intellegens

Alchemite™ machine learning

Gareth Conduit

Alchemite™ machine learning tool to

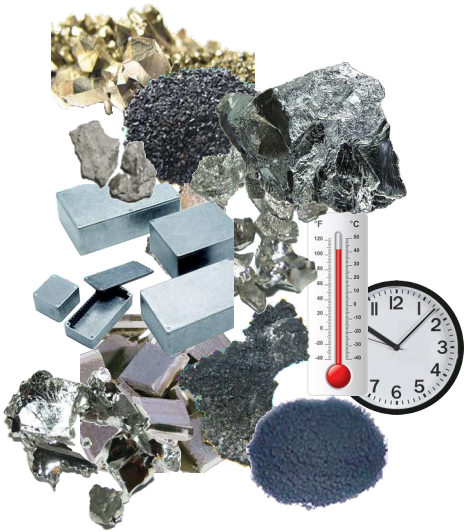
Utilise **all available** information: computer simulations and real-life measurements

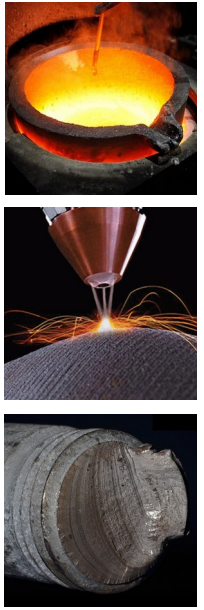
Impute values from sparse data

Reduce the need for experiments and **accelerate** discovery

Broadly applicable with **proven** applications in drug design, industrial chemicals, and materials

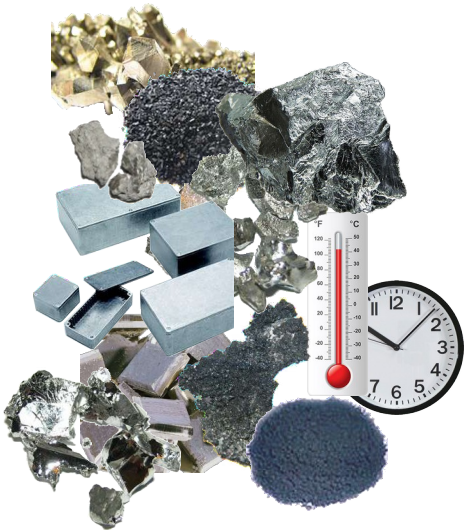
Machine learning black box predictions

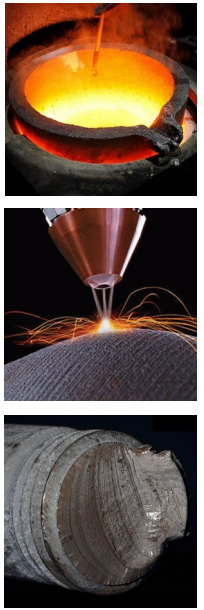




Train the machine learning from existing data

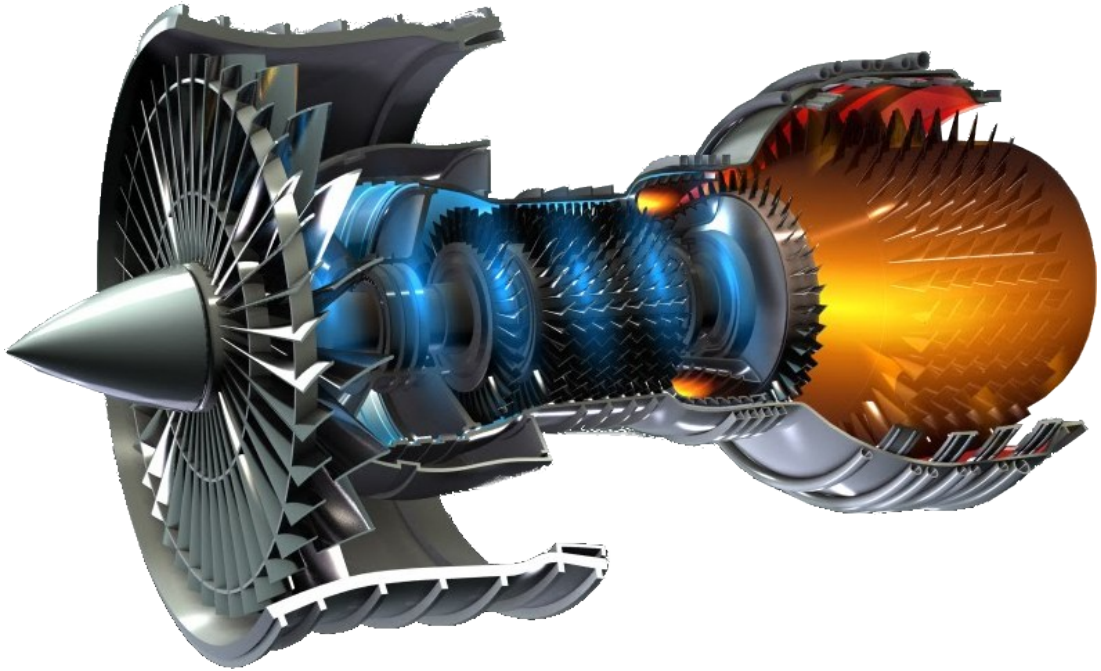
Machine learning predicts the properties of materials





Handling missing data

High-temperature alloys for a jet engine



Composition of the proposed alloy

Cr 19%

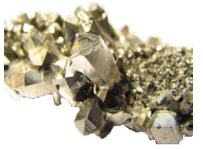
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



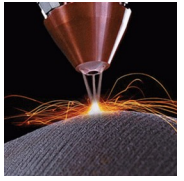
Al 2.9%

C 0.04%

B 0.01%

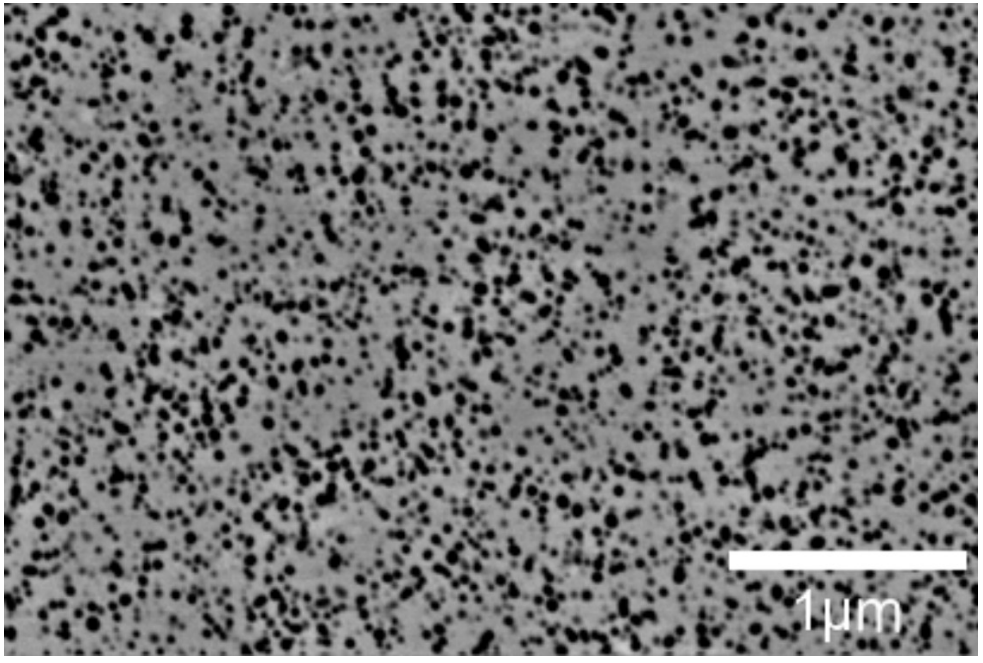
Ni

Expose 0.8



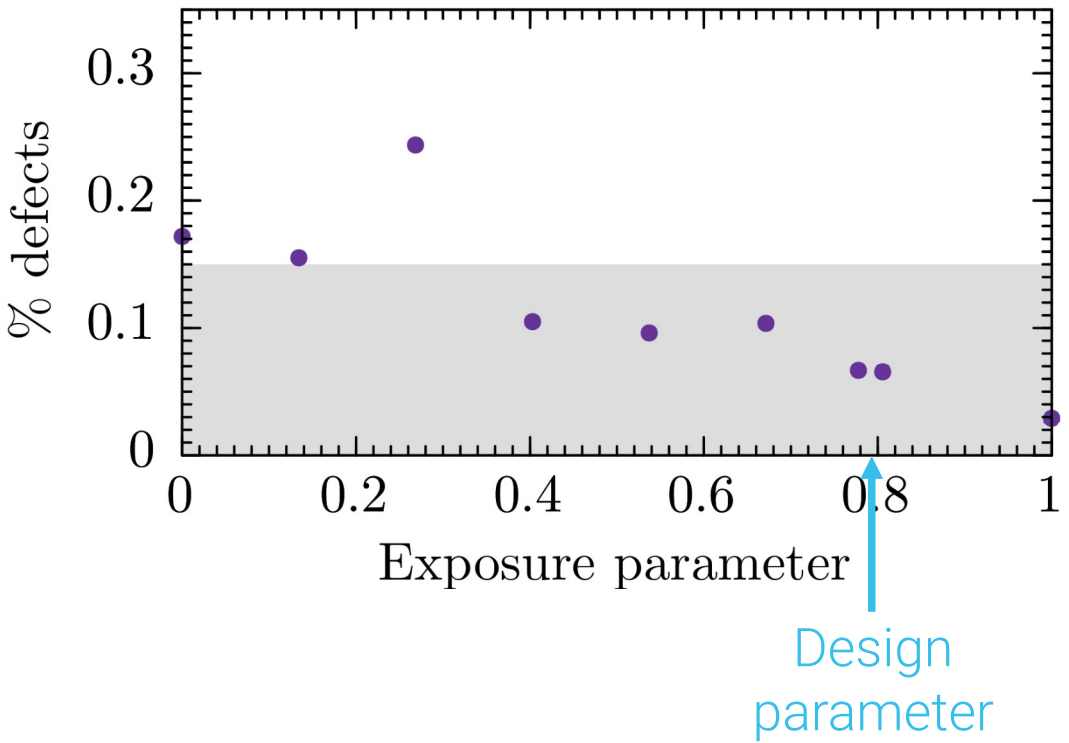
T_{HT} 1300ºC

Microstructure



Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design 168, 107644 (2019)

Defects formed on 3D printing



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Other materials and industrial chemicals

Battery cathodes

Lubricants

Ink

Summary

Train machine learning models on sparse data

Merge computational and experimental data

Model physically relevant properties of materials and industrial chemicals

Taken to materials and industrial chemicals market by Intellegens

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Demo	https://app.intellegens.ai/steel_optimise
Papers	https://www.intellegens.ai/paper.html