

# Alchemite™ machine learning

Gareth Conduit

# Alchemite™ machine learning tool to



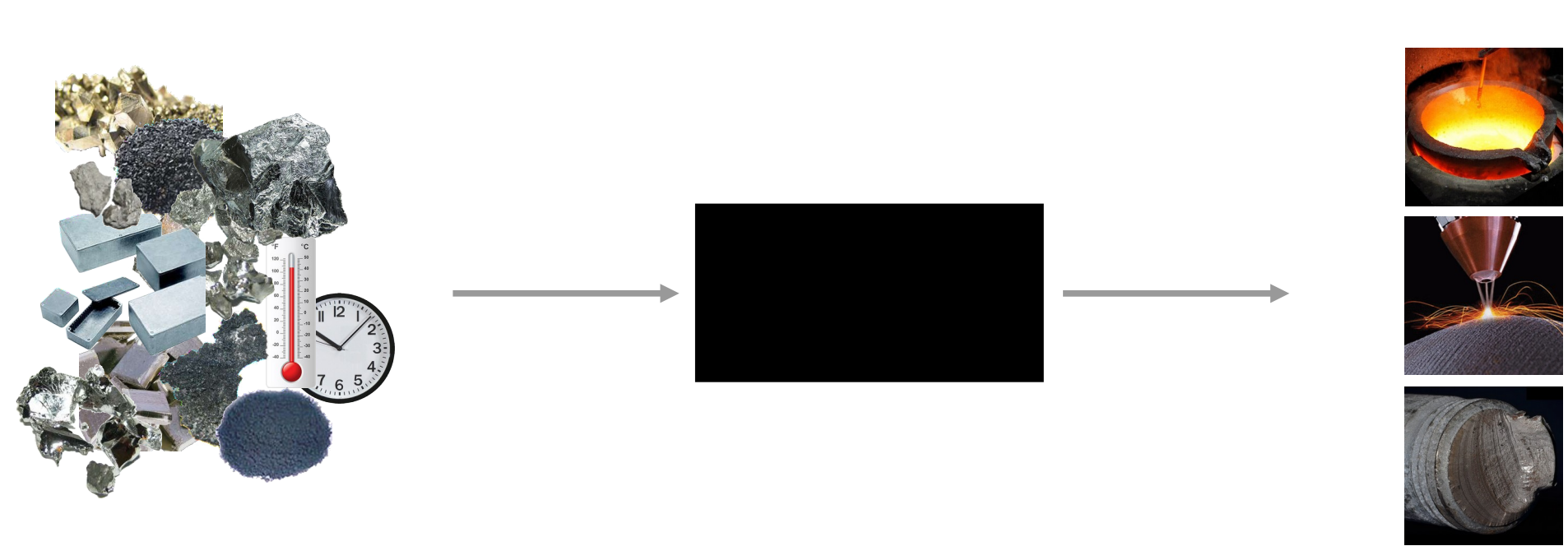
Utilise **all available** information: computer simulations and real-life measurements

**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



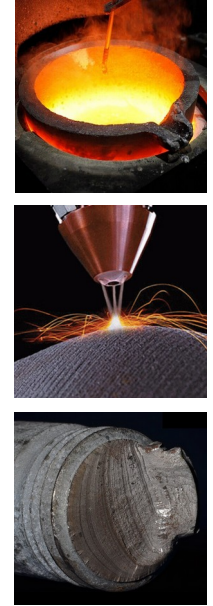
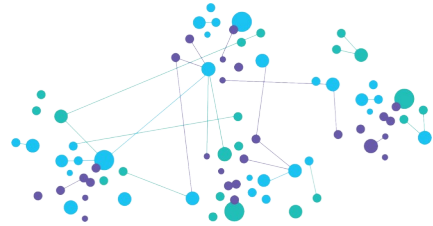
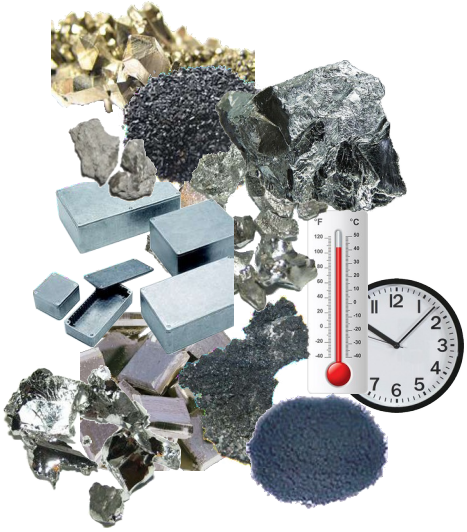
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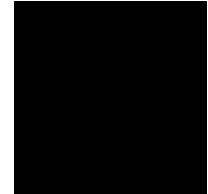
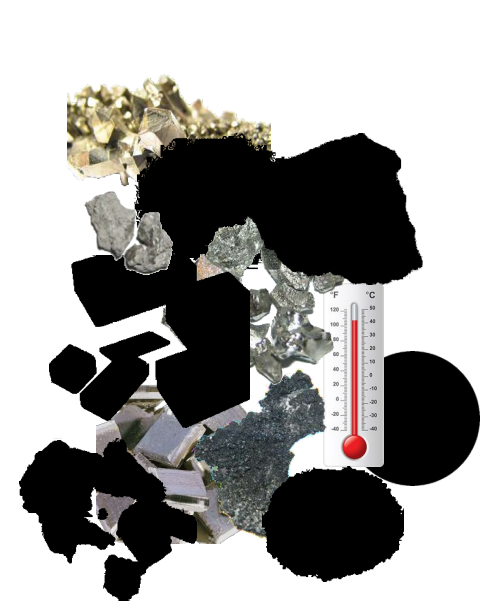
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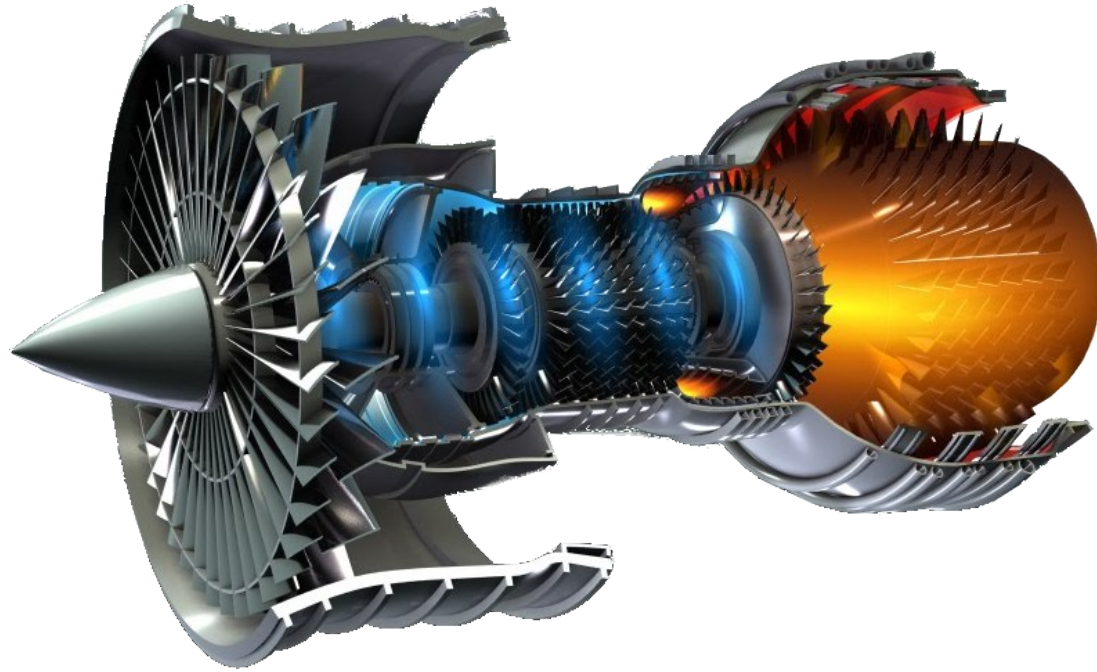
# Machine learning predicts the properties of materials



# Handling missing data



# High-temperature alloys for a jet engine



# Composition of the proposed alloy



Cr 19%



Co 4%



Mo 4.9%



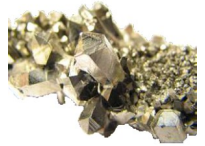
W 1.2%



Zr 0.05%



Nb 3%



Al 2.9%



C 0.04%



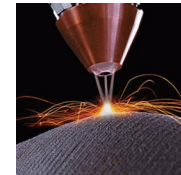
B 0.01%



Ni



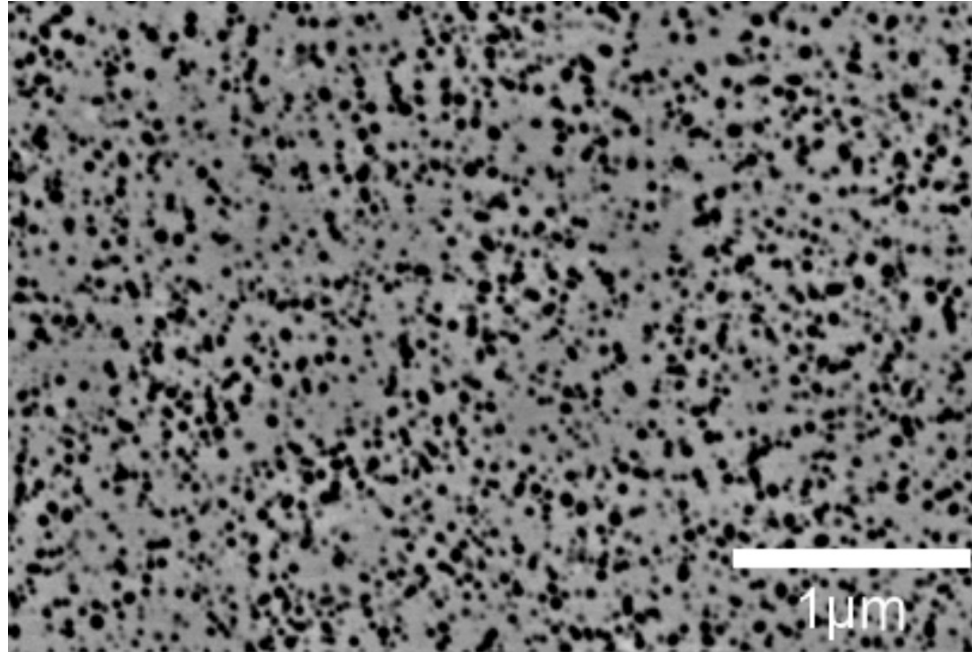
Expose 0.8



$T_{HT}$  1300°C

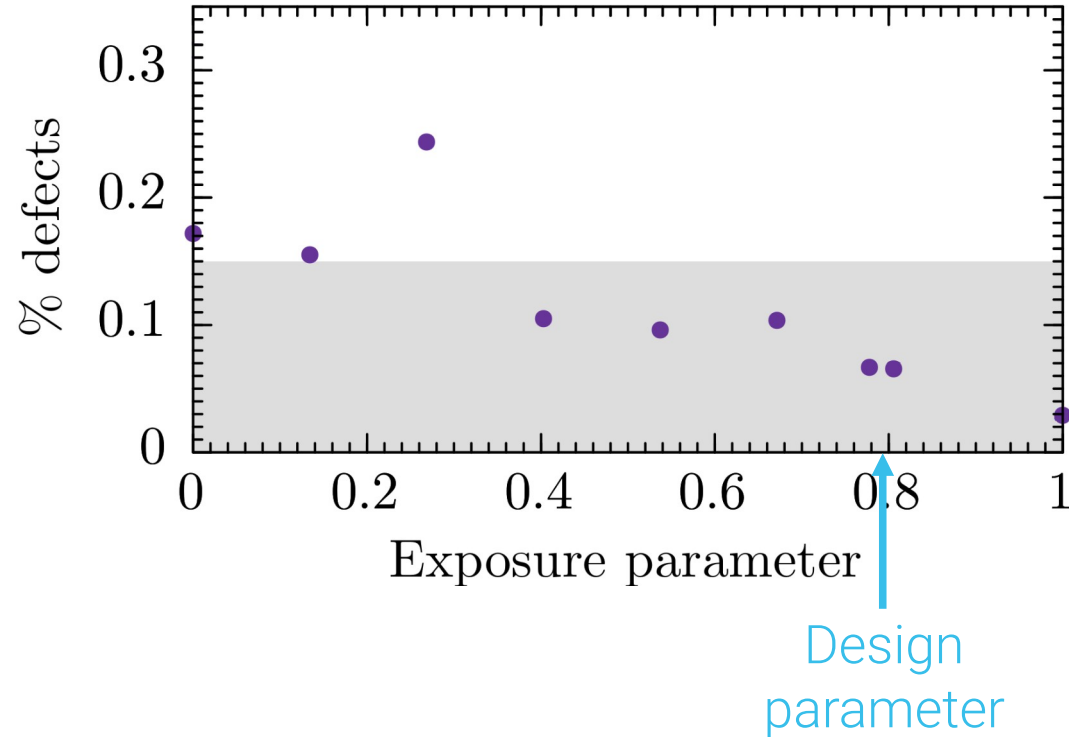






Probabilistic neural network identification of an alloy for direct laser deposition  
Materials & Design 168, 107644 (2019)

# Defects formed on 3D printing



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



# 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**

**Contact**

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**Website**

<https://intellegens.ai>

**Demo**

[https://app.intellegens.ai/steel\\_optimise](https://app.intellegens.ai/steel_optimise)

**Papers**

<https://www.intellegens.ai/paper.html>