# The modern day blacksmith

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# Neural network algorithm to

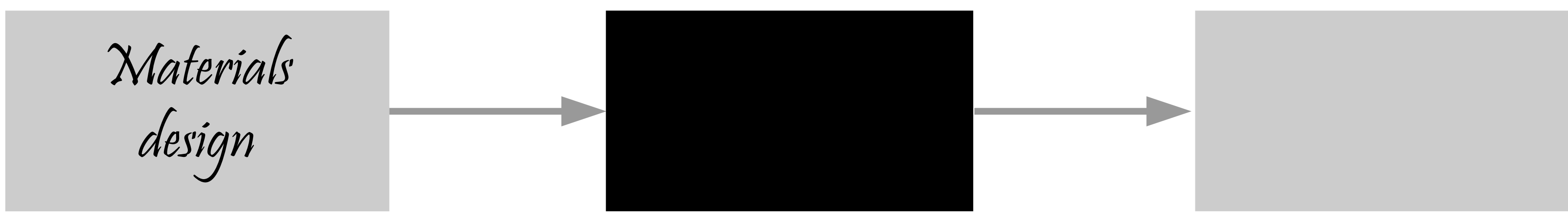
**Reduce** development costs

**Accelerate** materials discovery

**Merge** simulations, physical laws, and experimental data

**Generic** with **proven** applications in multiple material domains

# A black box



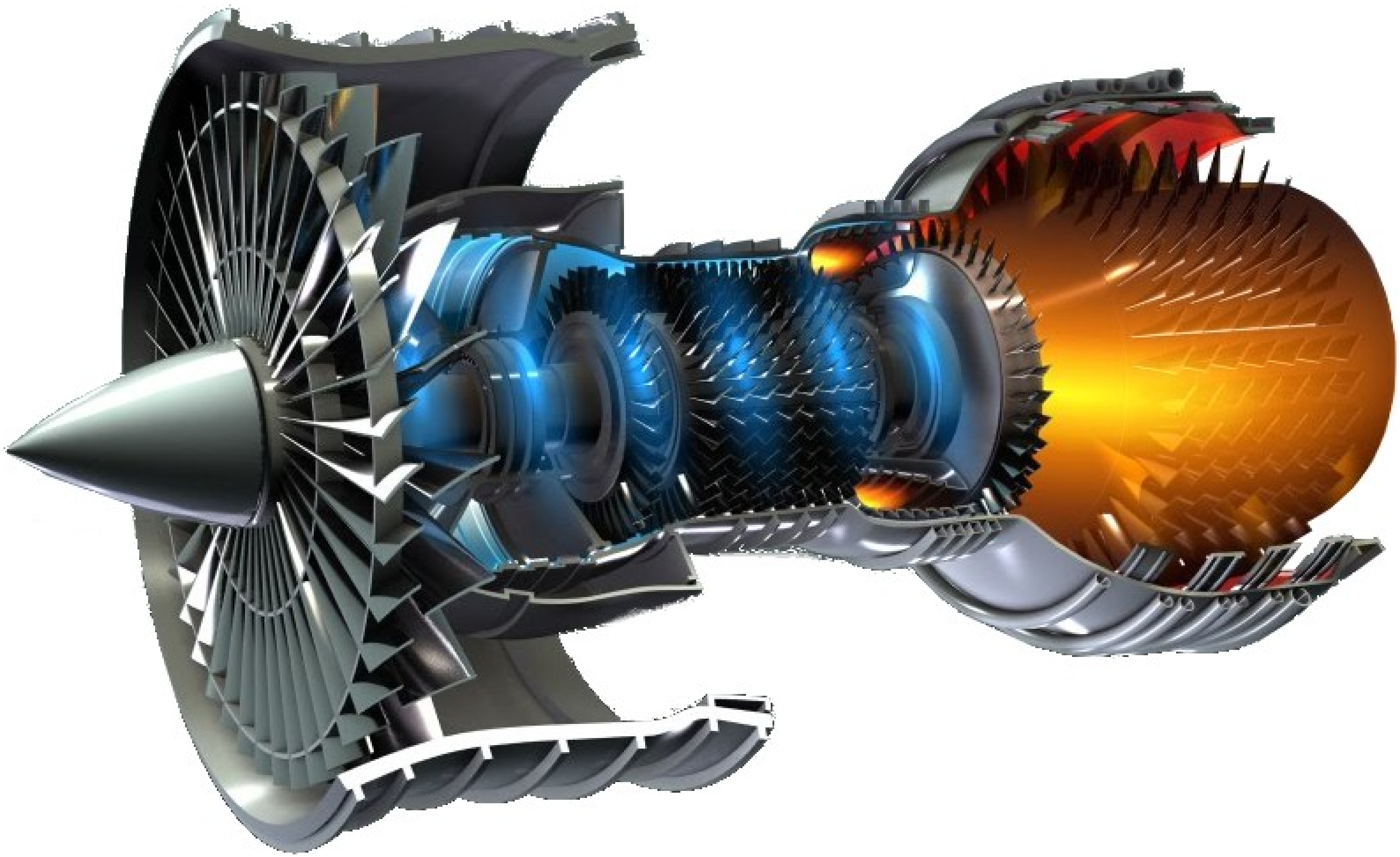
# Train with complete data

# Predict with complete data

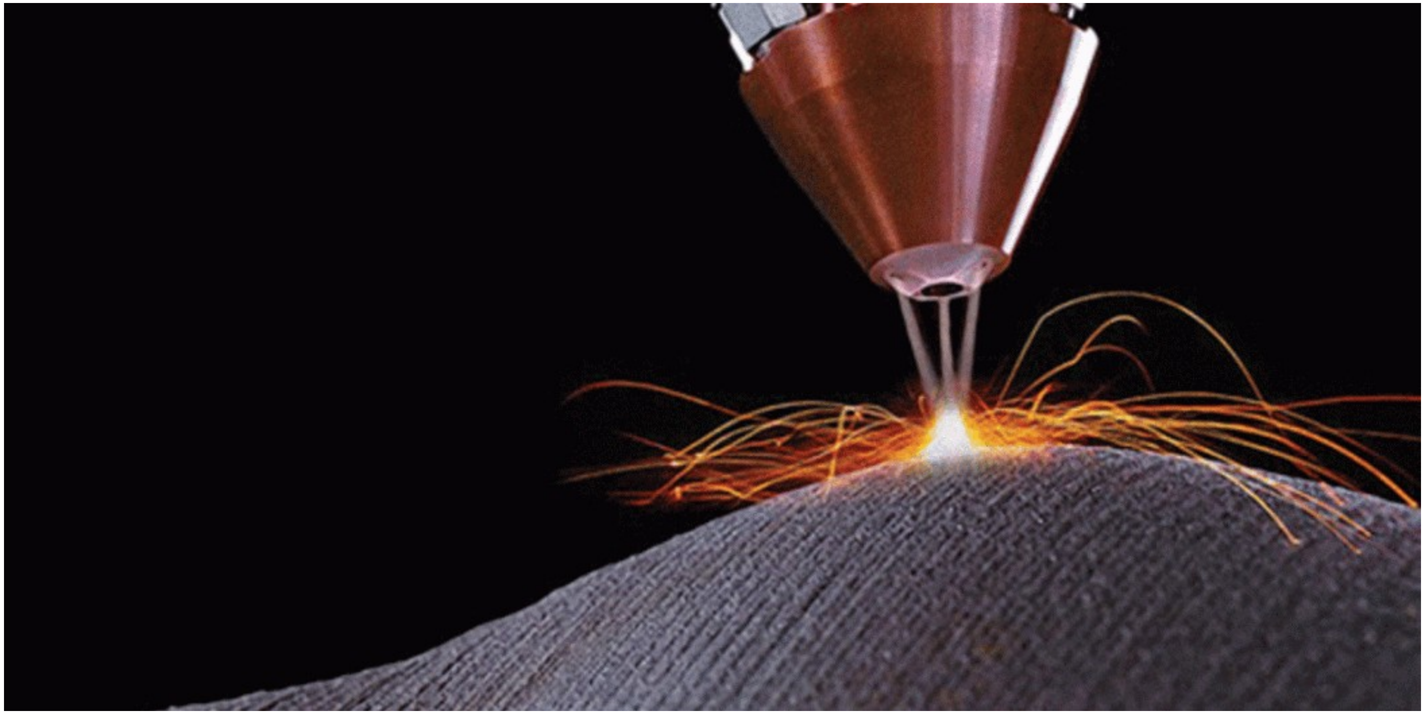
# Train with fragmented data

# Predict with fragmented data

# Schematic of a jet engine

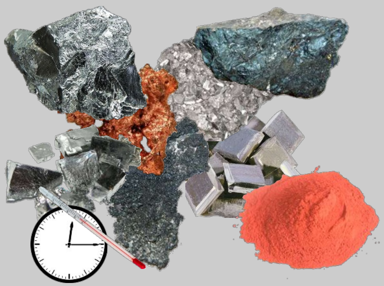


# Direct laser deposition requires new alloys



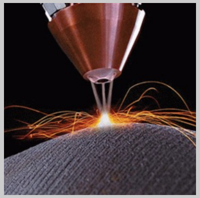
# Neural network for materials design

Composition



Properties

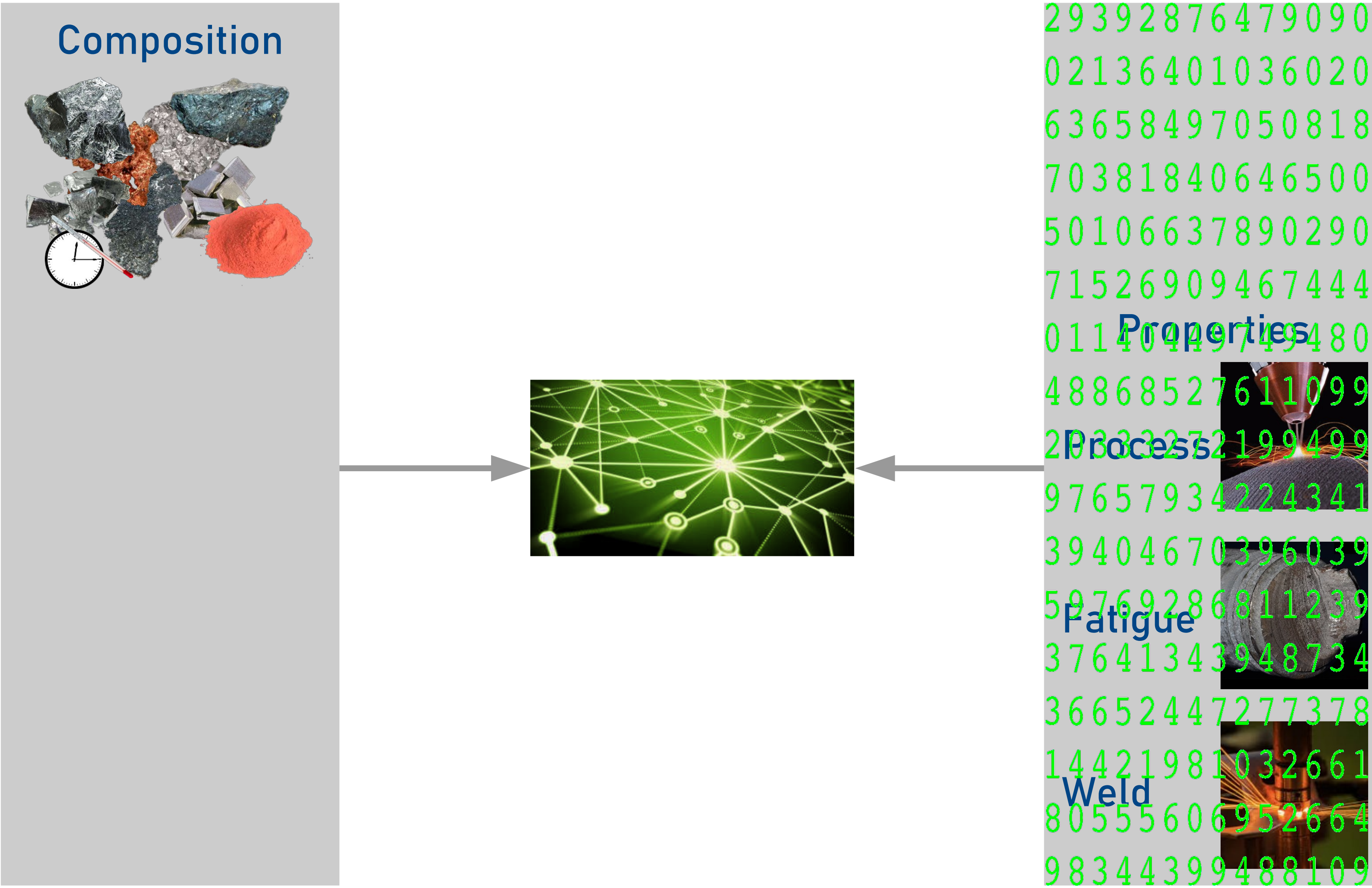
Process



Fatigue

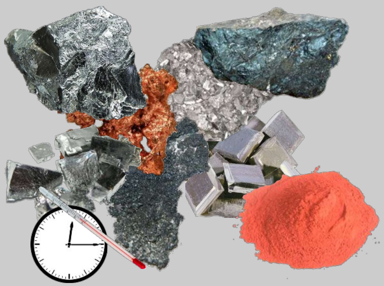
Weld

# Train the network



# Predict and design new materials

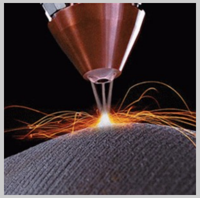
## Composition



## Composition

## Properties

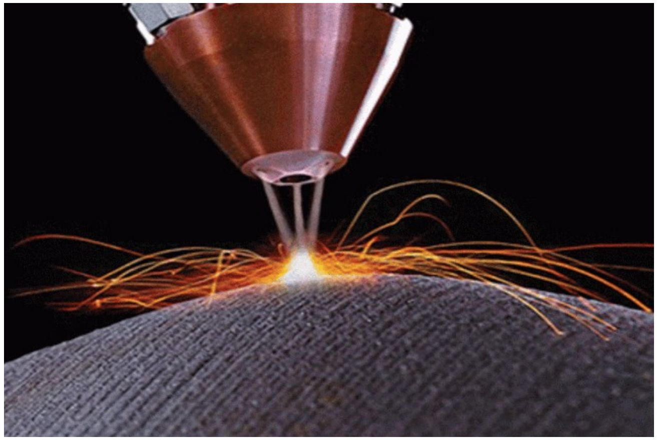
Process



Fatigue

Weld

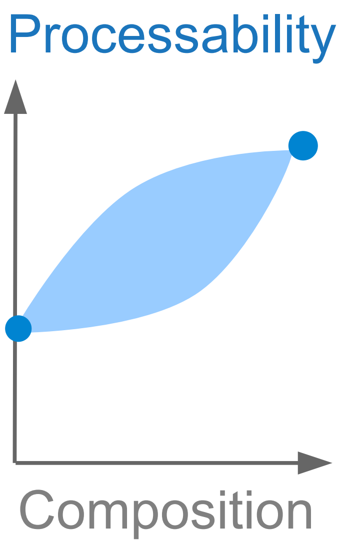
# Direct laser deposition and melting



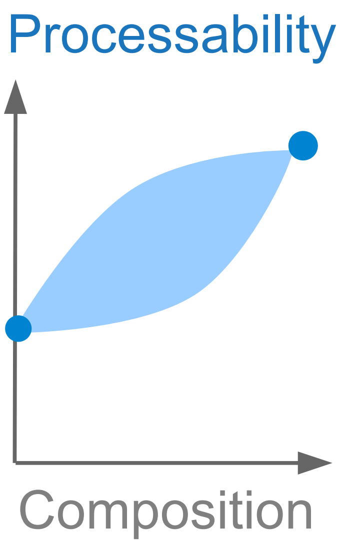
Laser

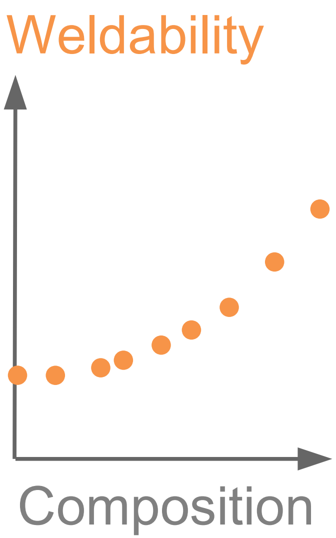
Electricity

# Direct laser deposition is analogous to welding

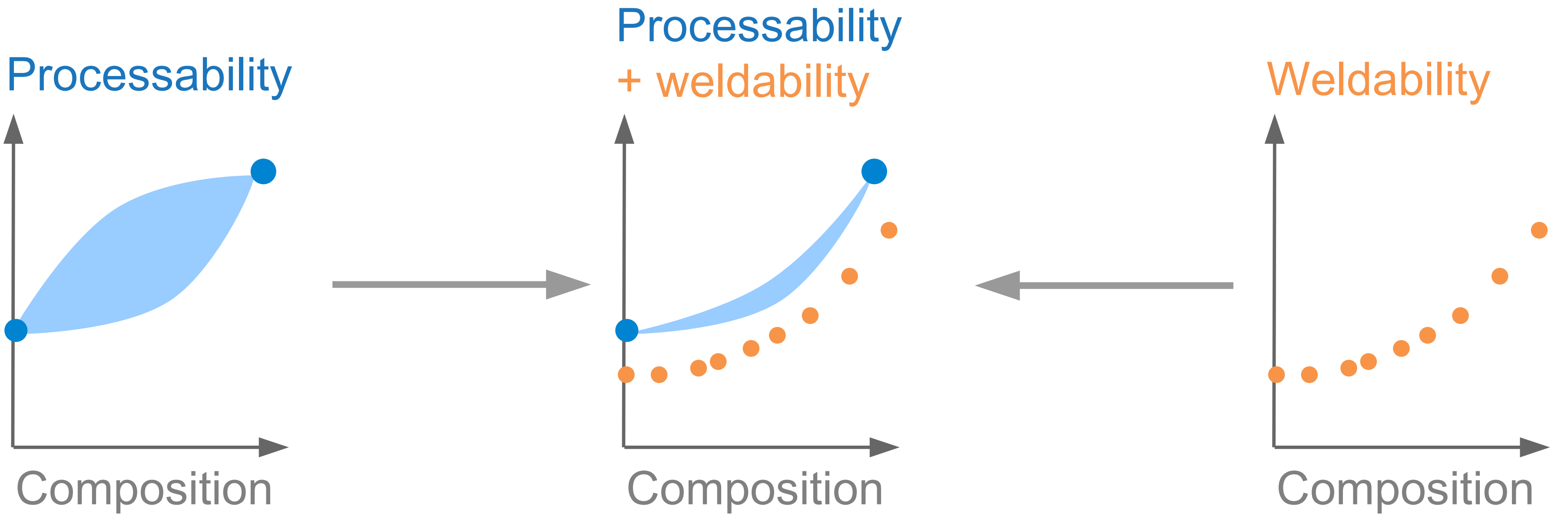


# Merge properties with a neural network



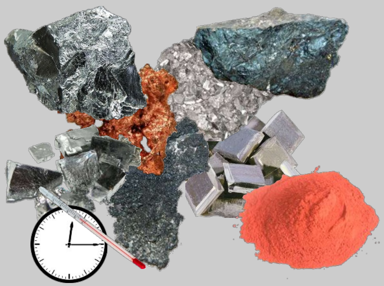



# Merge properties with a neural network



# Standard neural network

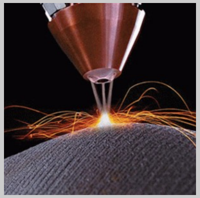
Composition



Composition

Properties

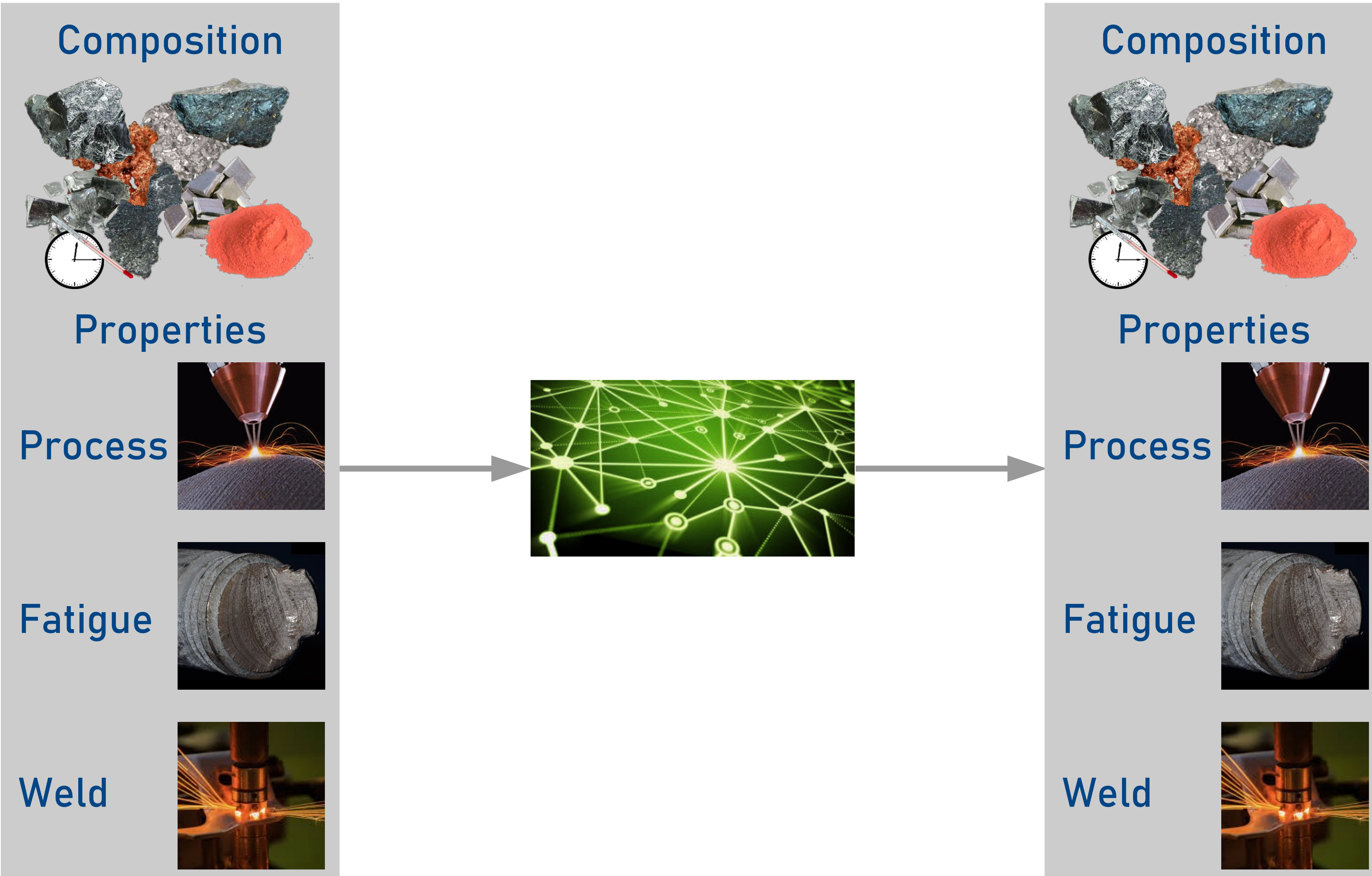
Process



Fatigue

Weld

# Neural network learns property-property link



# Target properties

| | |
|---|---|
| Elemental cost | $< 25\ \$kg^{-1}$ |
| Density | $< 8500\ kgm^{-3}$ |
| gamma’ content | < 25 wt% |
| Oxidation resistance | $< 0.3\ mgcm^{-2}$ |
| Processability | < 0.15% defects |
| Phase stability | > 99.0 wt% |
| gamma’ 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 |

# Material designed

19% Cr

4% Co

4.9% Mo

1.2% W

0.05% Zr

3% Nb

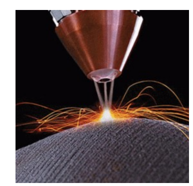
2.9% Al

0.04% C

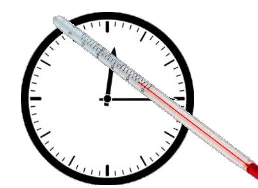
0.01% B

Ni

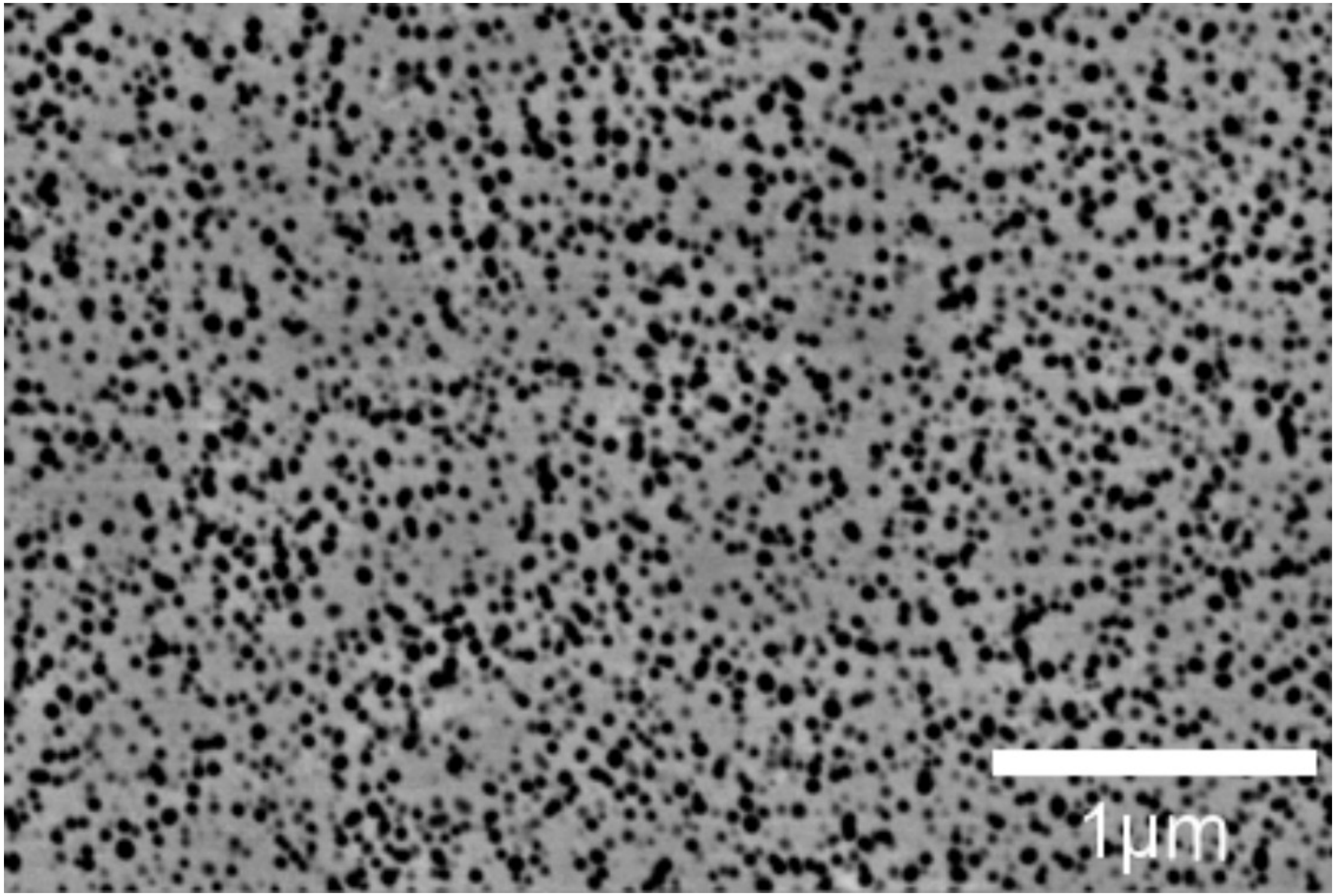
Expose 0.8



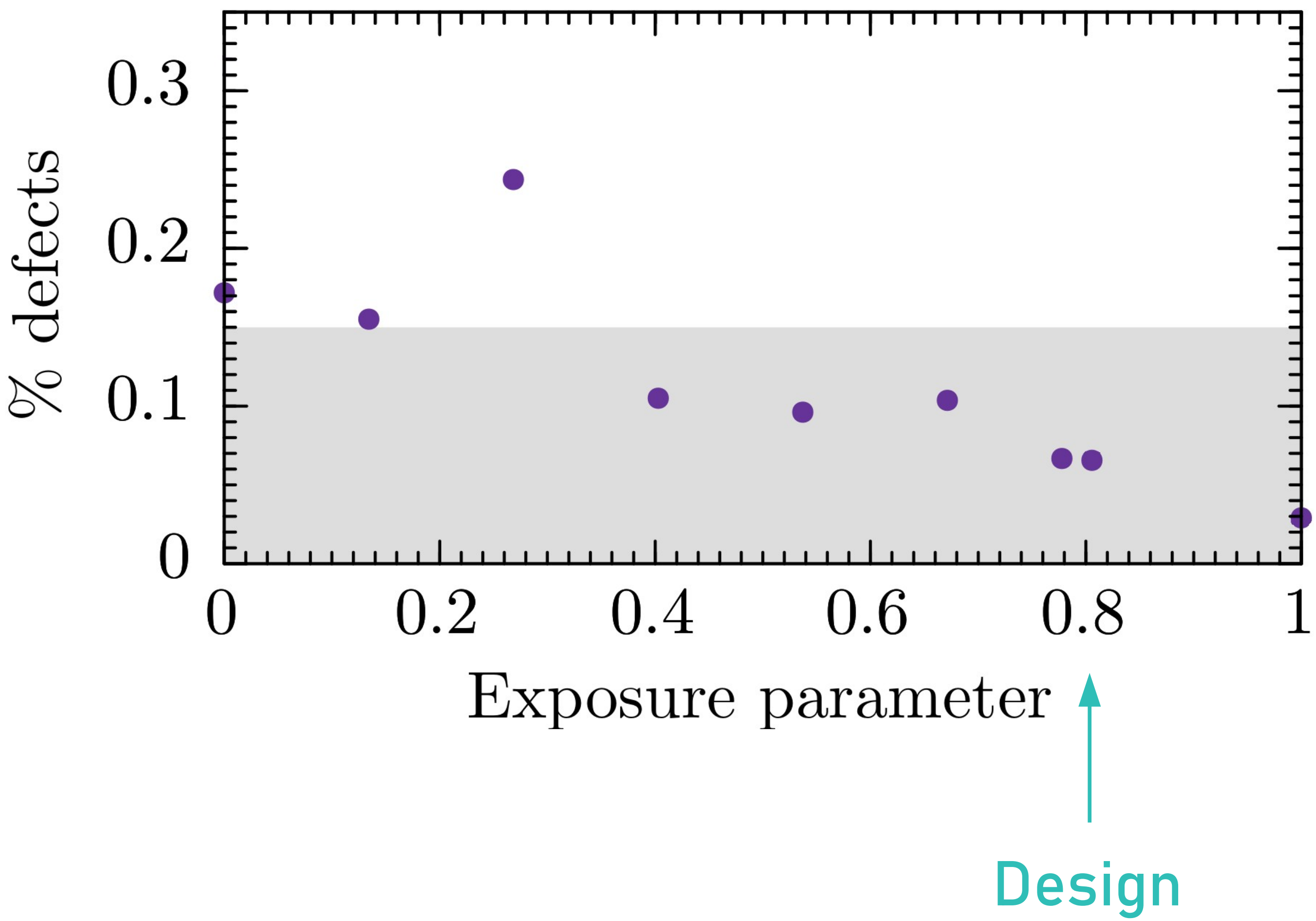
$T_{HT}$ 800°C



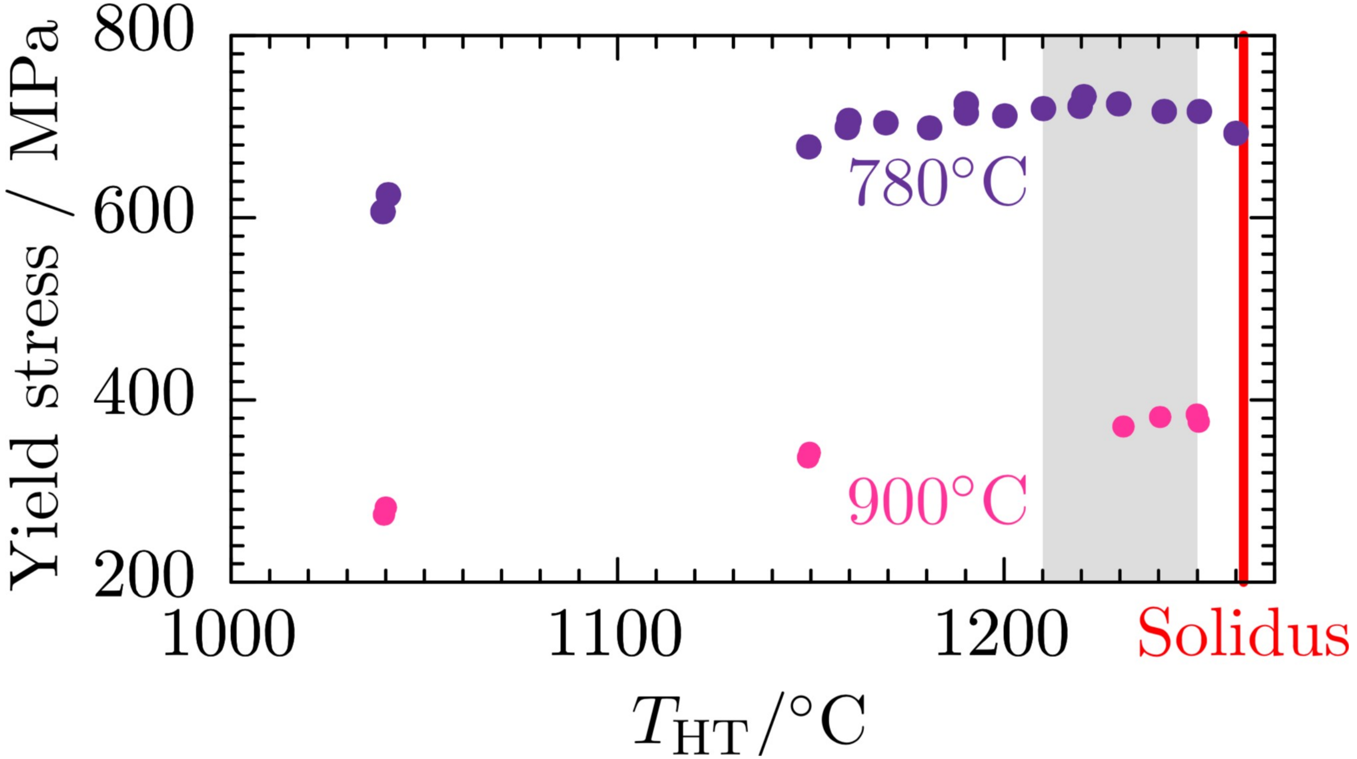
# Microstructure



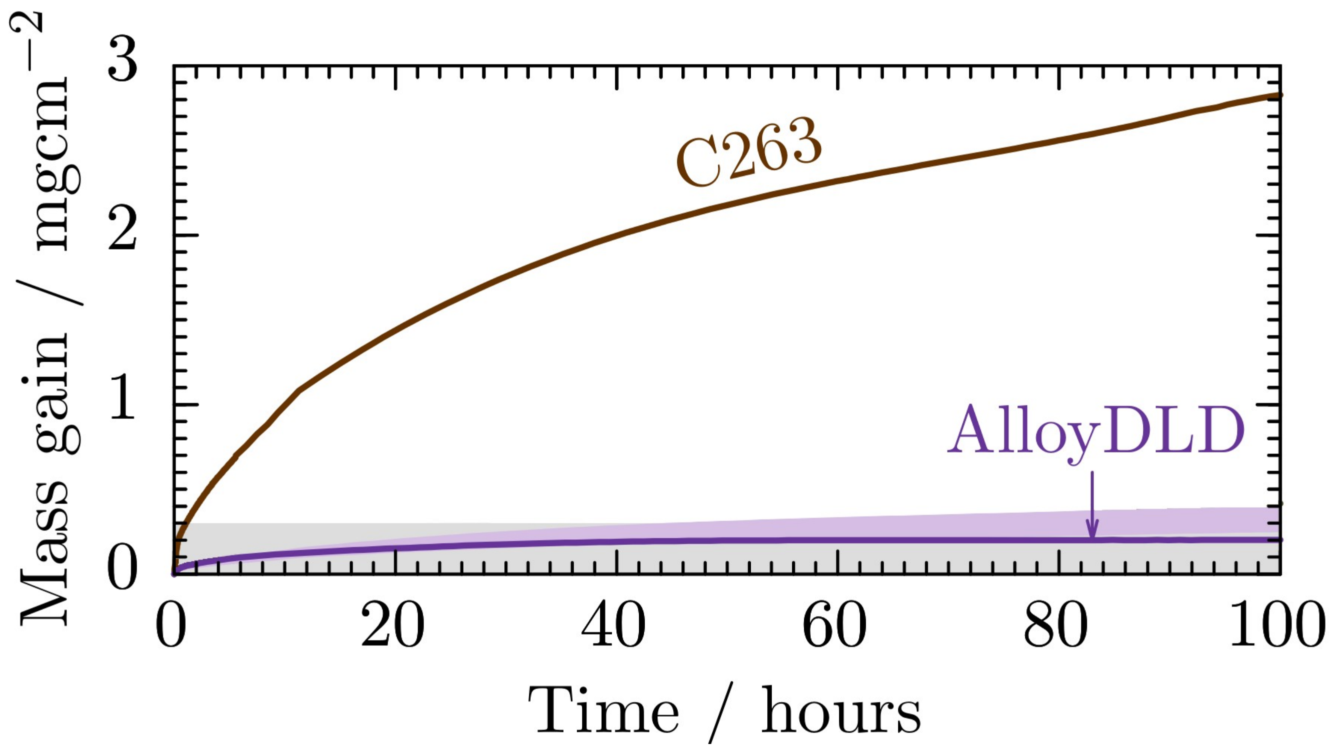
# Testing the processability



# Verifying the yield stress



# Verifying the oxidation resistance

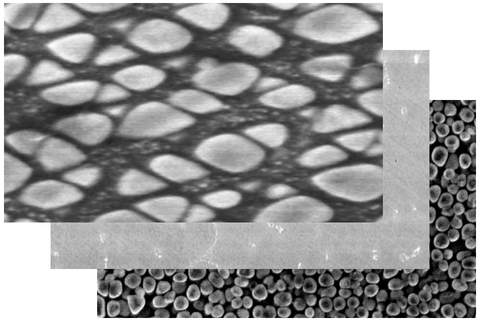


# Printing a component

# Materials designed

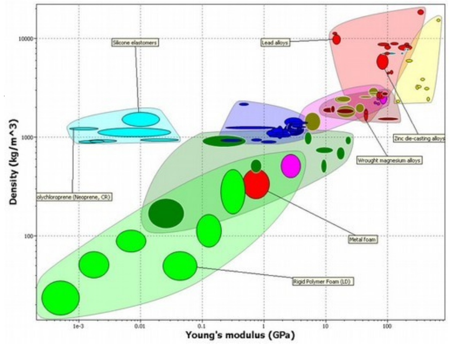
## Nickel and molybdenum alloys

Scripta Materialia 146, 82 (2018)
Materials & Design 131, 358 (2017)
EP14157622, US2013/0052077A2
EP14153898, US2014/177578
EP14161255, US2014/223465



## Identified and corrected errors in material database

Computational Materials Science 147, 176 (2018)



# Merging data

Linked the ability for direct laser deposition to weldability

Can also link experimental data to computational simulations

Merge quality with quantity

# Materials designed with simulations

Lubricants with experiments and molecular dynamics simulations

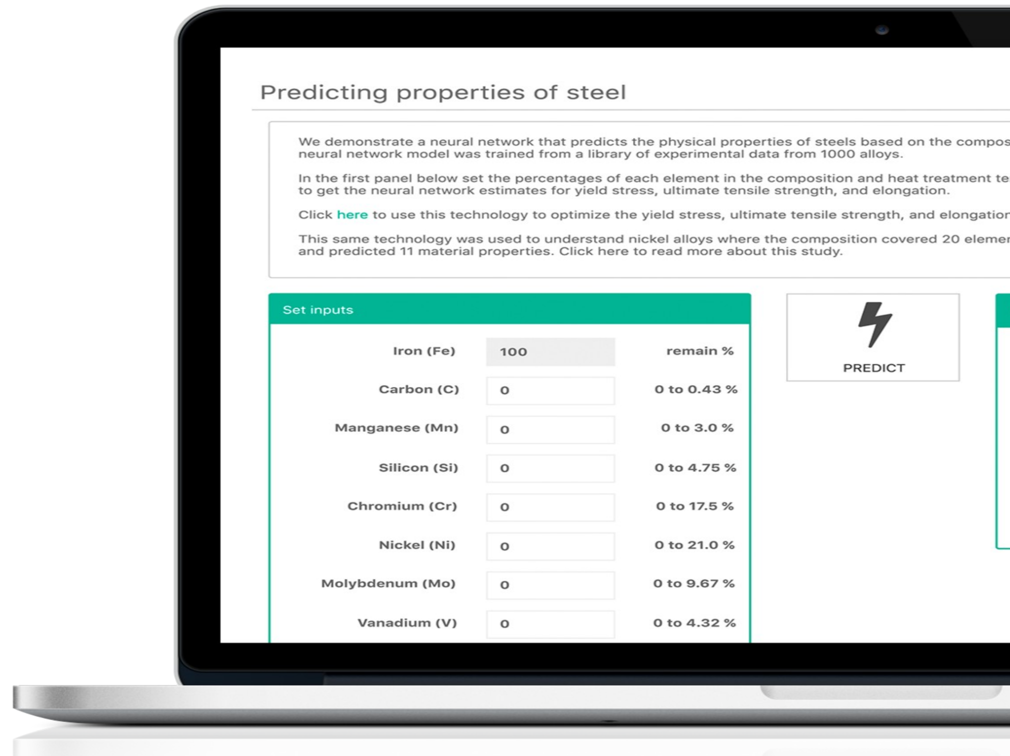
Batteries with experiments and Density Functional Theory

# Integrated software by Intellegens

Data load and transform

Train the neural network

Use model to design new materials




https://app.intellegens.ai/steel_search

# Summary

Designed and experimentally verified alloy for direct laser deposition

Reduce development costs

Accelerate materials discovery

Enable concurrent materials design

Intellegens

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