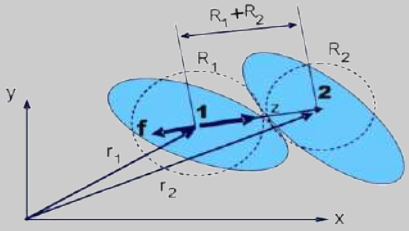


Video

Experimental

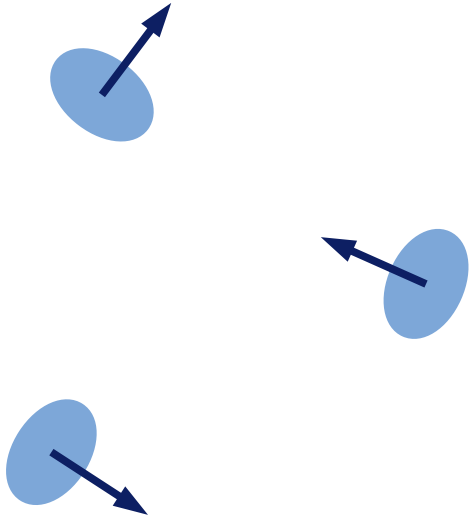
Person dynamics



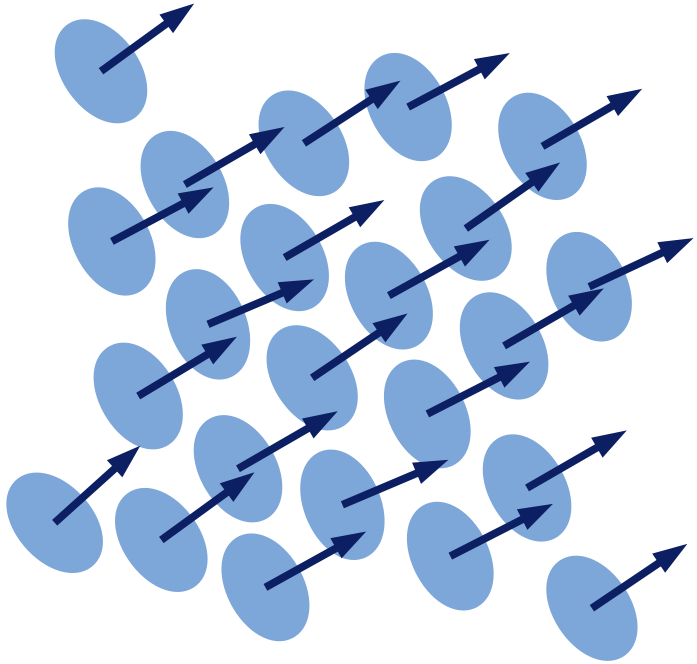


Fluid model of crowd behavior with Julian Hewitt

Sparse crowd
Independent motion



Dense crowd
Collective motion



Boundary condition of pedestrian flux

Calibrate against Legion model

Summary

Merge different experimental quantities and computer simulations into a holistic design tool

Designed and experimentally verified alloy for direct laser deposition

Further applications in materials and drug design, now being commercialized by Intellegens

Apply neural networks to crowd behavior