

A melting pot for data: machine learning for materials design and beyond

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Machine learning algorithm to

Merge simulations, physical laws, and experimental data

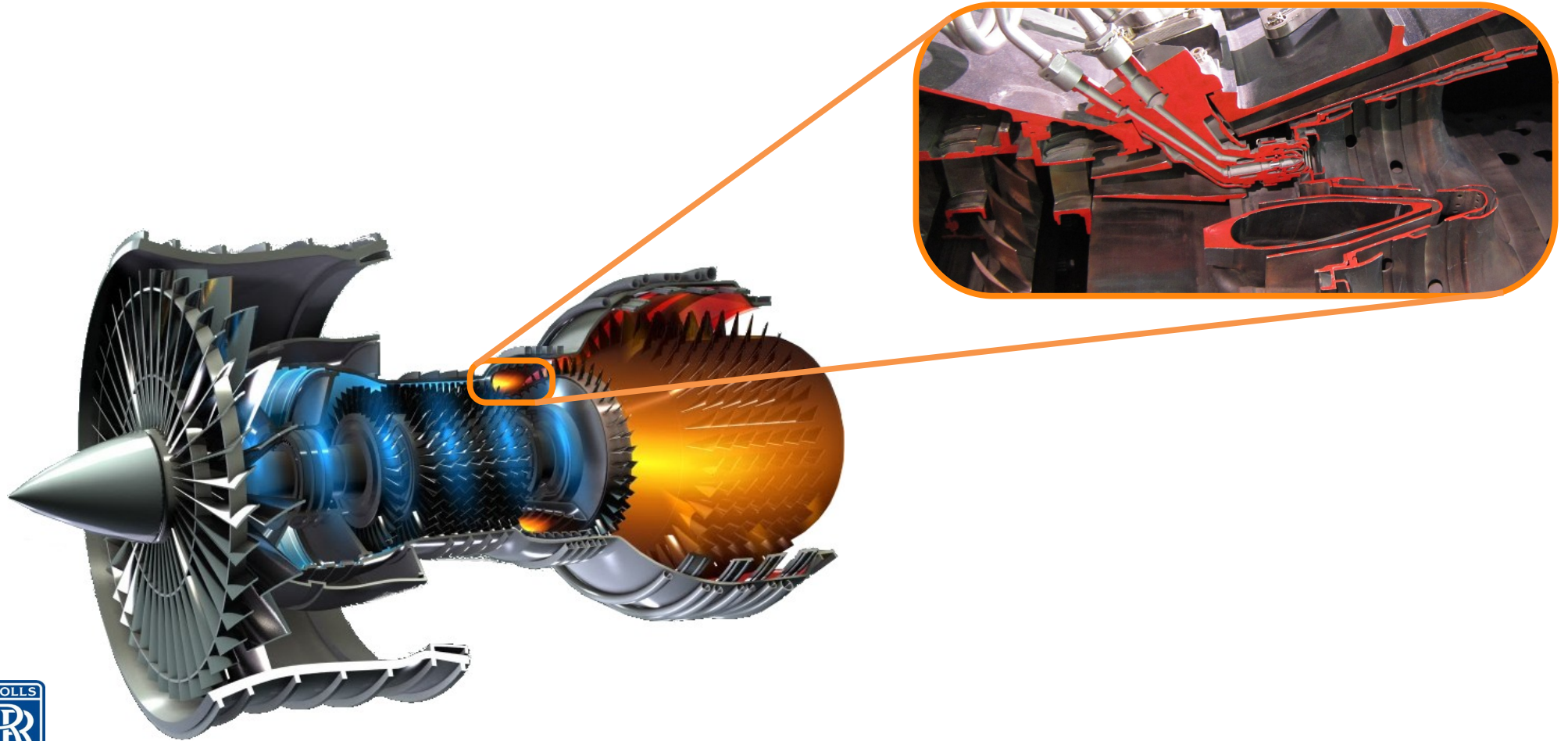
Train from **sparse** datasets

Exploit **property-property** correlations

Probabilistic design focuses on material **most likely** to work

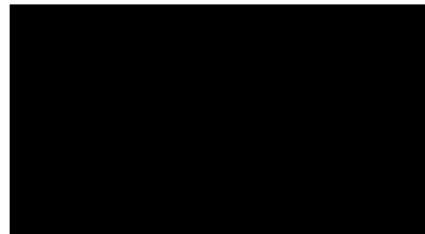
Reduce costly experiments to **accelerate** discovery

Combustor in a jet engine



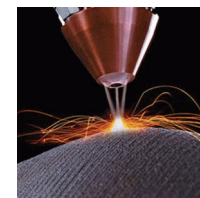
Black box machine learning for materials design

Composition



Properties

Defects



Fatigue



Strength



Train the machine learning

Composition

70	38	18	40	64	65	00
50	10	66	37	89	02	90
71	52	69	09	46	74	44
01	14	04	49	74	94	80
48	86	85	27	61	10	99
20	33	32	72	19	94	99
97	65	79	34	22	43	41
39	40	46	70	39	60	39



Properties

29	39	28	76	47	90	90
02	13	64	40	10	36	020
63	65	84	97	05	08	18
70	38	18	40	64	65	00
50	10	66	37	89	02	90
71	52	69	09	46	74	44
01	14	04	49	74	94	80
48	86	85	27	61	10	99
20	33	32	72	19	94	99
97	65	79	34	22	43	41
39	40	46	70	39	60	39
59	76	92	86	81	12	39
37	64	13	43	94	87	34
36	65	24	47	27	53	78
14	42	19	81	03	26	61
80	55	56	06	95	26	64
98	34	43	99	48	81	09

Defects

Fatigue

Strength

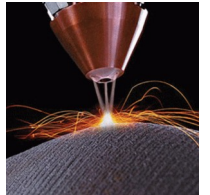
Machine learning predicts material properties

Composition



Properties

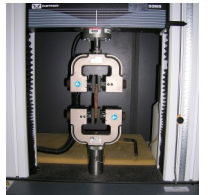
Defects



Fatigue



Strength



Data available to model defect density

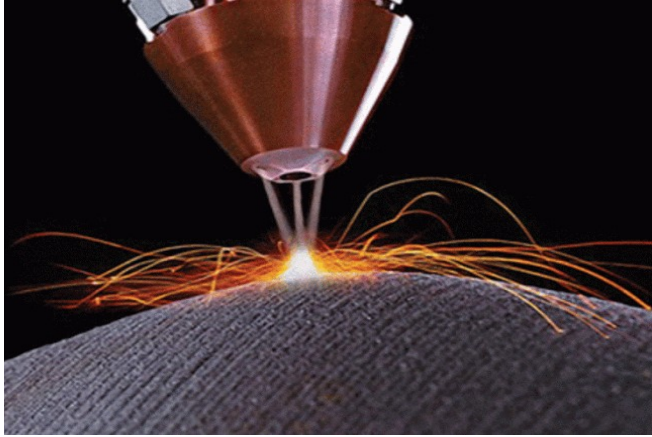


Composition and heat treatment space **30** dimensions

Requires **31** points to fit a hyperplane

Just **10** data entries available to model defect density

Ability for printing and welding are strongly correlated

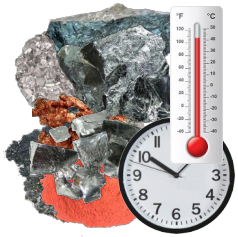


Laser

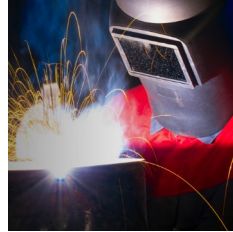


Electricity

First predict weldability

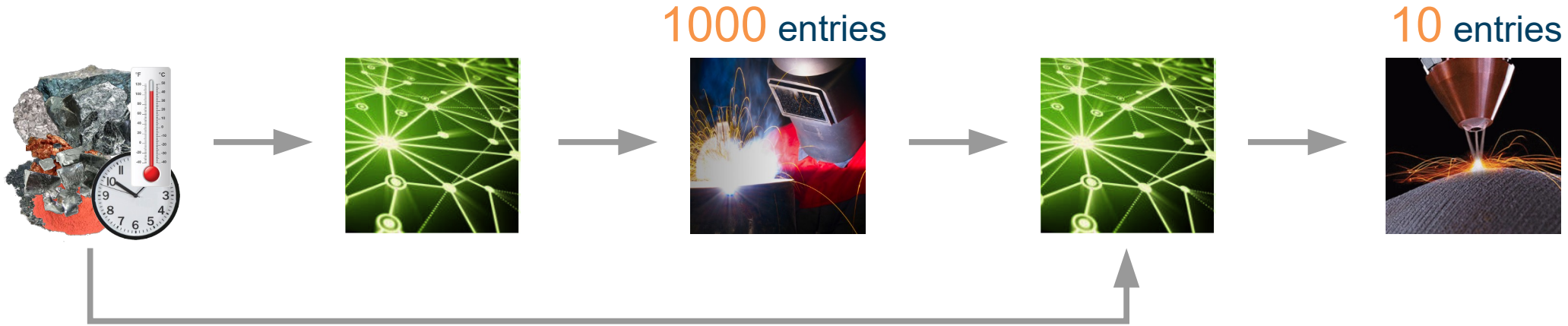


1000 entries



Use 1000 weldability entries to understand complex composition → weldability model

Use weldability to predict defects formed



Use **1000** weldability entries to model complex composition → weldability

10 defects entries capture the simple weldability → defect relationship

Two interpolations give composition → defects **extrapolation**

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⁻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 and processing variables

Cr 19%



Co 4%



Mo 4.9%



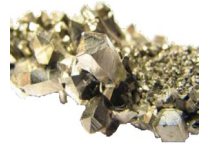
W 1.2%



Zr 0.05%



Nb 3%



Al 2.9%



C 0.04%



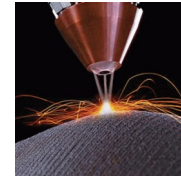
B 0.01%



Ni



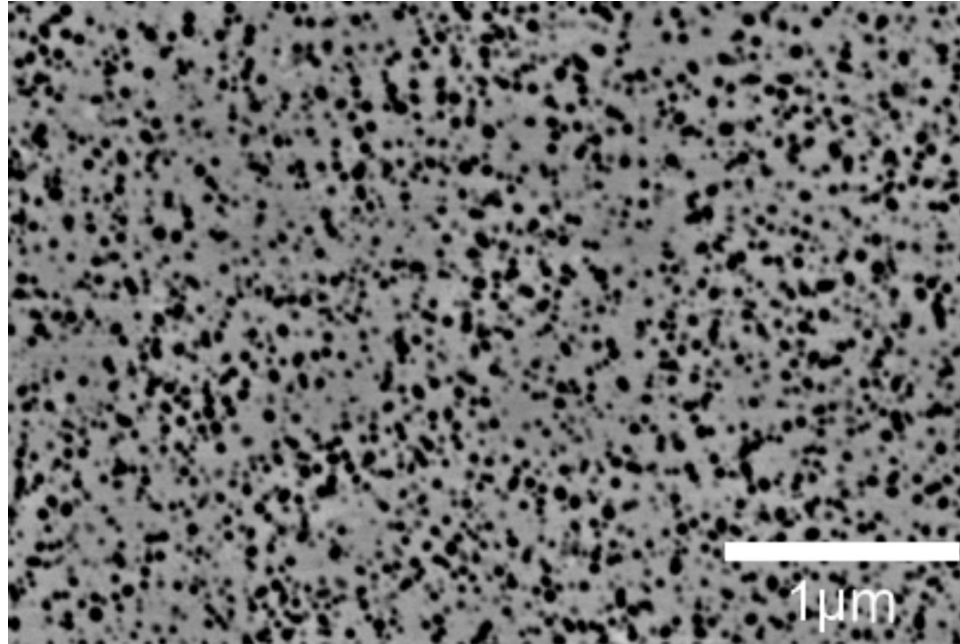
Expose 0.8



T_{HT} 1300°C

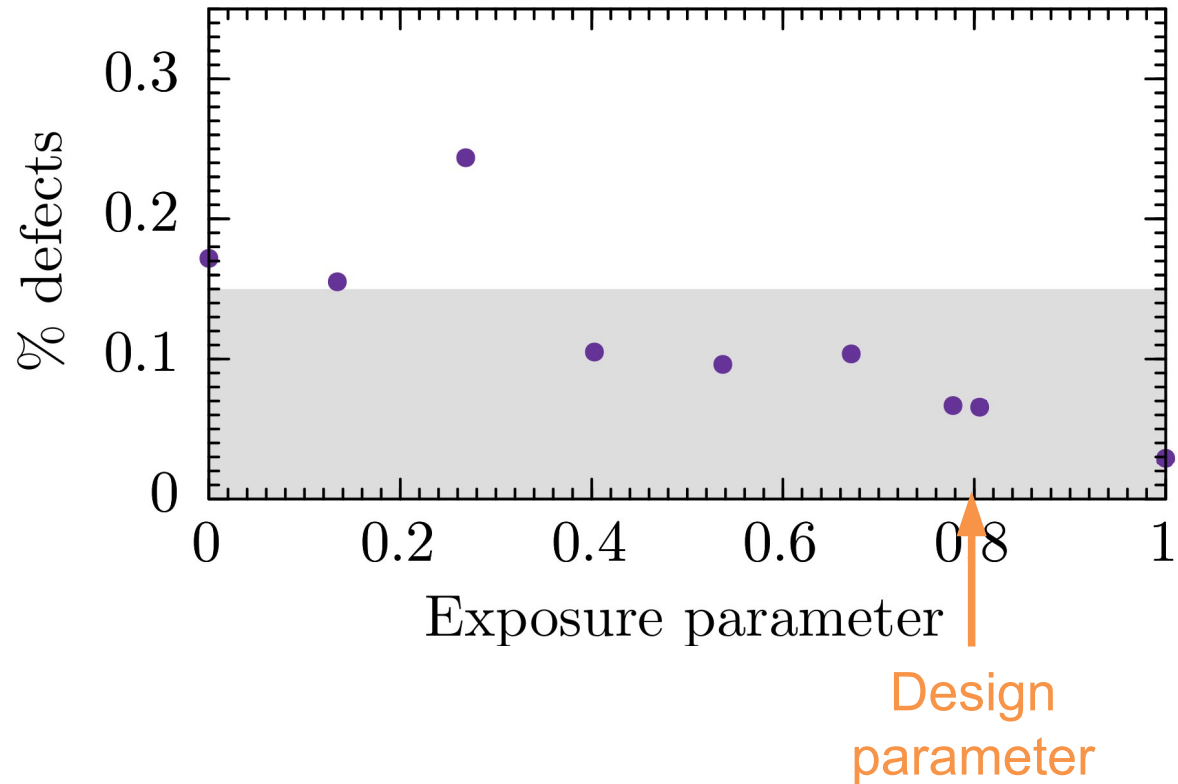


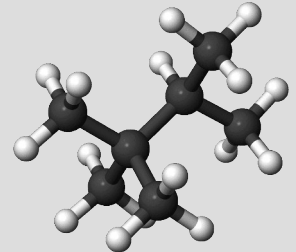
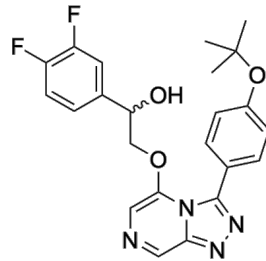
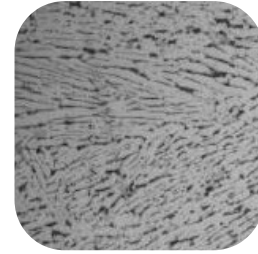
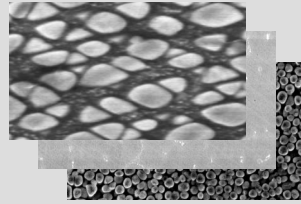
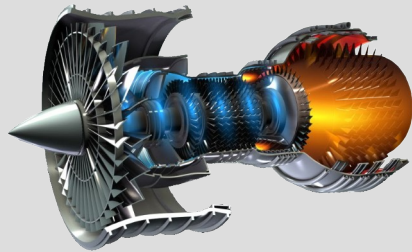
Microstructure



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

Testing the defect density





Commercialization



Alchemite Analytics™ platform for materials and chemicals with Intellegens released in **September 2020**



Machine learning tool embedded into **Cerella™** released in **October 2020**



Integrate machine learning into **Granta MI™**

Summary

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

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

Taken to market through startup **Intellegens**

Future drive to extract **all possible information** from the data