

A decorative graphic at the top of the slide consists of a network of blue circles of various sizes connected by thin lines, resembling a molecular or data network structure.

intellegens

Applied machine learning

Modern-day blacksmith

Dr Gareth Conduit



Model **sparse** datasets

Exploit **property-property** relationships

Merge data, computer simulations, and physical laws

Reduce costly experiments to **accelerate** discovery

Black box machine learning for materials design

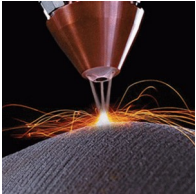


Composition



Properties

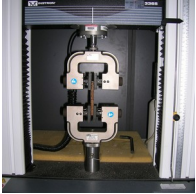
Defects



Fatigue



Strength



Train the machine learning



63658497050818
70381840646500
50106637890290
71526909467444
01140449749480
48868527611099
20333272199499
97657934294341
39404670396039
59769286811239
37641343948734

Composition



29392876479090
02136401036020
63658497050818
70381840646500
50106637890290
71526909467444
01140449749480
48868527611099
20333272199499
97657934294341
39404670396039
59769286811239
37641343948734
36652447275378
144219981032661
80555606952664
98344399488109

Properties

Defects

Fatigue

Strength



Machine learning predicts material properties

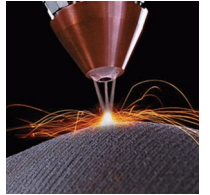


Composition



Properties

Defects



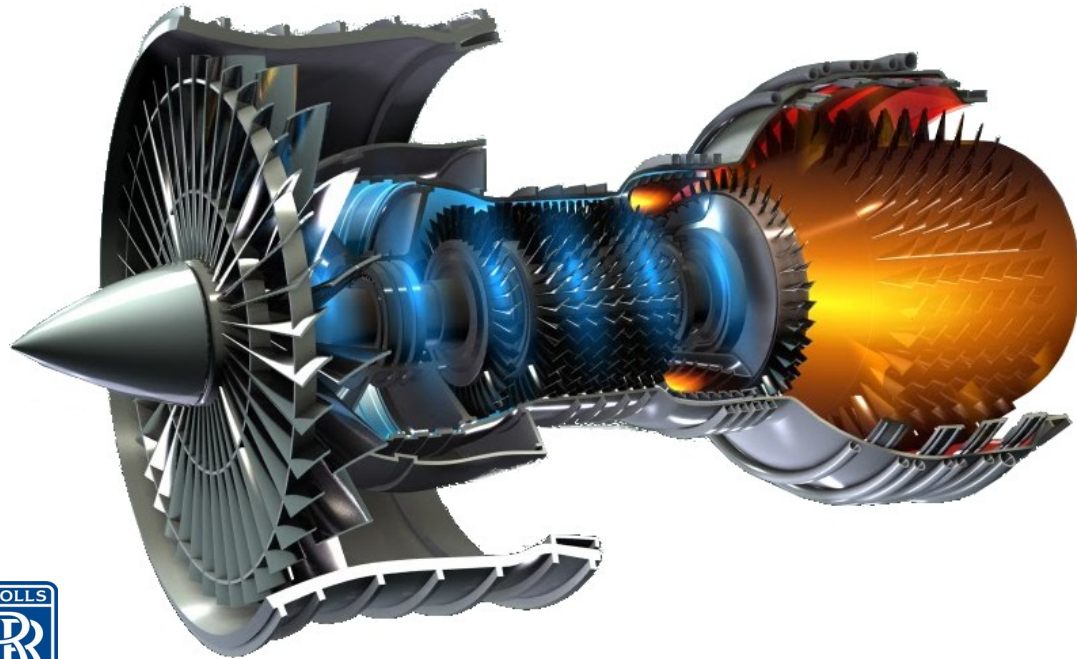
Fatigue



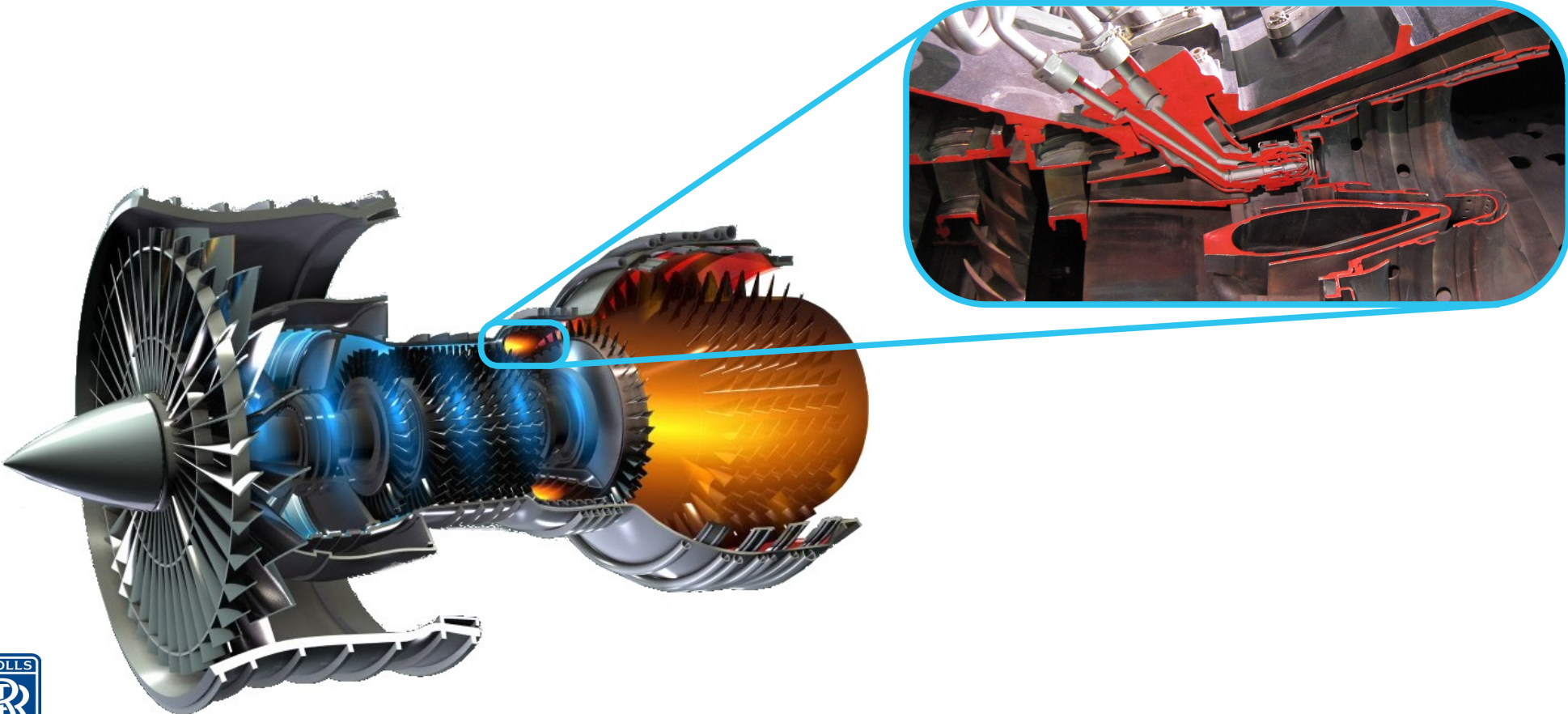
Strength



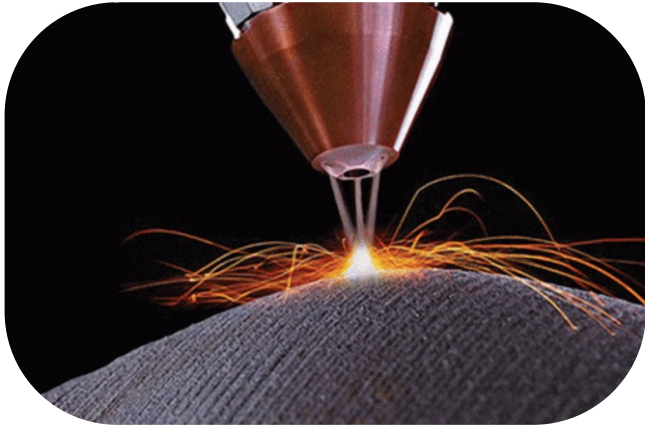
Jet engine schematic



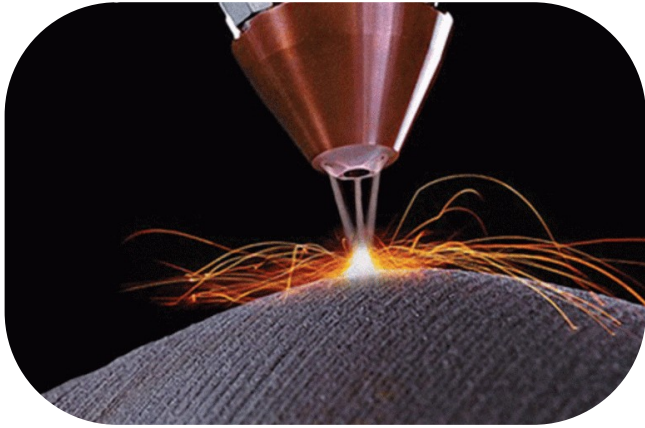
Combustor in a jet engine



Direct laser deposition



Ability for printing and welding are strongly correlated



Laser



Electricity

Target properties



Elemental cost	< 25 \$kg ⁻¹
Density	< 8500 kgm ⁻³
γ' content	< 25 wt%
Oxidation resistance	< 0.3 mgcm ⁻²
Defects	< 0.15% defects
Phase stability	> 99.0 wt%
γ' solvus	> 1000 °C
Thermal resistance	> 0.04 KΩ ⁻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 and processing variables



Cr 19%



Co 4%



Mo 4.9%



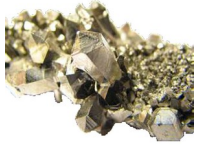
W 1.2%



Zr 0.05%



Nb 3%



Al 2.9%



C 0.04%



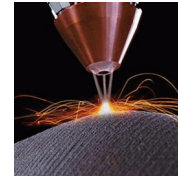
B 0.01%



Ni

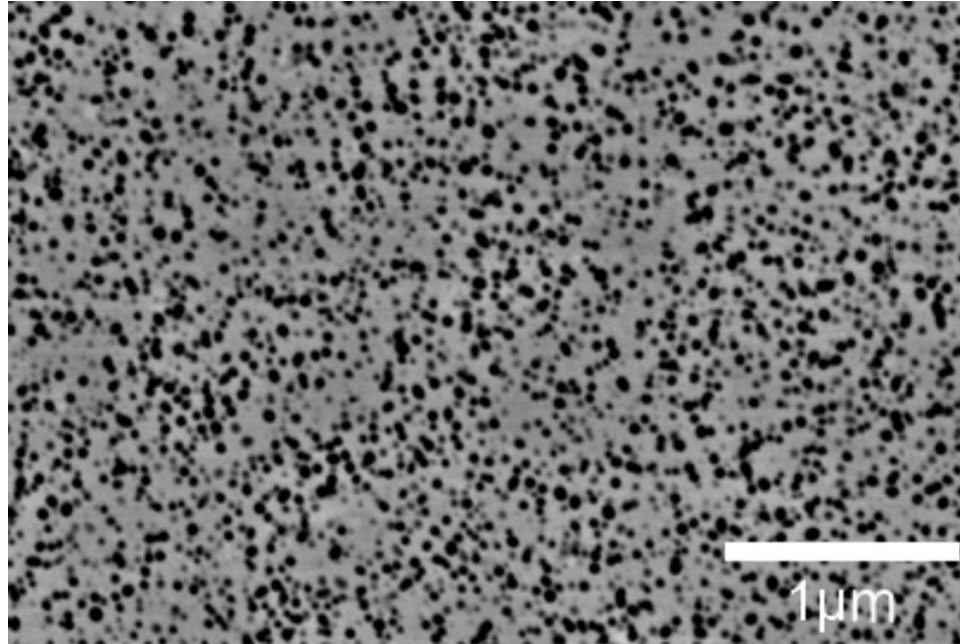


Expose 0.8

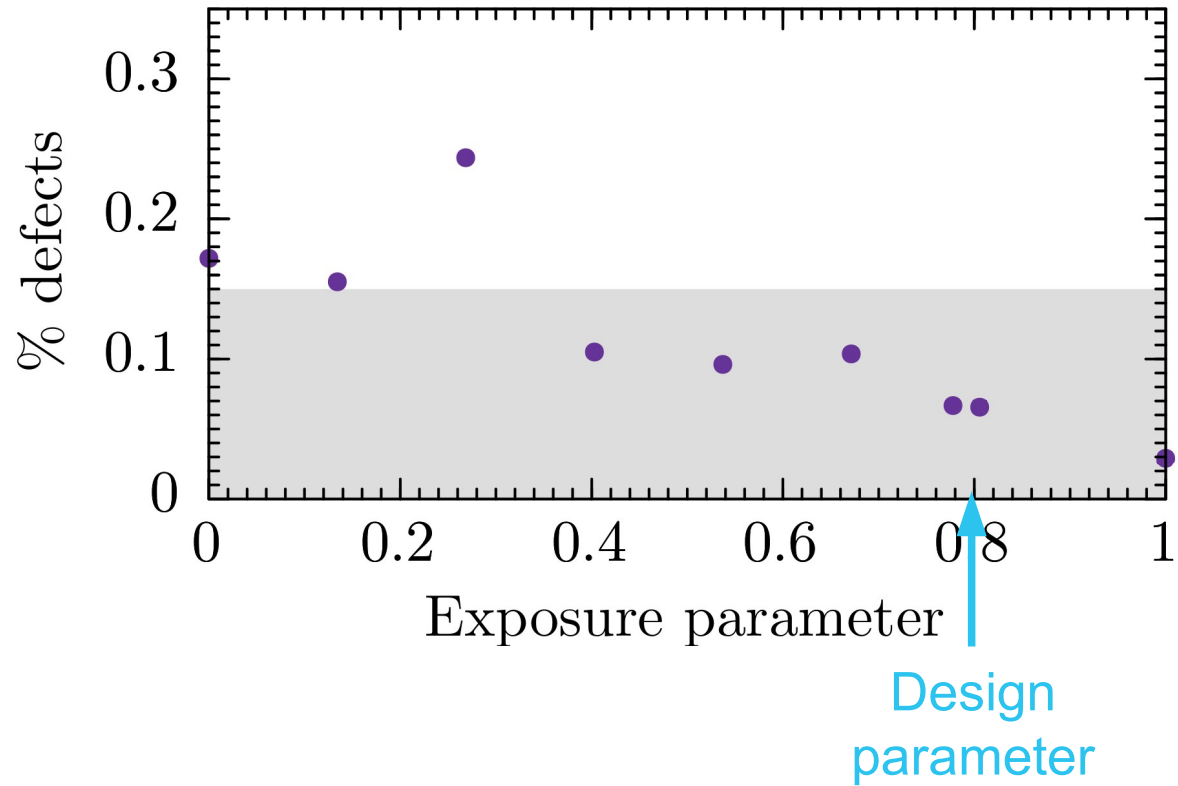


T_{HT} 1300°C

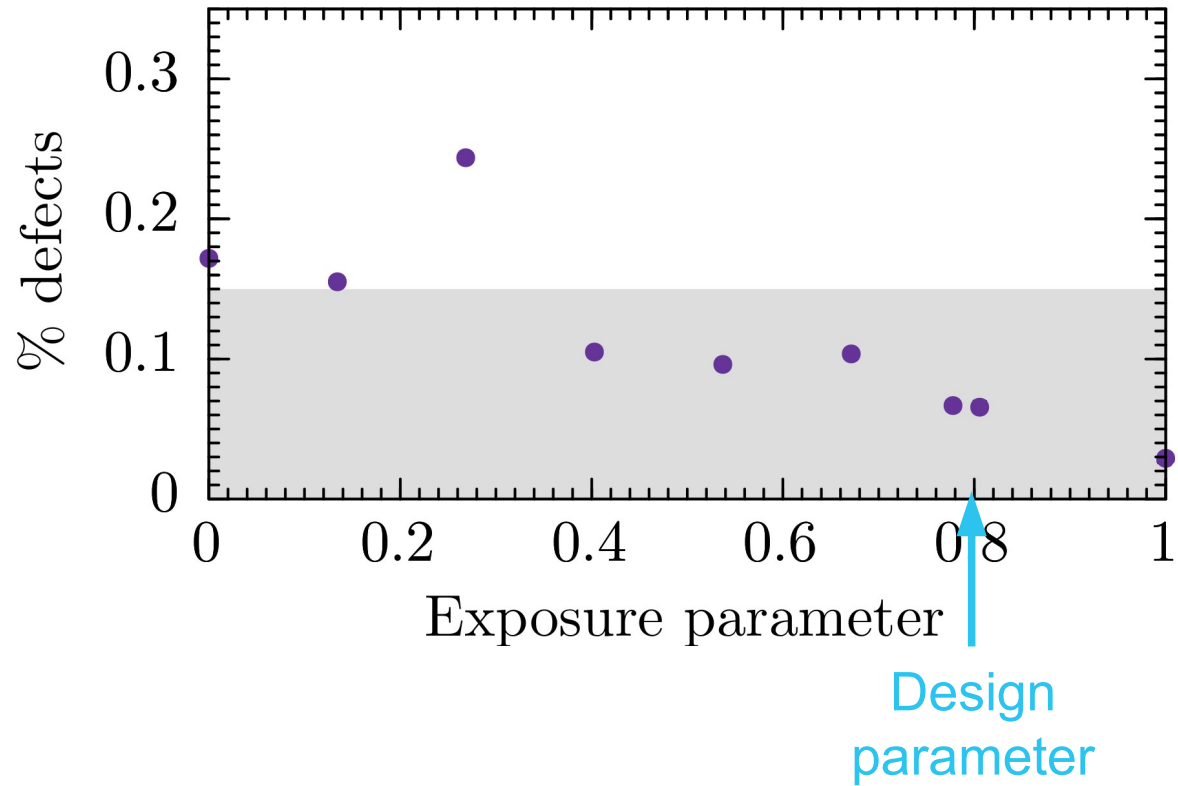




Testing the defect density



Testing the defect density



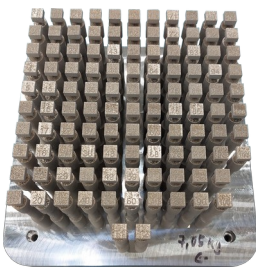
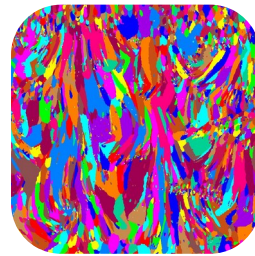
Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design **168**, 107644 (2019)




optibrium™



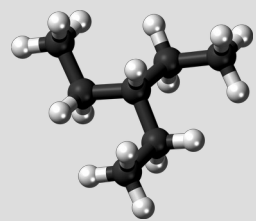

Journal of Computer-Aided Molecular Design **35**, 112501140 (2021)

Project MEDAL



NASA Technical Memorandum 20220008637 (2022)



nature machine intelligence

REVIEW ARTICLE
<https://doi.org/10.1038/s42256-020-0156-7>

Check for updates

Predicting the state of charge and health of batteries using data-driven machine learning

Man-Fai Ng¹, Jin Zhao², Qingyu Yan², Gareth J. Conduit³ and Zhi Wei Seh⁴

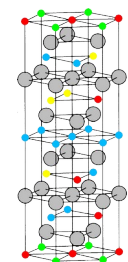


Fluid Phase Equilibria **501**, 112259 (2019)



Journal of Chemical Physics **153**, 014102 (2020)





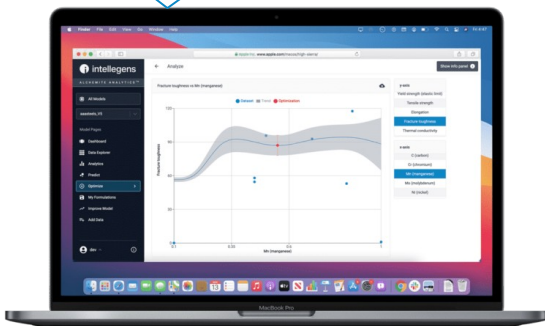
Johnson Matthey Technology Review **66**, 130 (2022)



Alchemite™ product family

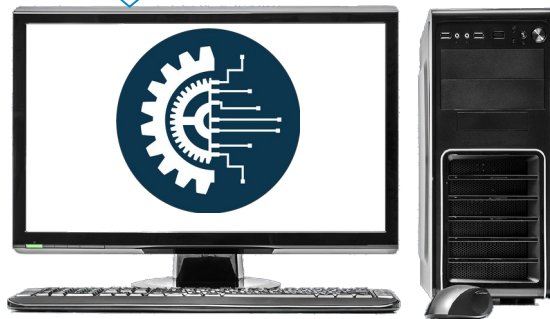


Engineers



←
Deploy models

Data scientists



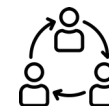
Optional connectors



Lab systems



Software & scripts



Collaboration

Alchemite™ Analytics

Deep data insights on your desktop
Guide experiments, predict, design

Alchemite™ Engine

Integrate into your workflow (API, Python)
Advanced configuration, enterprise deployment

Alchemite™
Success

Apply Intellegens deep learning expertise
Advice to your data science team or full project management

Summary



Merge computer simulations with experimental data and exploit **property-property** relationships to circumvent **missing data**

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

Generic approach applied to materials, batteries, chemicals, and beyond

Taken to market through by **Intellegens** as **Alchemite Analytics™**, **Optibrium**, and **ANSYS Granta**

<https://intellegens.com>