UNIVERSITY OF CAMBRIDGE

The modern-day blacksmith

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Theory of Condensed Matter group

Neural network algorithm to

Train from sparse datasets

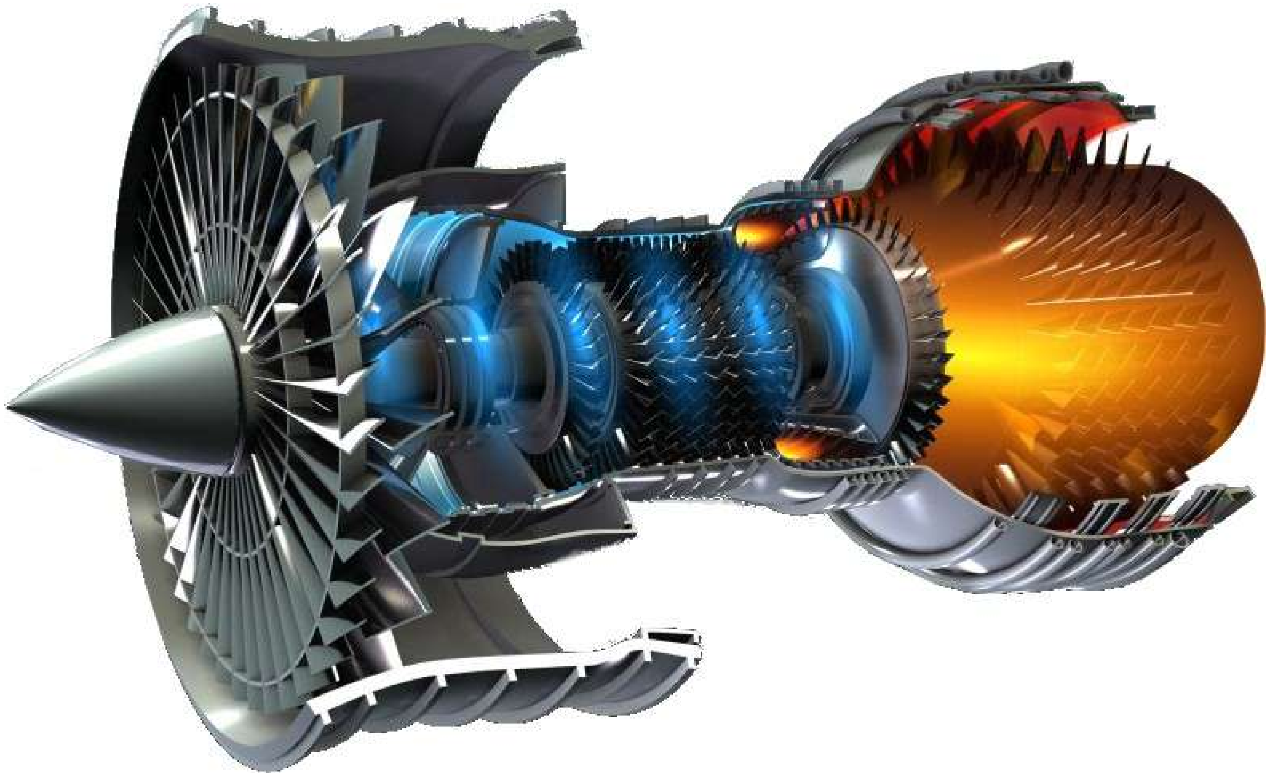
Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

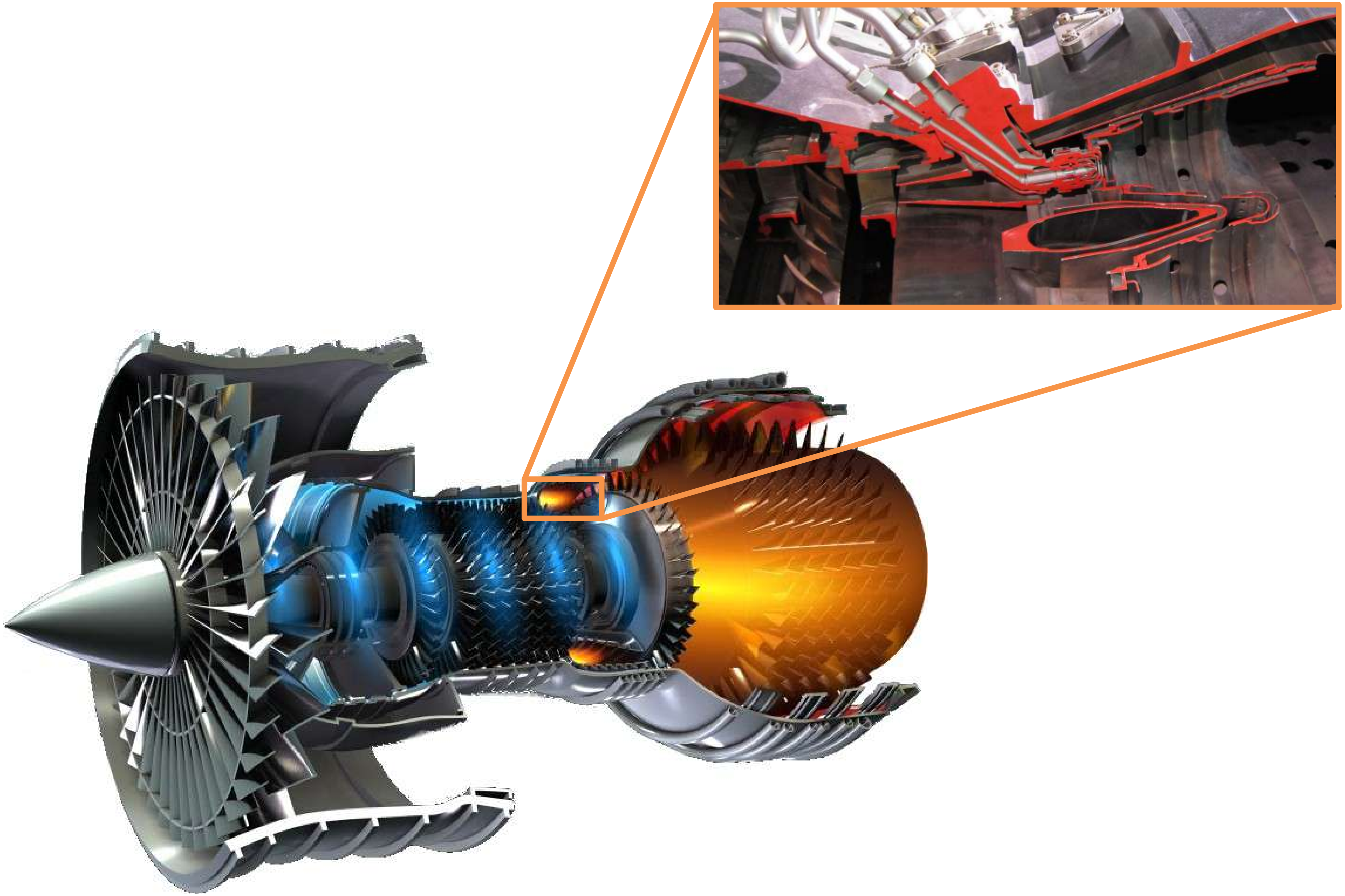
Accelerate materials discovery

Generic with proven applications in materials discovery and drug design

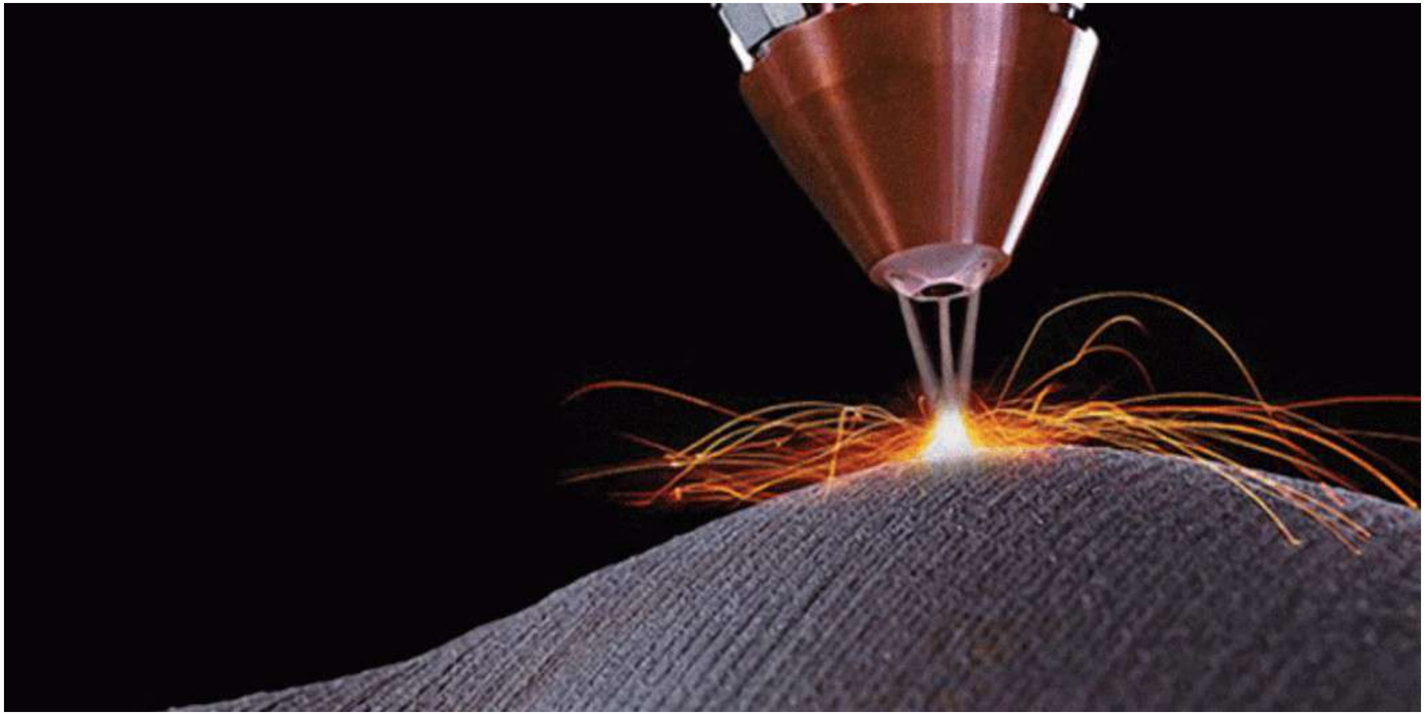
Schematic of a jet engine



Combustor in a jet engine

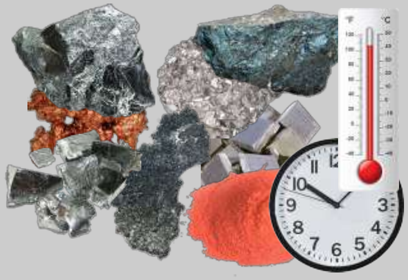


Direct laser deposition requires new alloys



Neural networks for materials design

Composition



Properties

Process

Fatigue

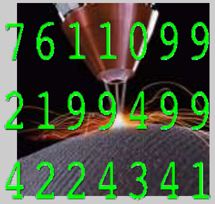
Welding

Neural networks for materials design

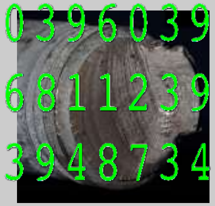
Composition

Properties

Process



Fatigue



Welding

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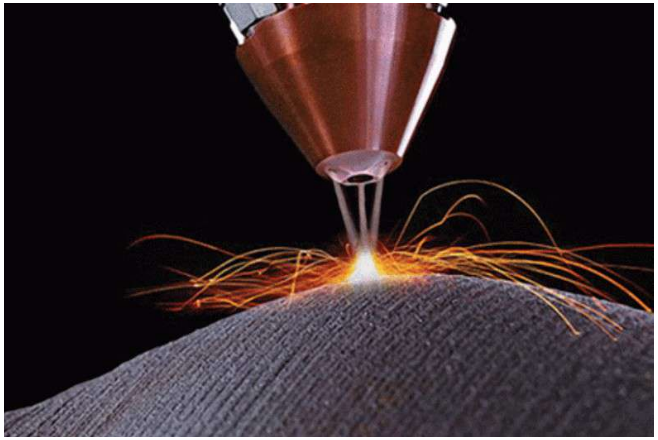
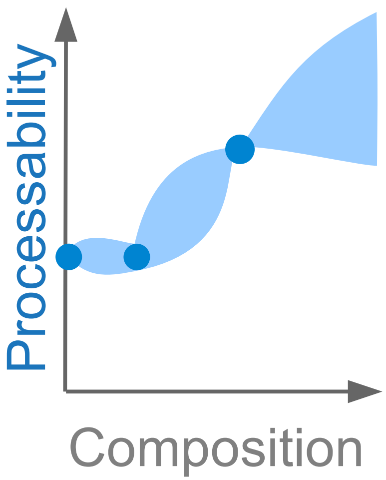


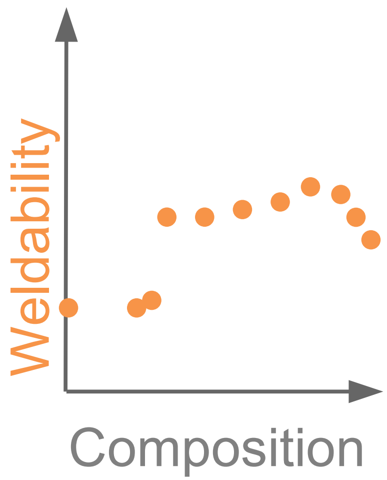
Laser

Electricity

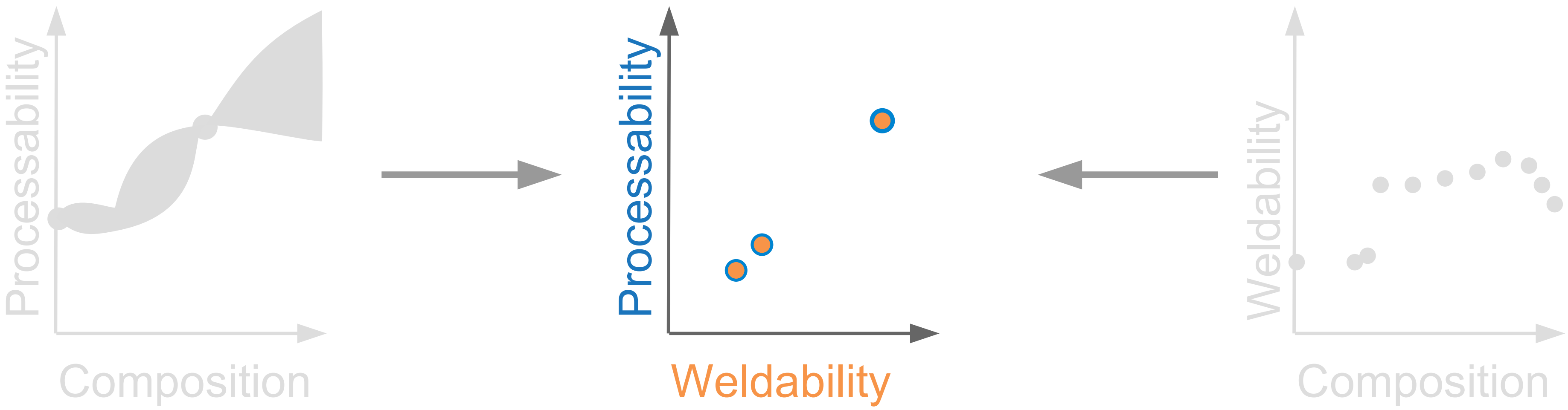
Insufficient data for processability



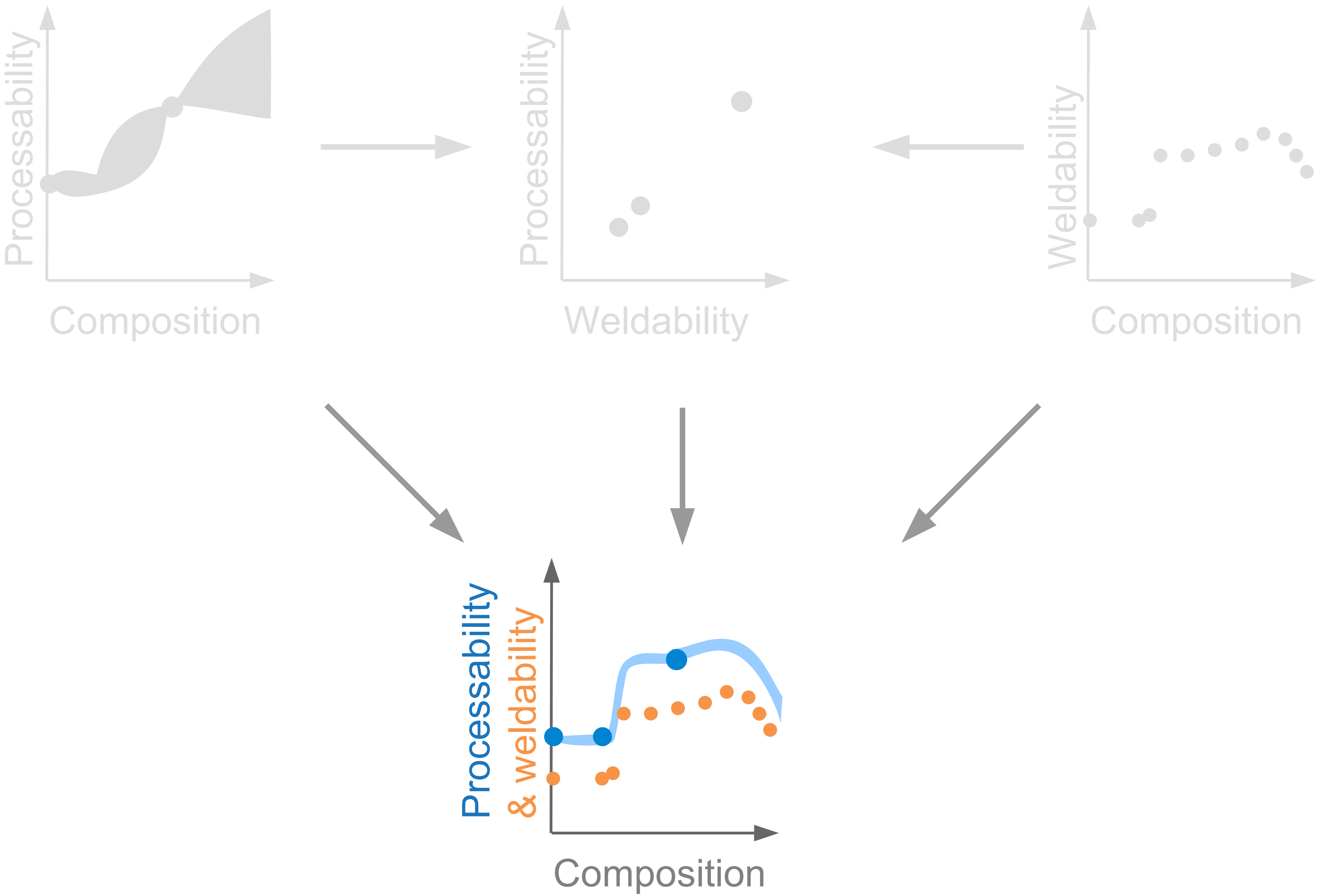
Welding is analogous to direct laser deposition



Simple processability-welding relationship



Merging properties with the neural network



Neural networks for materials design

Composition

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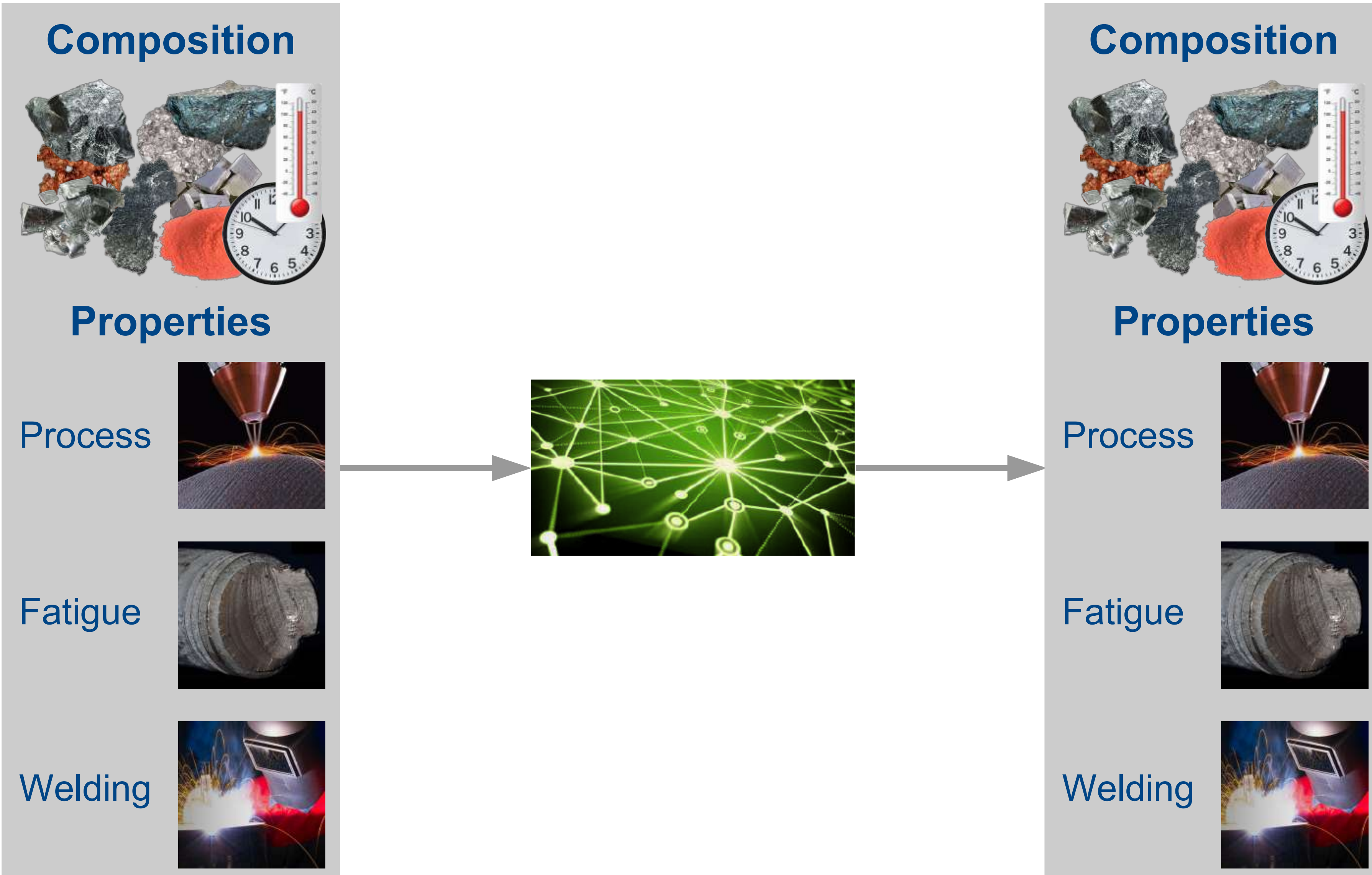
Neural networks for materials design



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%

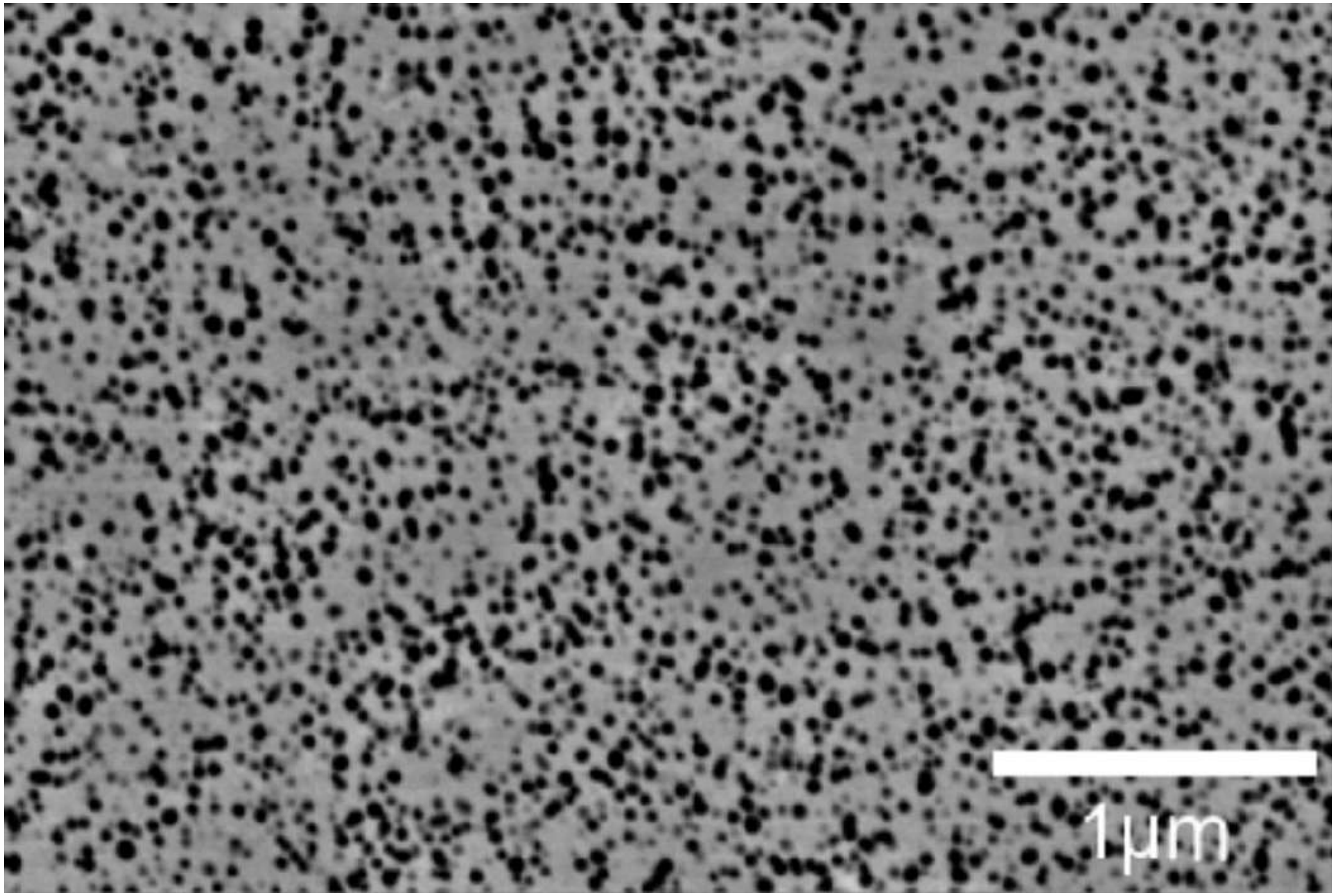
B 0.01%

Ni

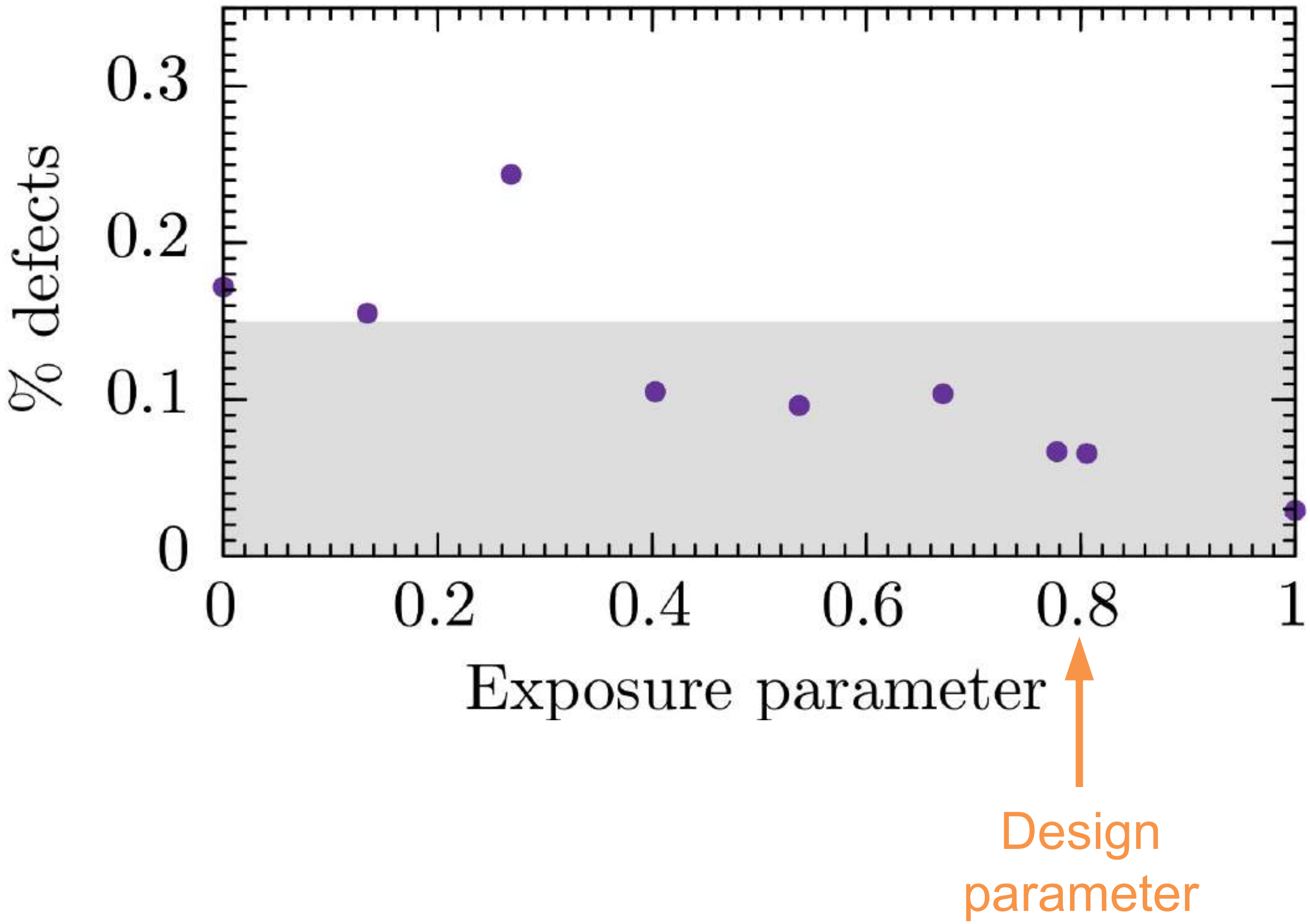
Expose 0.8

T_{HT} 1230ºC

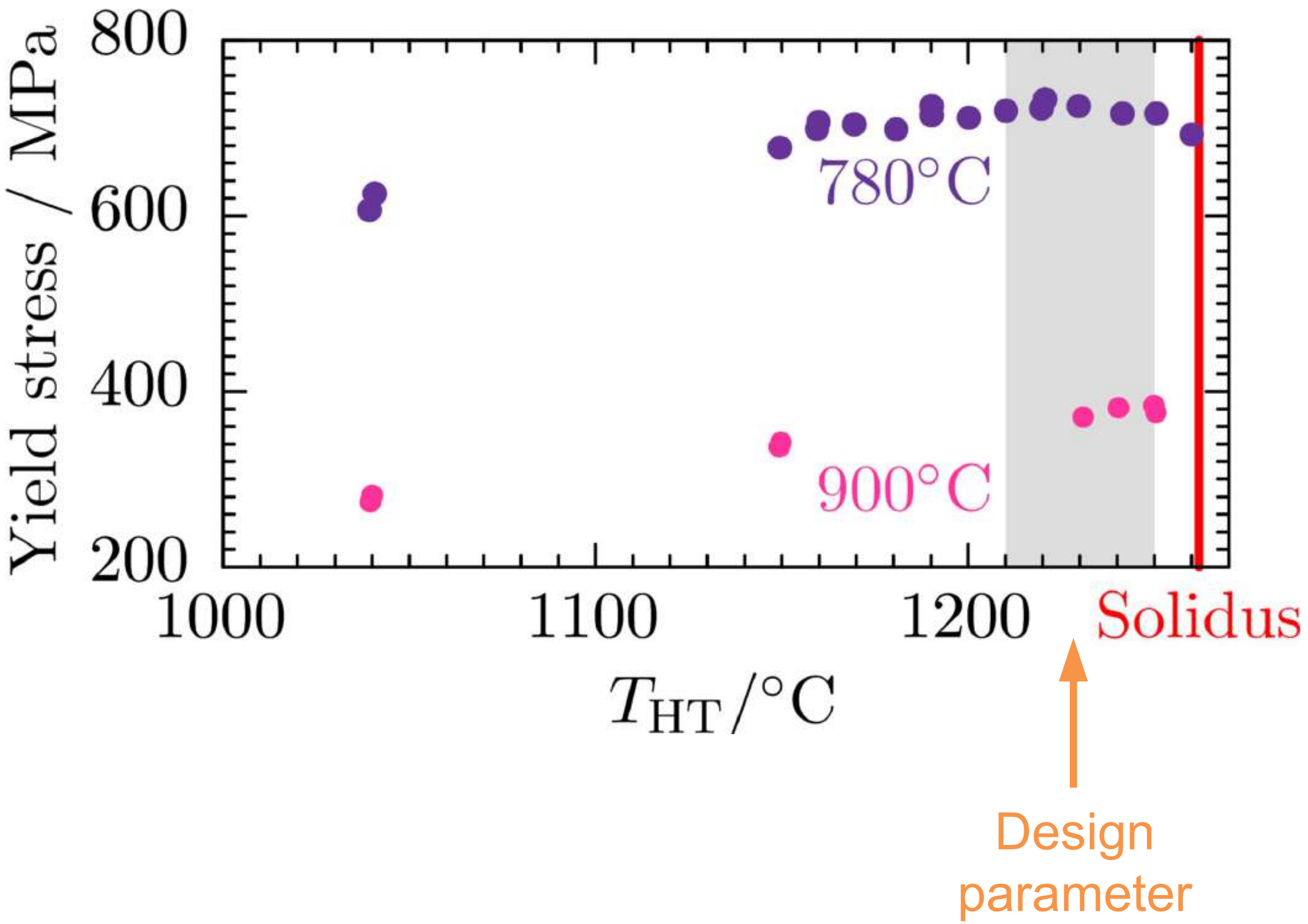
Microstructure



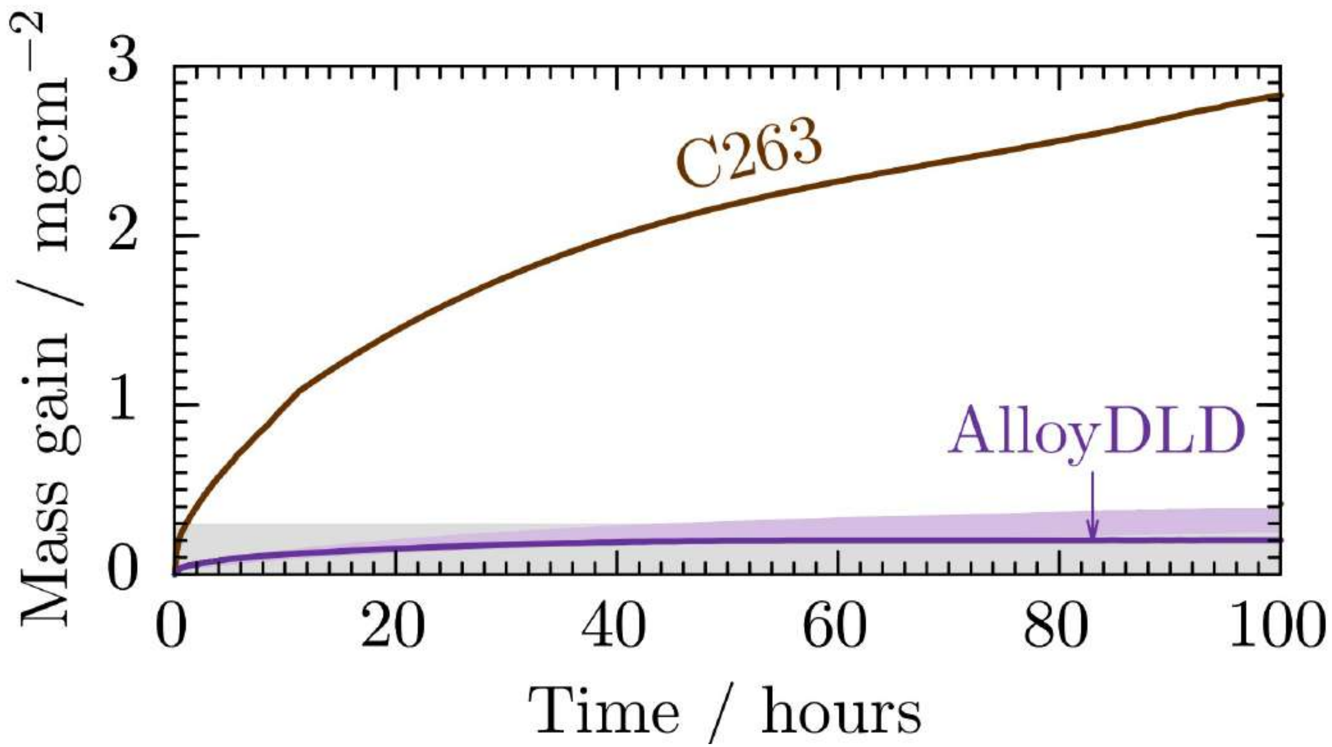
Testing the processability



Testing the yield stress

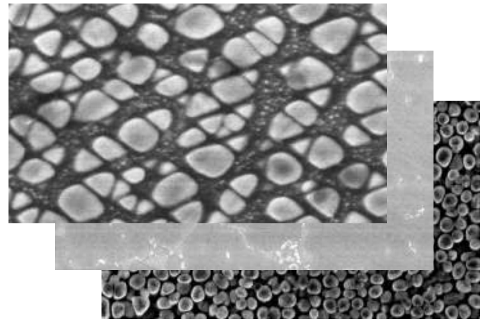


Testing the oxidation resistance



Materials designed

Nickel and molybdenum

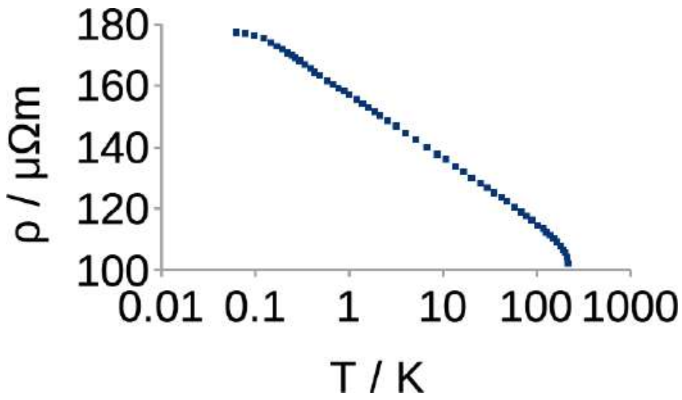


Experiment and DFT for batteries

Steel for welding

More materials

Quantum and experiment for thermometry



UNIVERSITY OF CAMBRIDGE
Cavendish Laboratory

Lubricants with molecular dynamics and experiments

bp

Drug design

e-therapeutics

optibrium

Takeda

Summary

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

Designed and experimentally verified alloy for direct laser deposition

Apply technology to other materials and drug design

Commercialized by startup Intellegens