

The modern day blacksmith

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Theory of Condensed Matter group

Neural network algorithm to

Train from **sparse** datasets

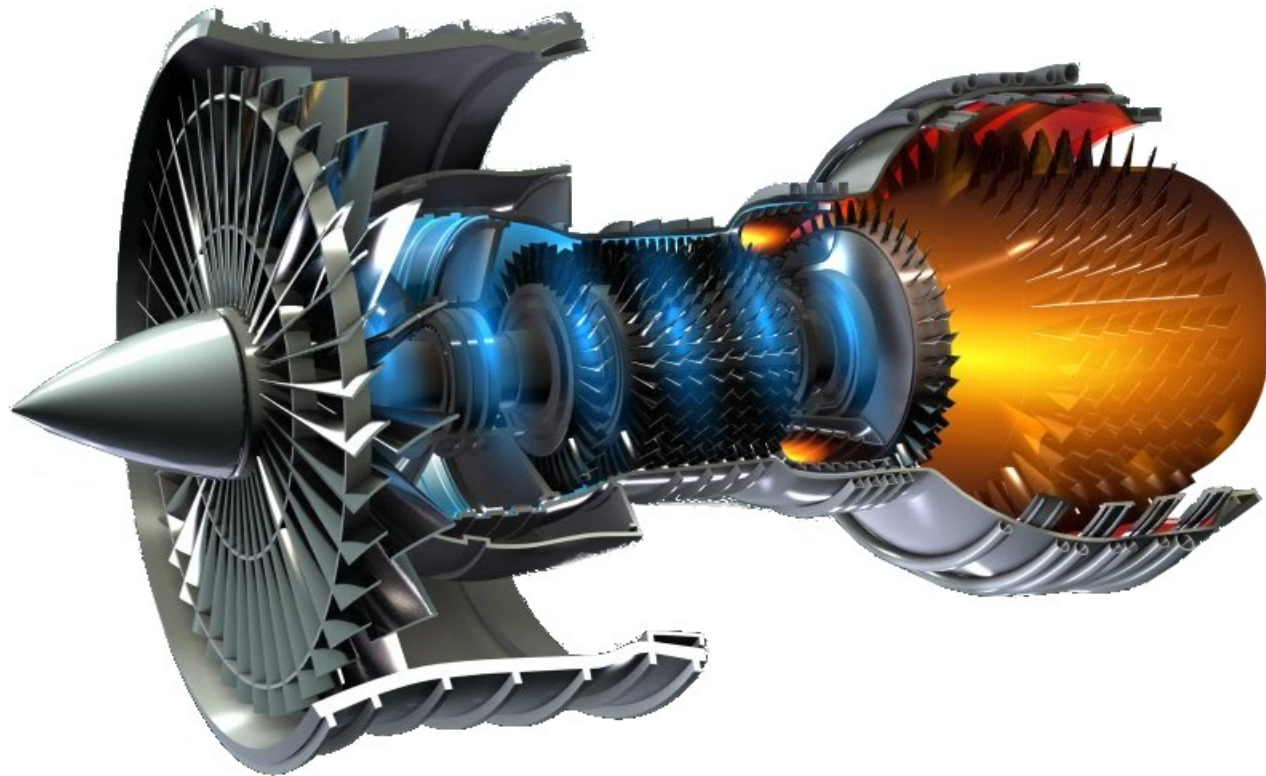
Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

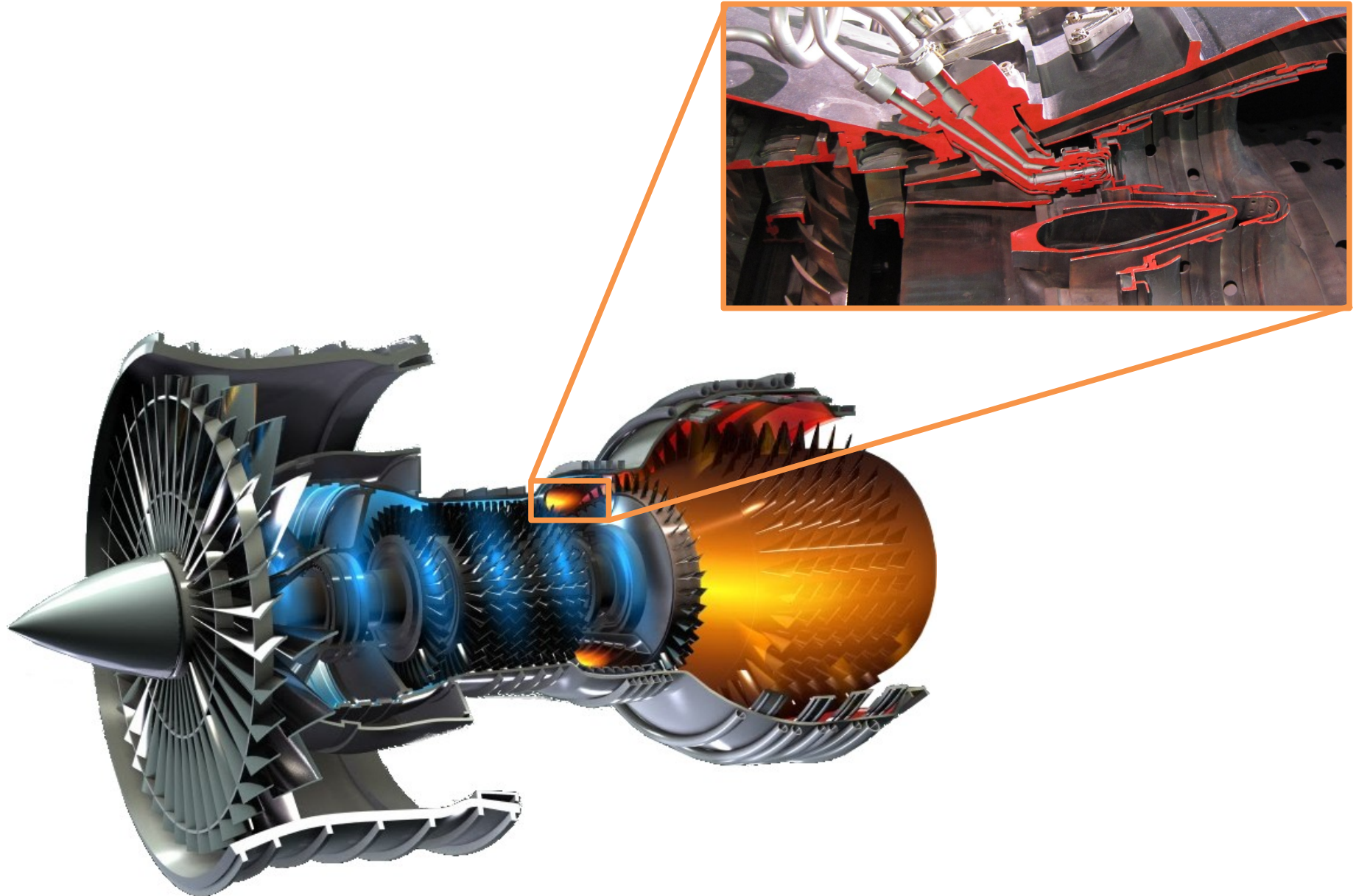
Accelerate materials discovery

Generic with **proven** applications in materials discovery and drug design

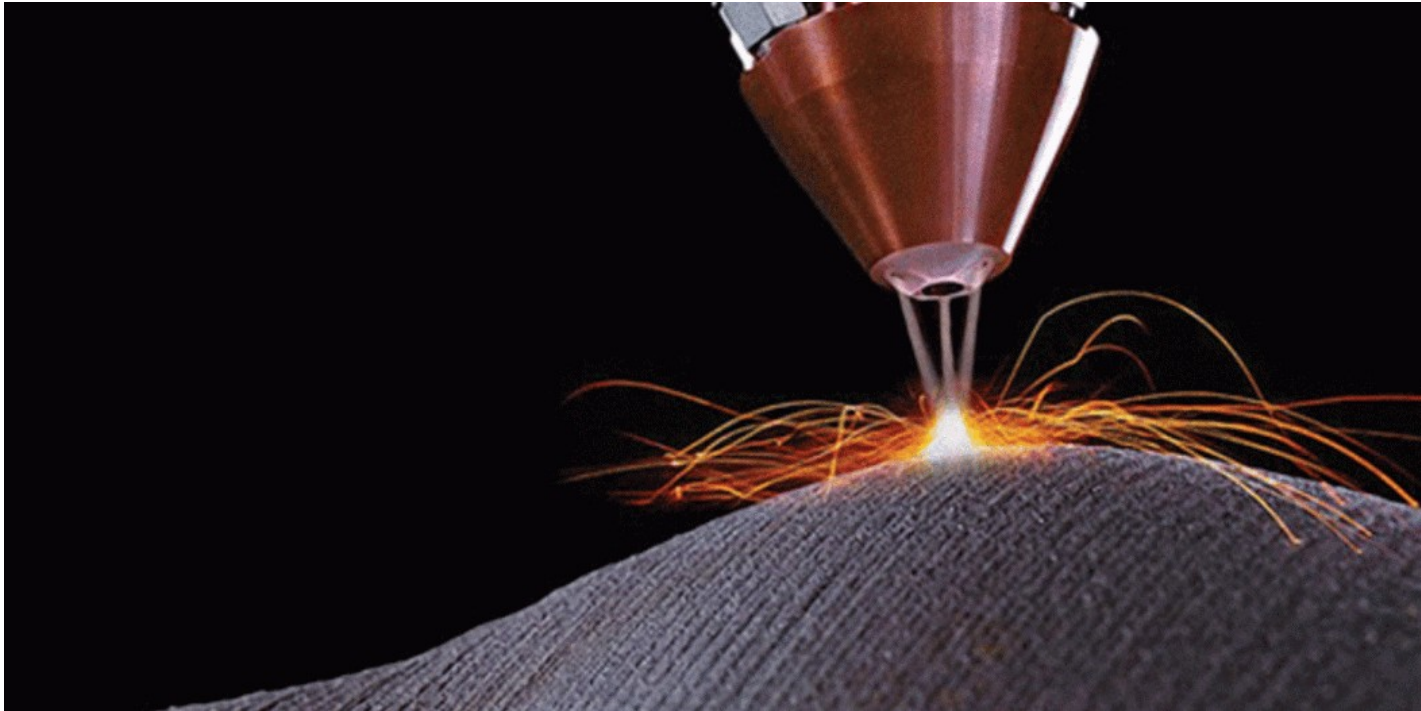
Schematic of a jet engine



Combustor in a jet engine

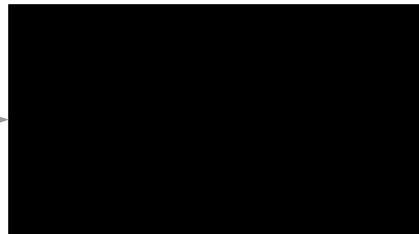


Direct laser deposition requires new alloys



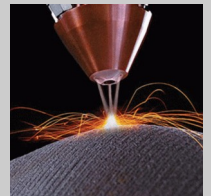
Neural networks for materials design

Composition



Properties

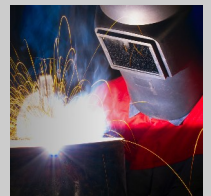
Process



Fatigue



Welding



Neural networks for materials design

Composition



Properties

293928764790904
021364010360202
636584970508183
703818406465007
501066378902903
715269094674449
011404497494802

Process

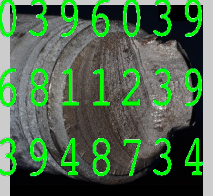
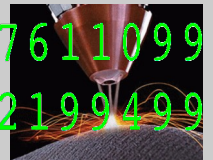
488685276110993
203332721994995
976579342243418

Fatigue

394046703960393
597692868112392
376413439487341

Welding

366524472773787
144219810326510
805556069526643
983443994881092



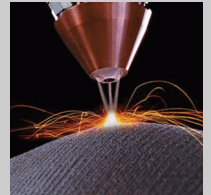
Neural networks for materials design

Composition



Properties

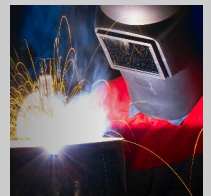
Process



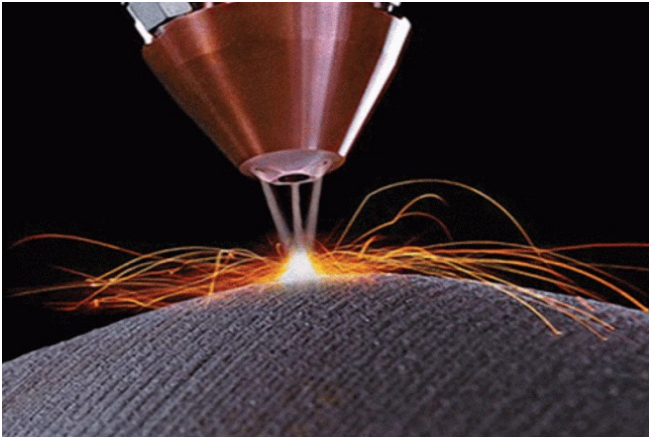
Fatigue



Welding



Neural networks for materials design

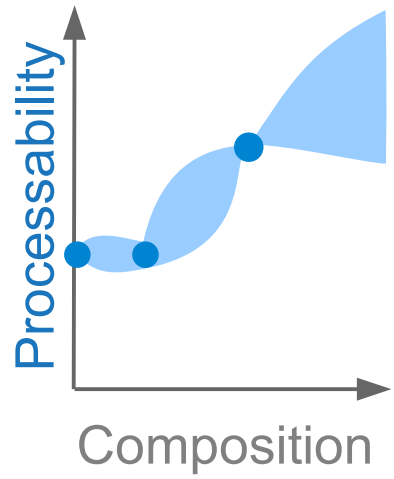


Laser

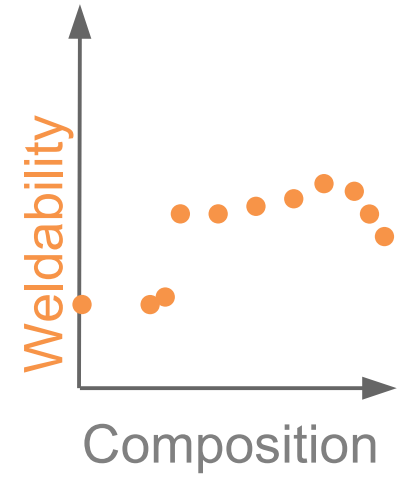


Electricity

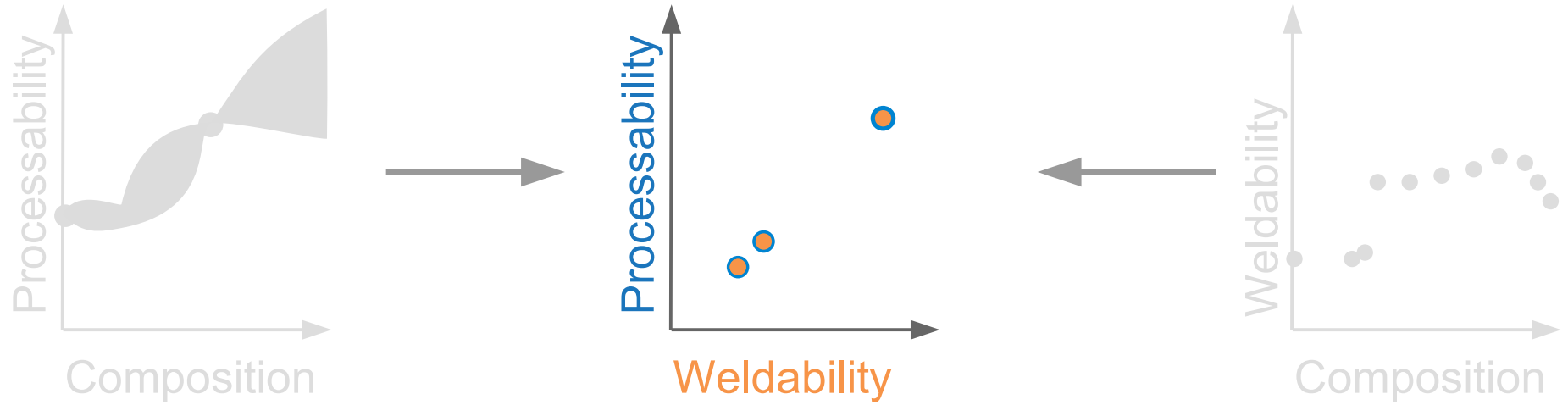
Insufficient data for processability



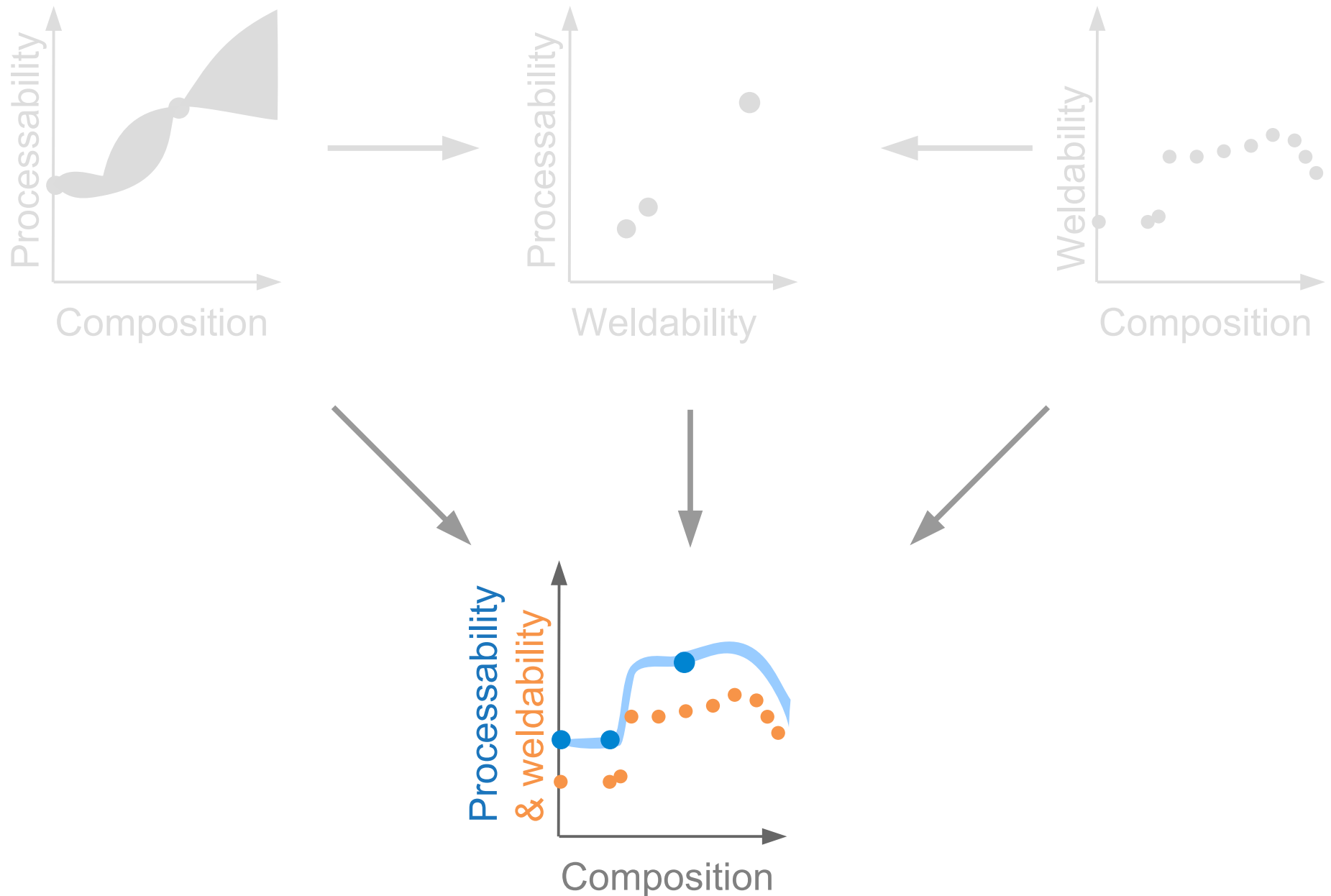
Welding is analogous to direct laser deposition



Simple processability-welding relationship



Merging properties with the neural network



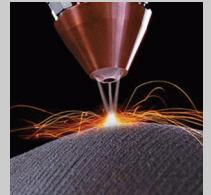
Neural networks for materials design

Composition



Properties

Process



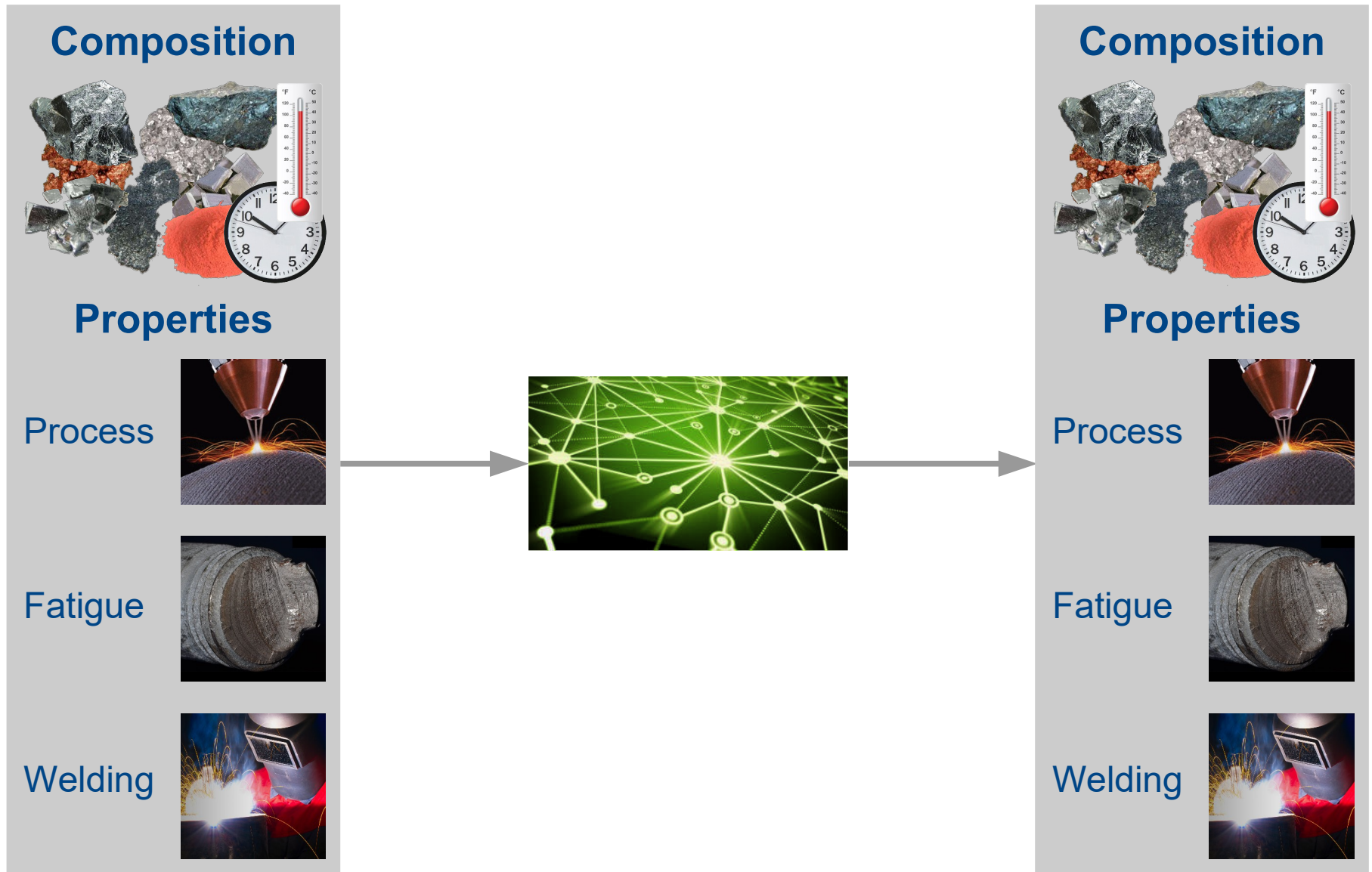
Fatigue



Welding



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 KΩ⁻¹m⁻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 > 10⁵ cycles

Composition

Cr 19%



Co 4%



Mo 4.9%



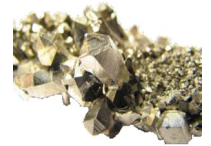
W 1.2%



Zr 0.05%



Nb 3%



Al 2.9%



C 0.04%



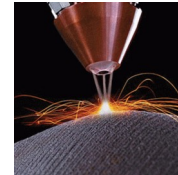
B 0.01%



Ni



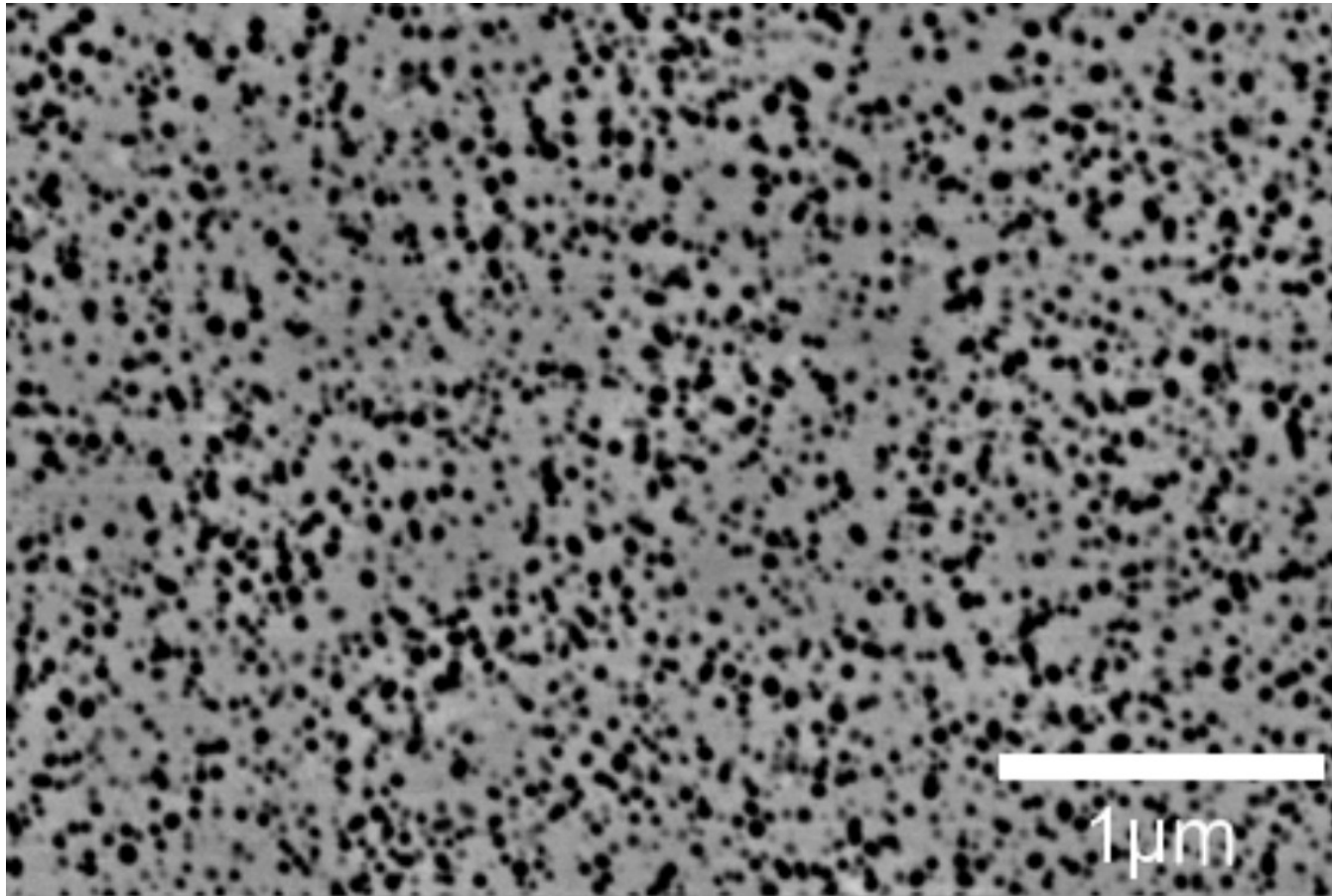
Expose 0.8



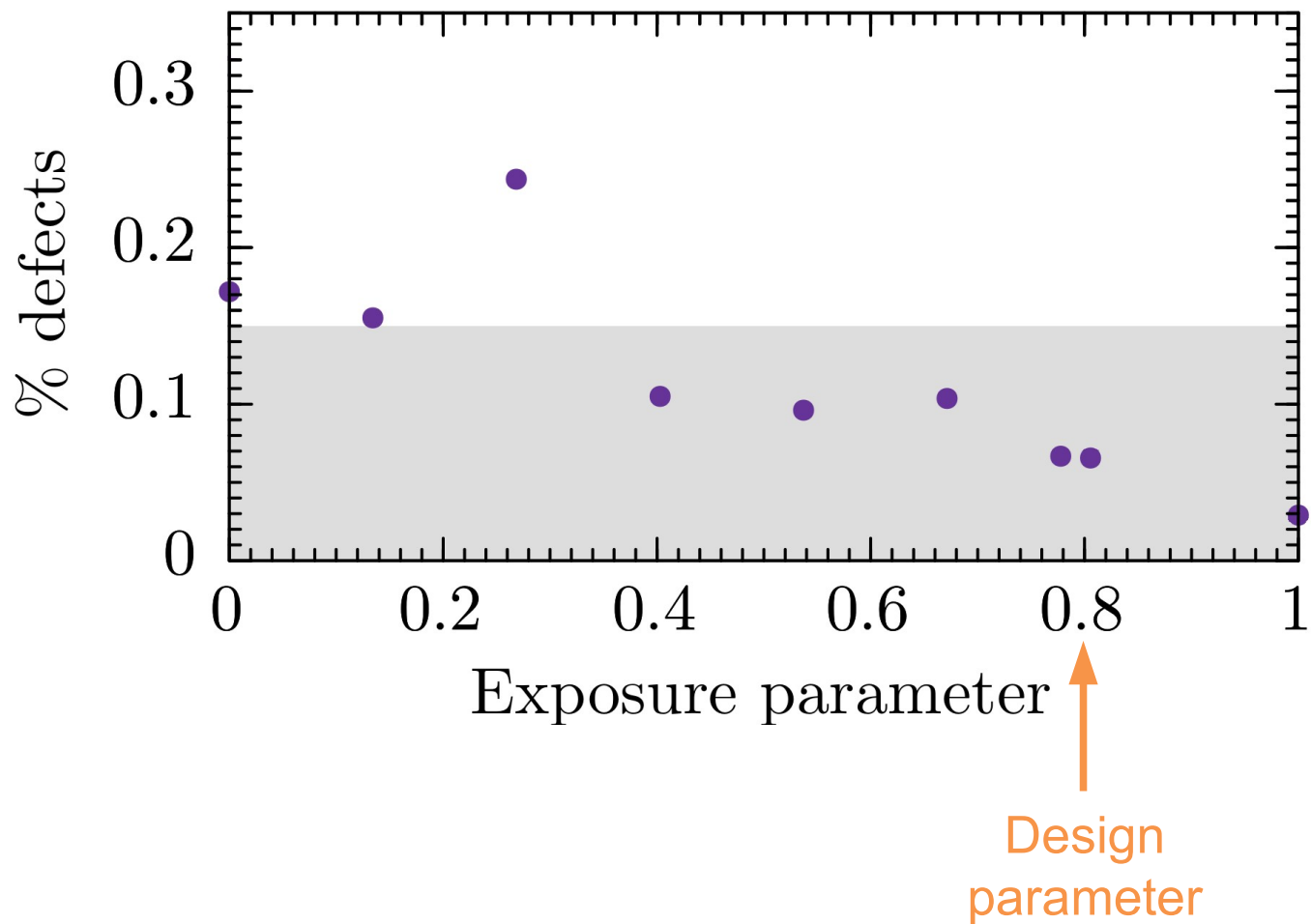
T_{HT} 1230°C



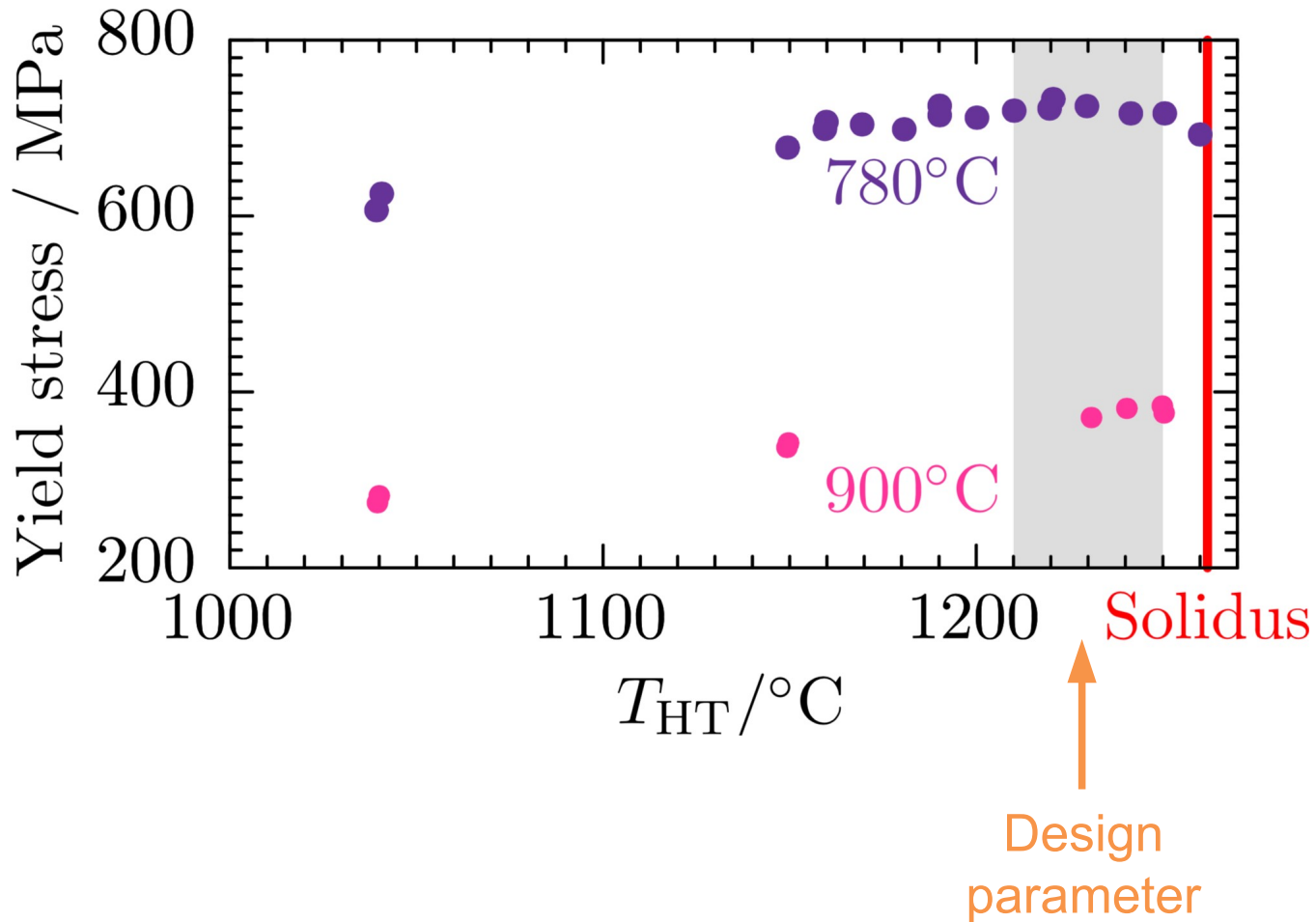
Microstructure



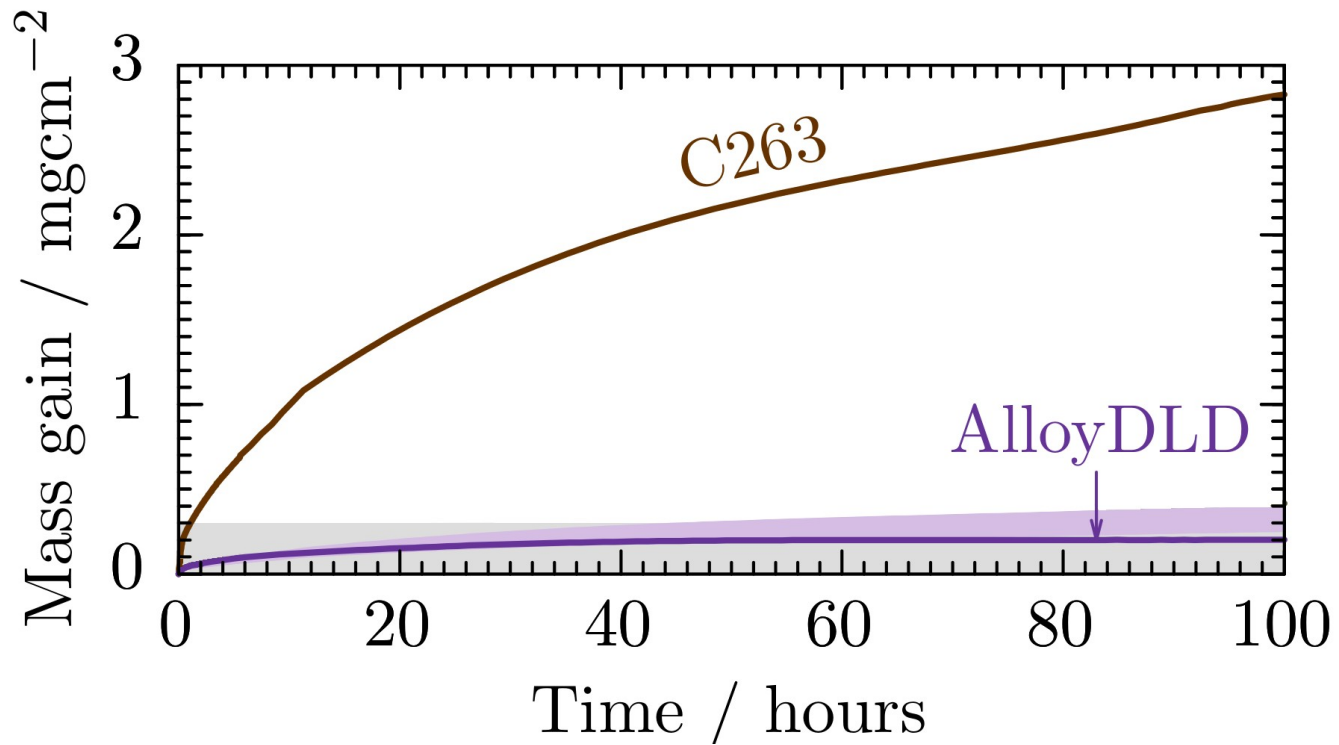
Testing the processability



Testing the yield stress

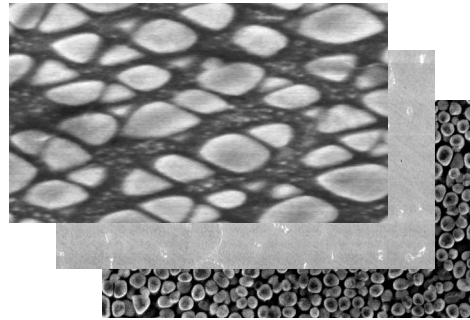


Testing the oxidation resistance



Materials designed

Nickel and molybdenum



Experiment and DFT for batteries

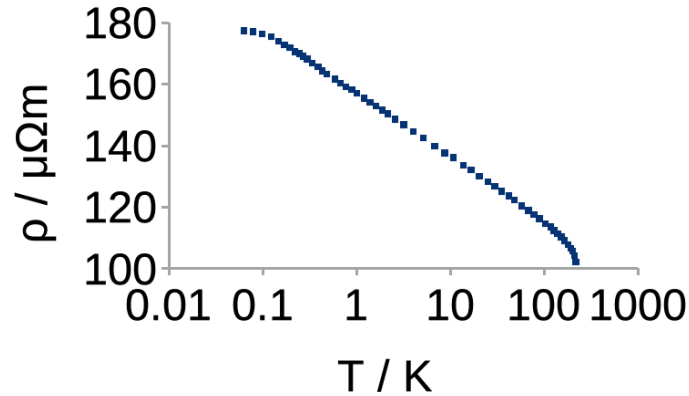


Steel for welding



More materials

Quantum and experiment for thermometry



Lubricants with molecular dynamics and experiments



Drug design



Summary

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

Designed and experimentally verified alloy for **direct laser deposition**

Applied technology to other materials and **drug design**

Commercialized by startup **Intellegens**