UNIVERSITY OF CAMBRIDGE

Concurrent materials design with artificial intelligence

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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 discovery

Generic with proven applications in materials discovery

A black box

Train with complete data

Materials design

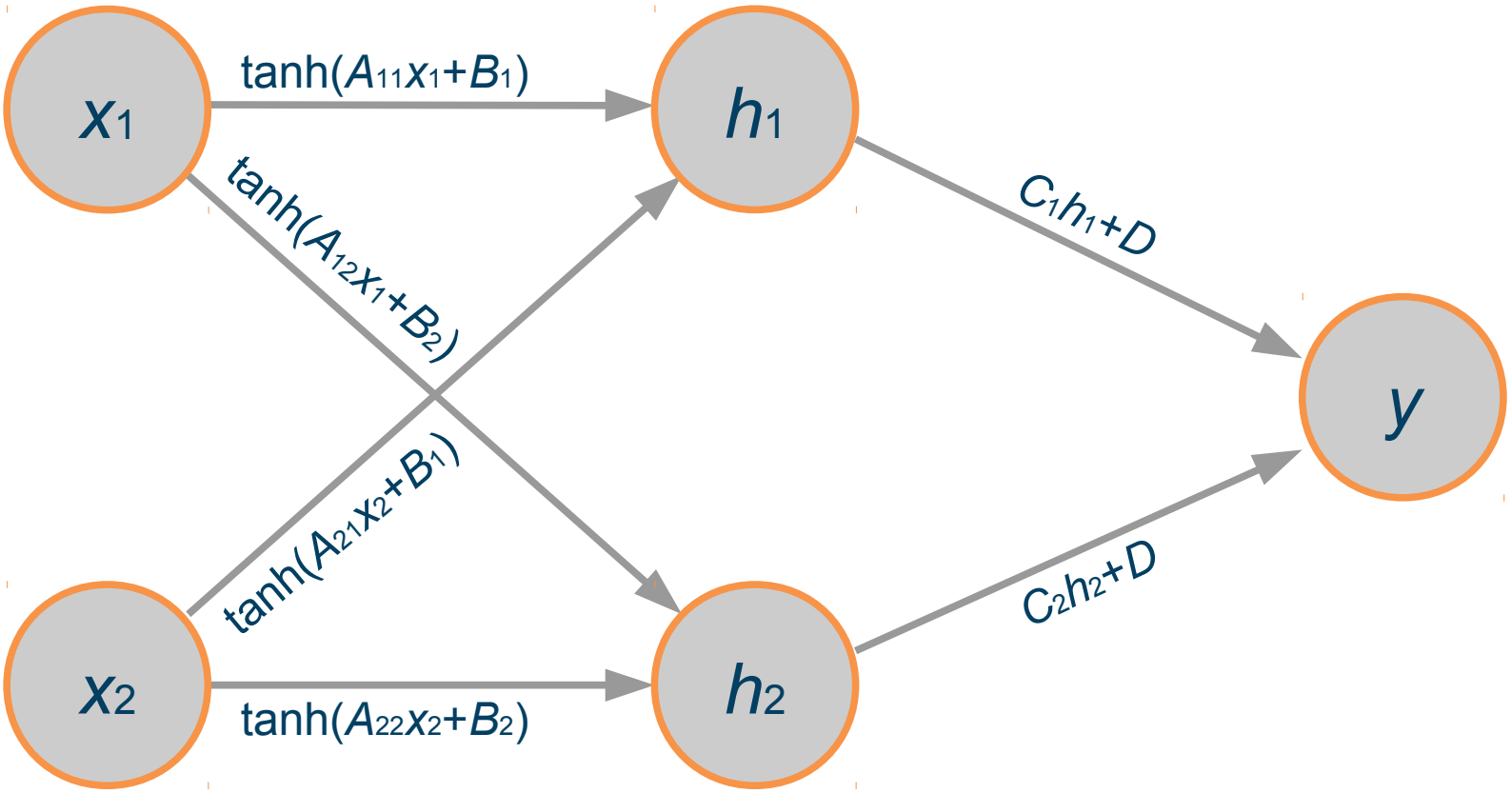
Materials design

Predict with complete data

Crystal structure

Crystal structure

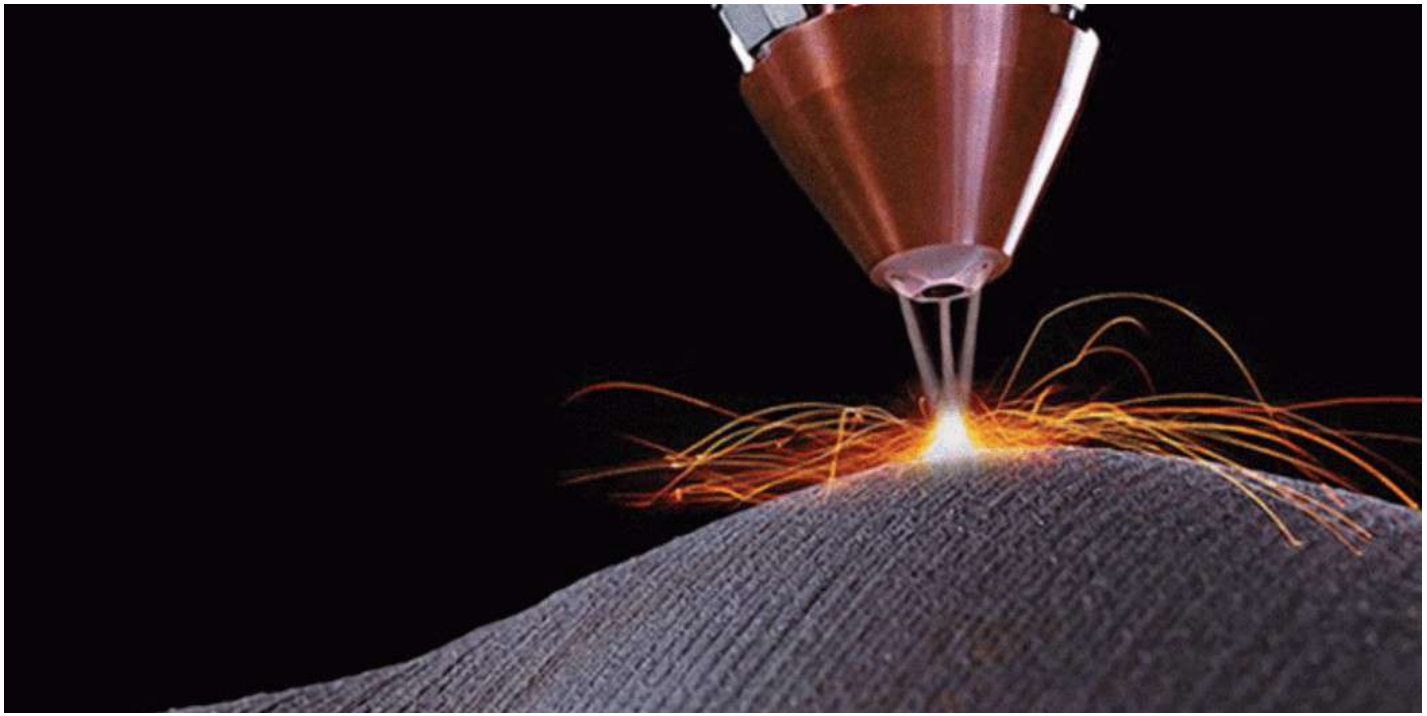
Architecture



Train with fragmented data

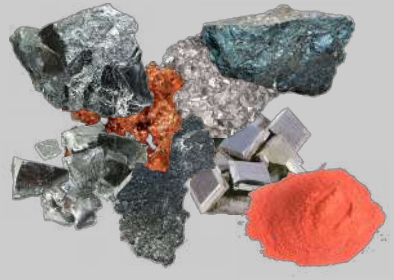
Predict with fragmented data

Direct laser deposition requires new alloys



Neural networks for materials design

Composition



Properties

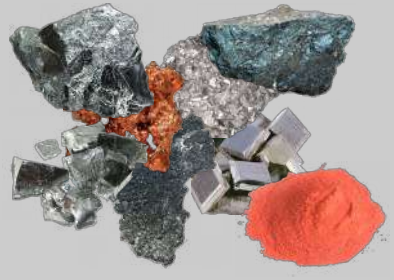
Process

Fatigue

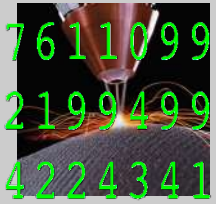
Welding

Neural networks for materials design

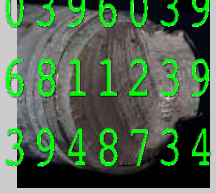
Composition



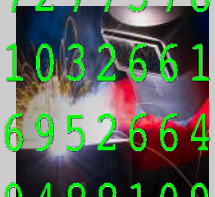
Properties



Process



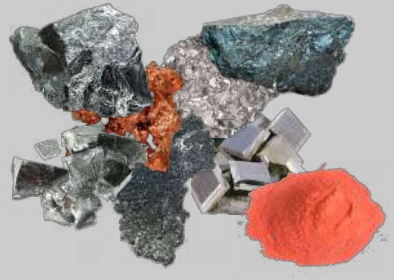
Fatigue



Welding

Neural networks for materials design

Composition



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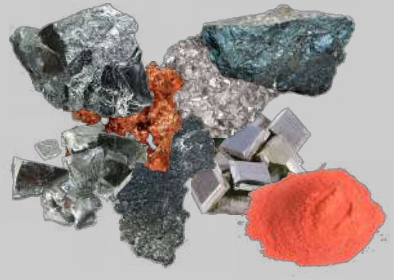

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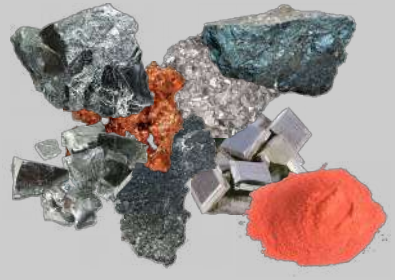


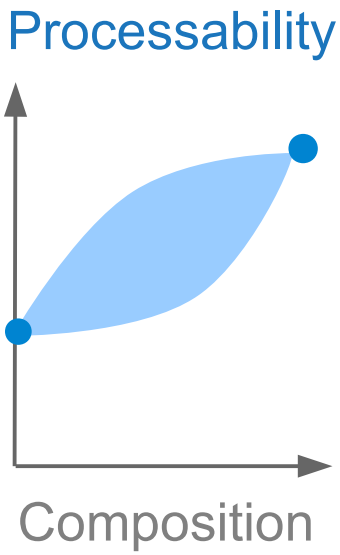
Properties

Process

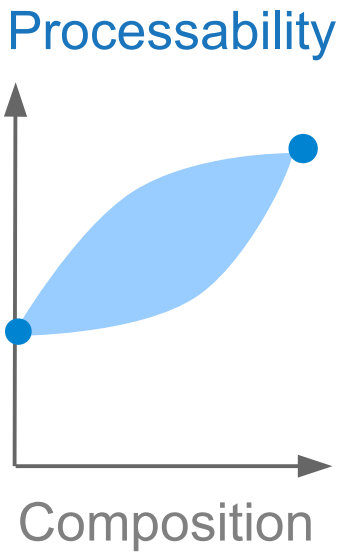
Fatigue

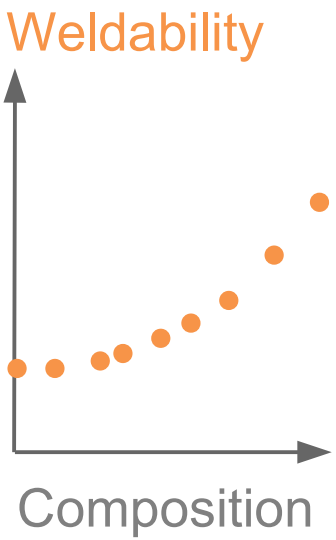
Welding

Insufficient processability results

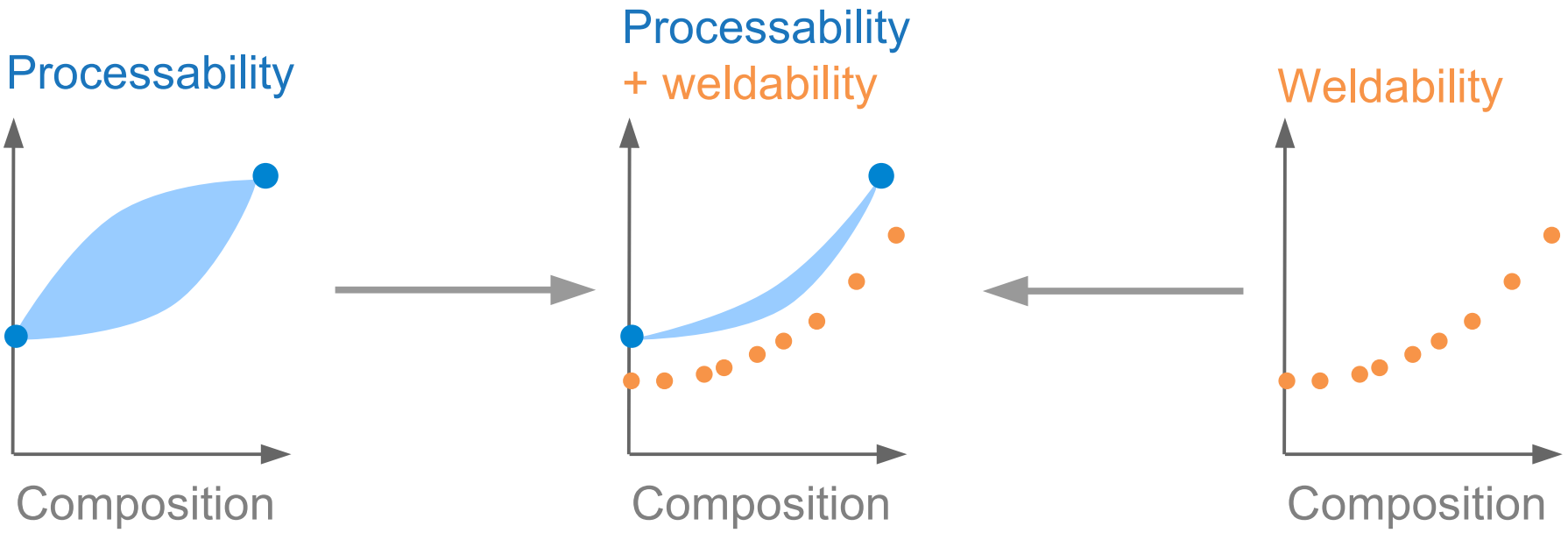


Welding is analogous to direct laser deposition

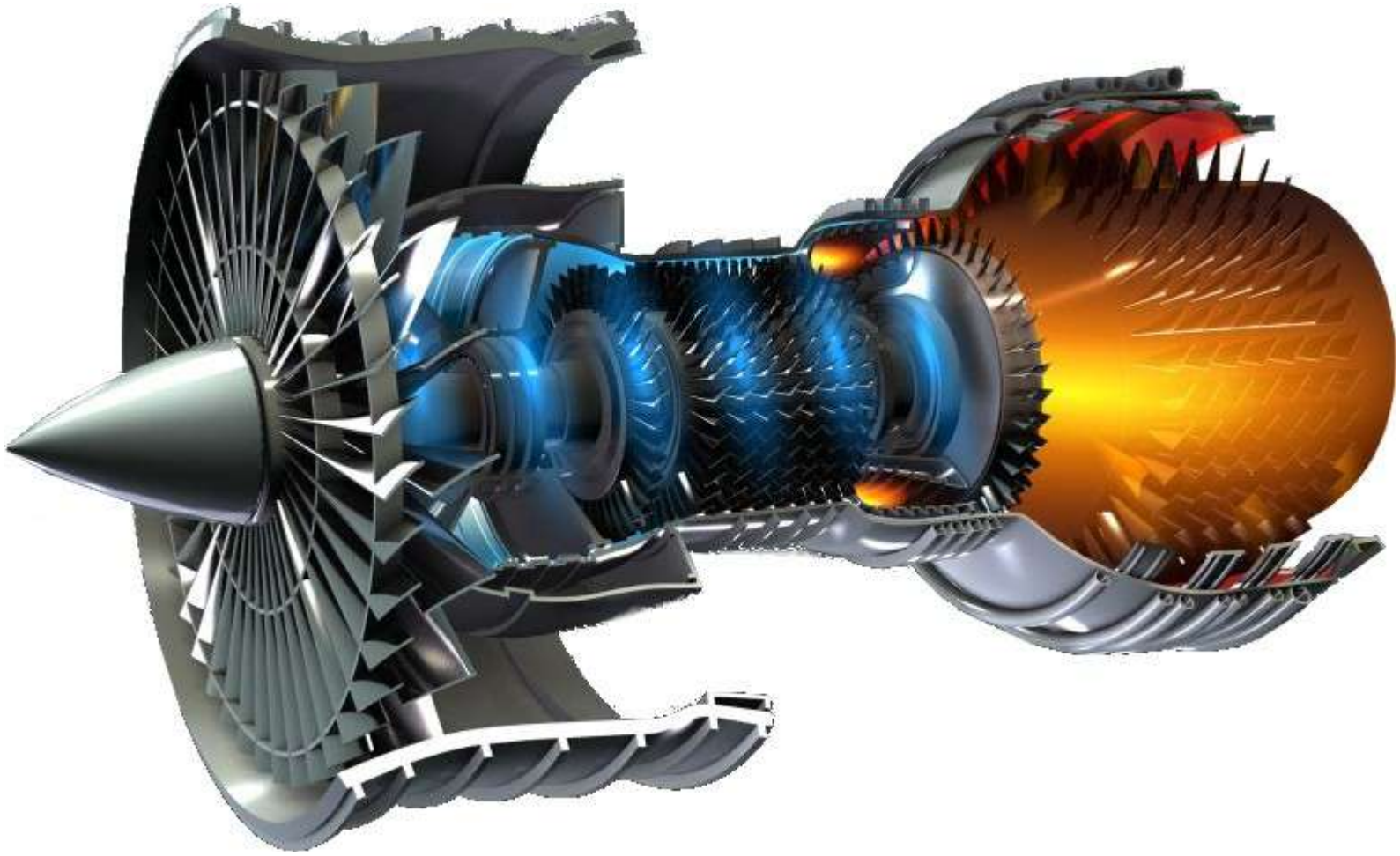




Merging properties with the neural network



Schematic of a jet engine



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%

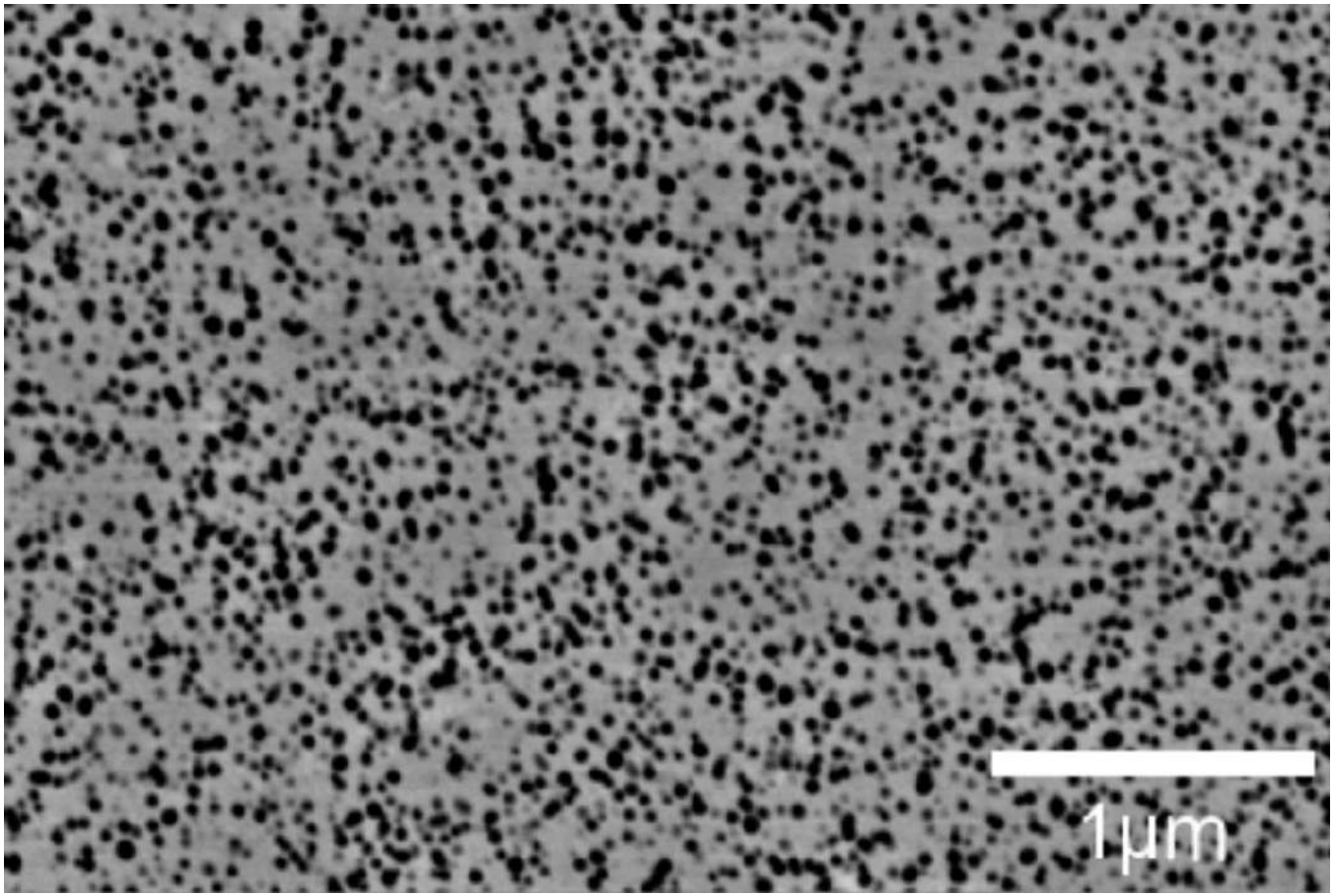
C: 0.04%

B: 0.01%

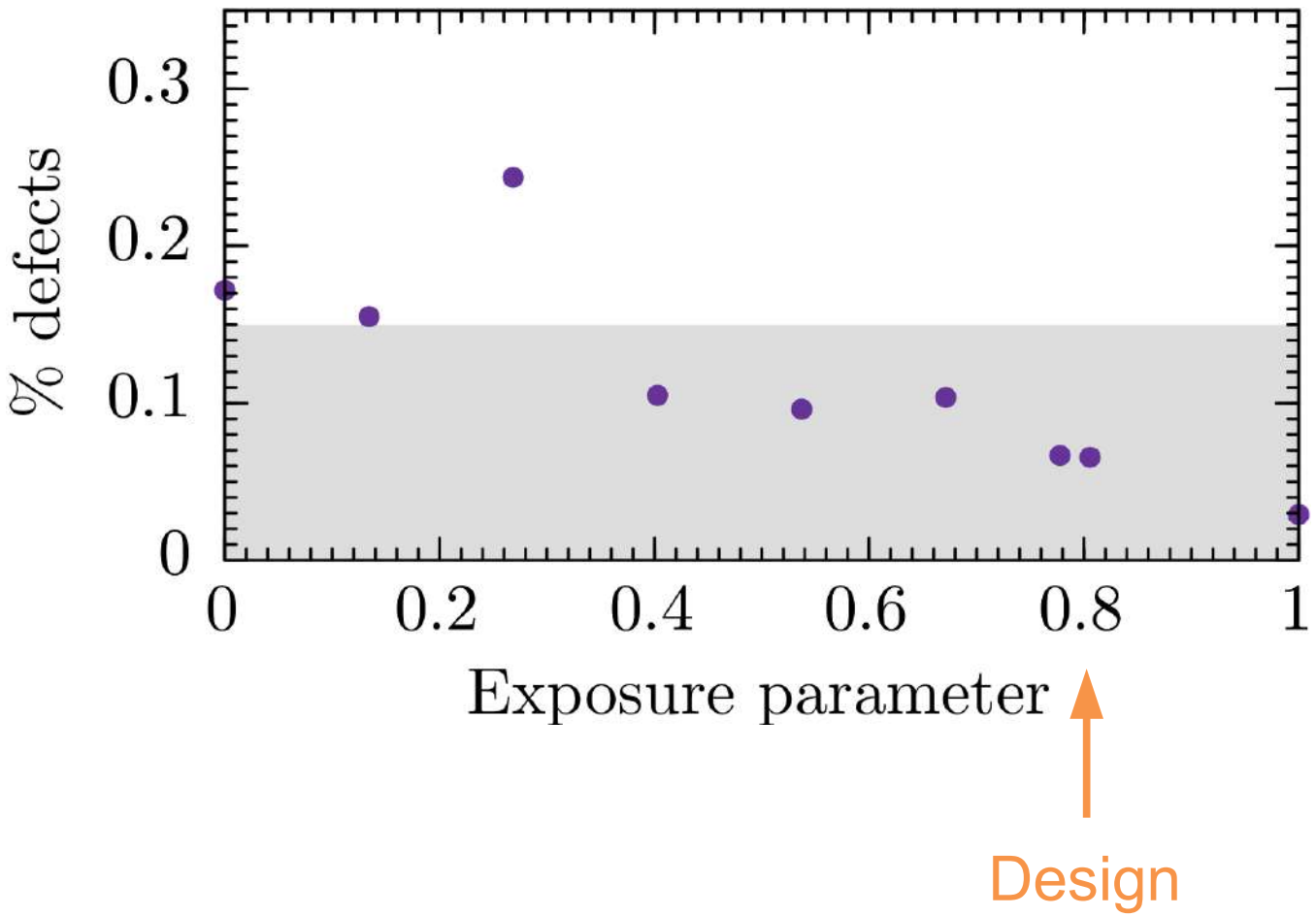
Ni

Expose 0.8

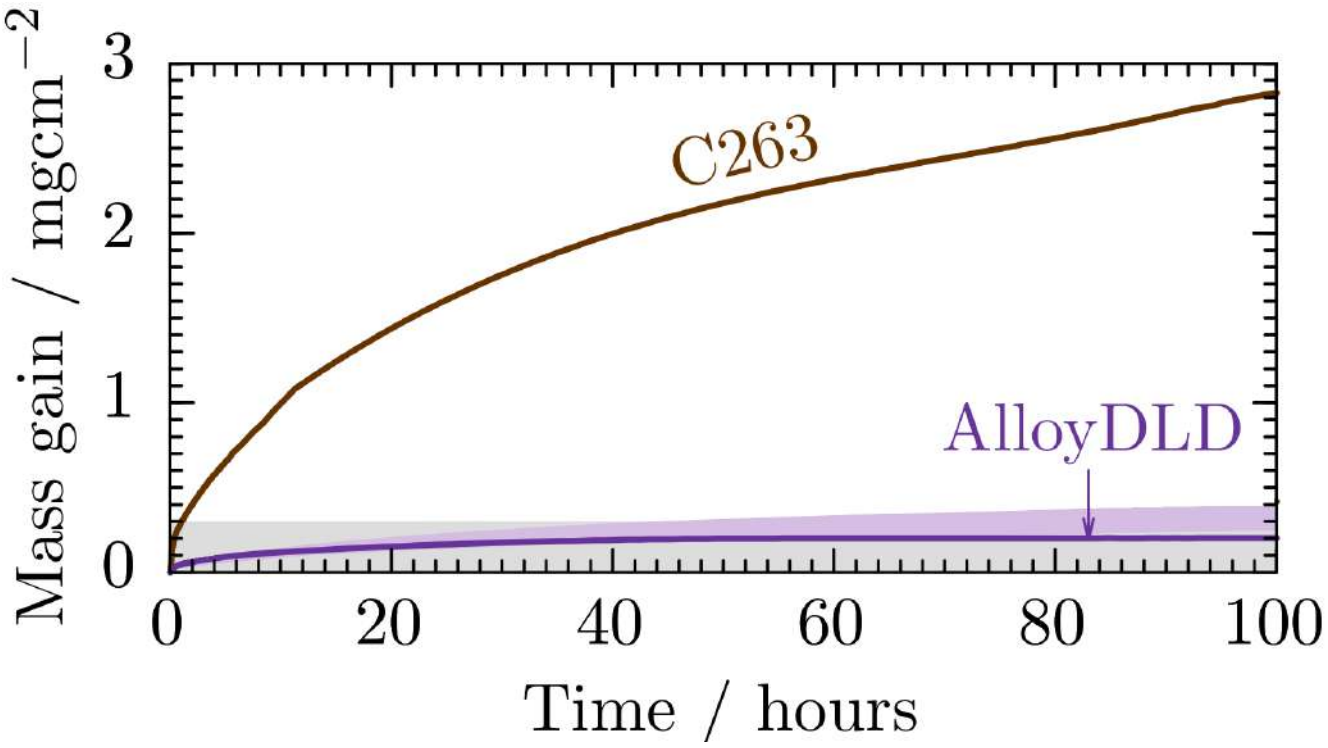
Microstructure



Testing the processability: horizontal printing



Testing the oxidation resistance



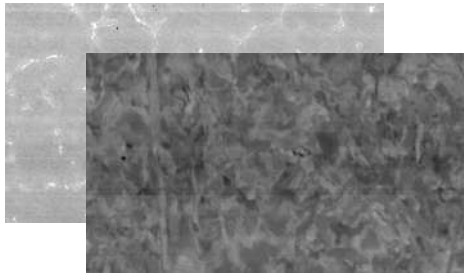
Printing a component for an engine

Materials Solutions

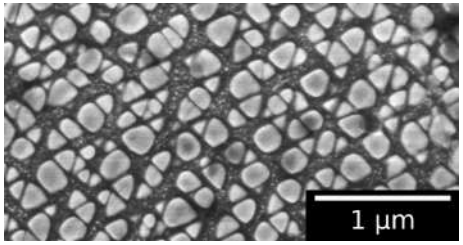
ROLLS ROYCE

More materials designed

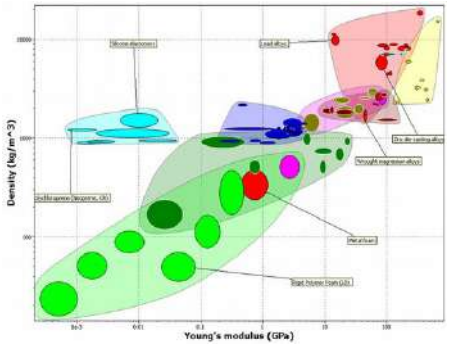
Molybdenum forging alloys



Ni-base alloy for discs



Found 192 errors in materials databases



GRANTA
MATERIAL INSPIRATION

even more materials designed

Battery design with DFT and experimental data

Designing lubricants with DFT and experimental data

In situ repair

Summary

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

Designed and experimentally verified alloy for direct laser deposition

Generic, applications in materials, drug design, and beyond