



Probabilistic neural network identification of an alloy for direct laser deposition

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Neural network algorithm to

Train from **sparse** datasets

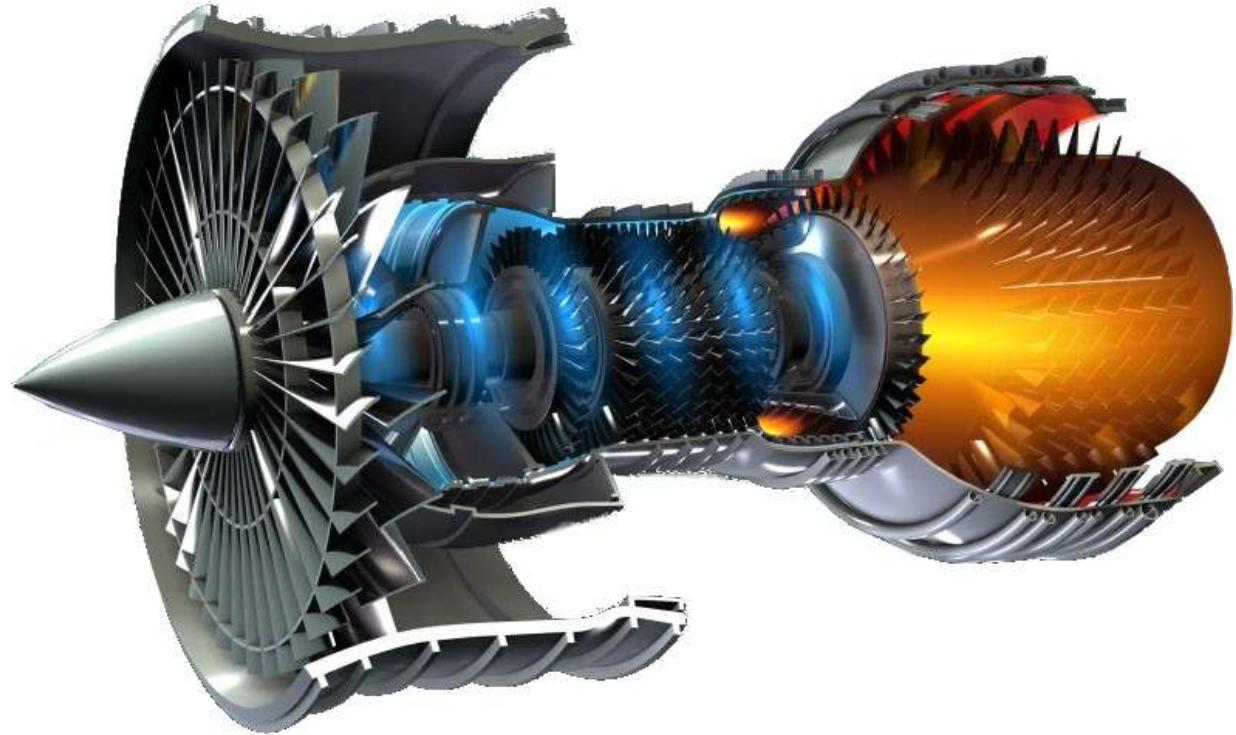
Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

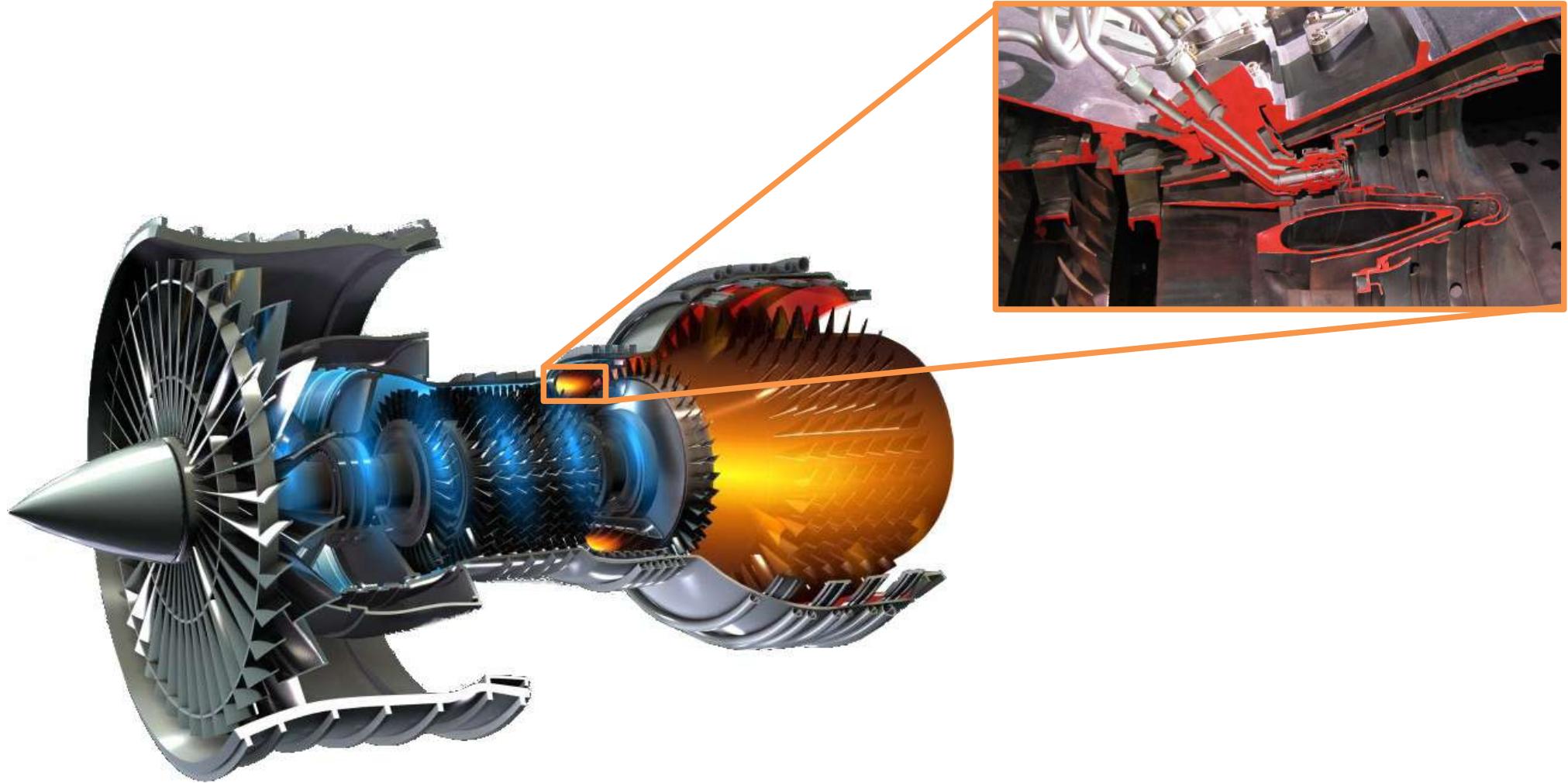
Accelerate materials and drugs discovery

Generic with **proven** applications in materials discovery and drug design

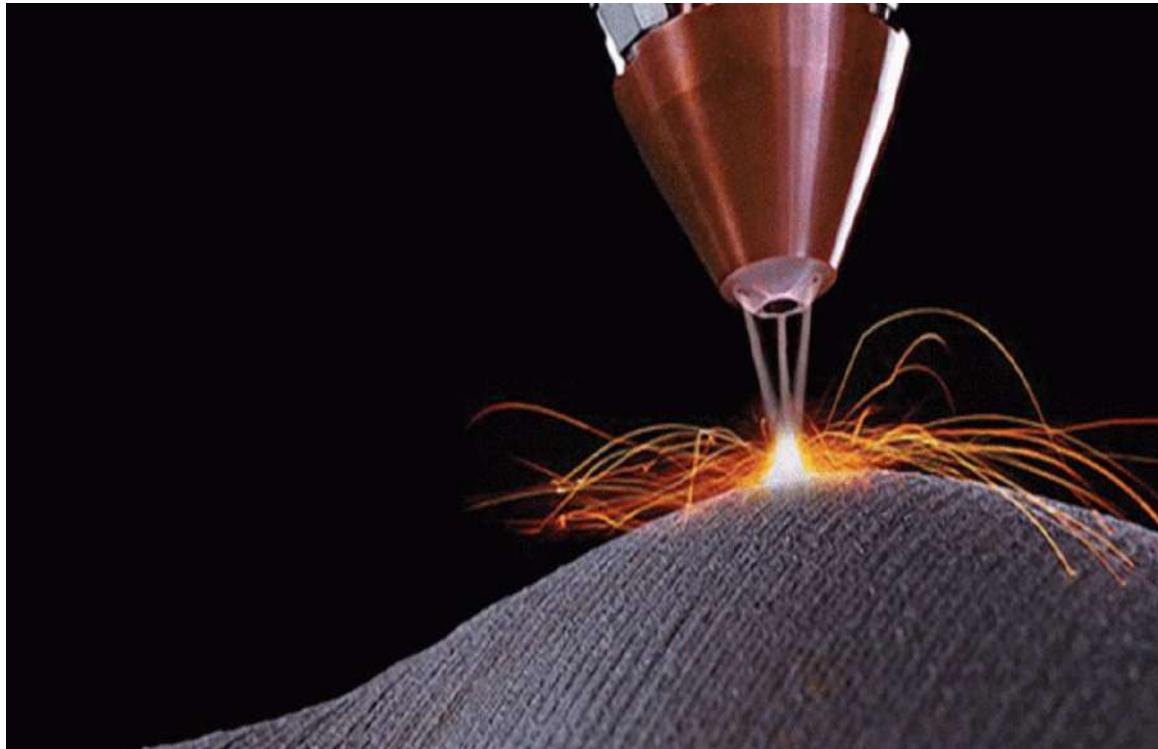
Schematic of a jet engine



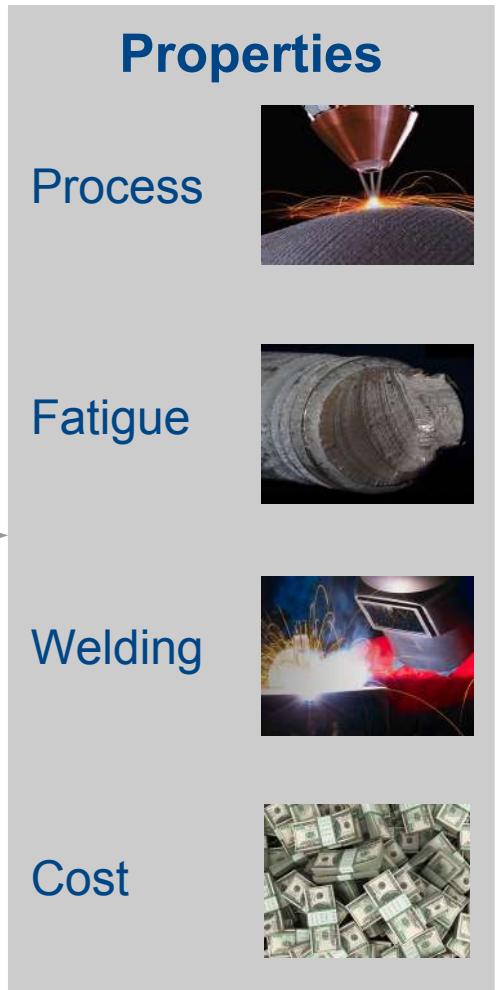
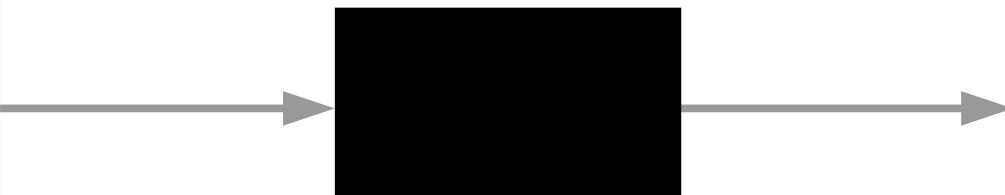
Combustor in a jet engine



Direct laser deposition requires new alloys

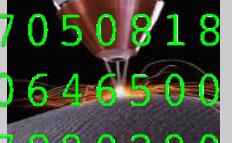
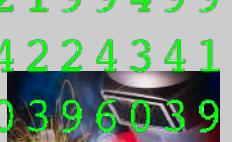
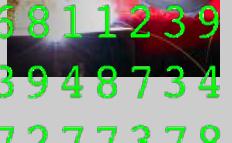


Neural networks for materials design

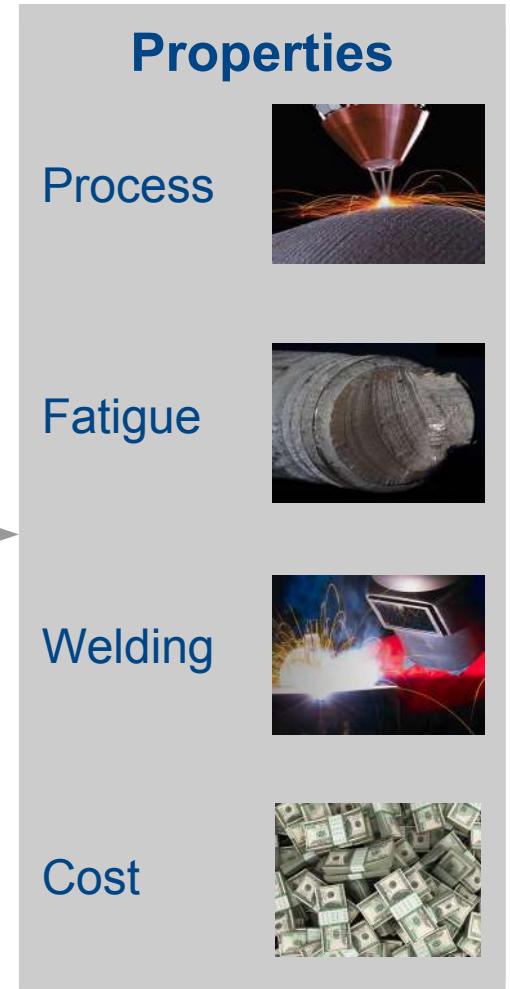


Neural networks for materials design

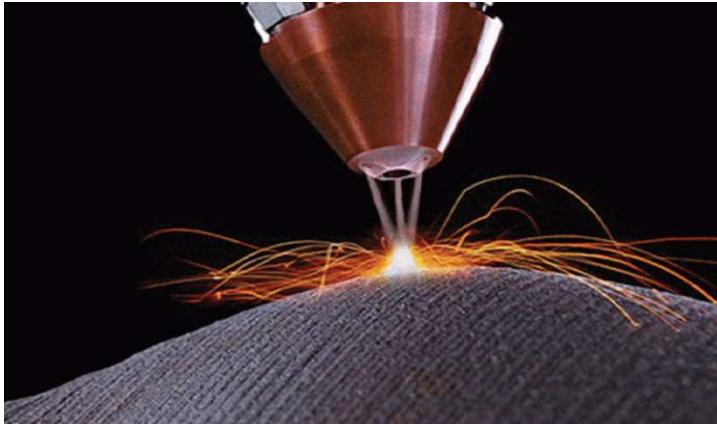


29	39	28	76	47	90	90	4	Properties	
02	13	64	01	03	60	20	2		
63	65	84	97	05	08	18	1	Process	
70	38	18	40	64	65	00	0		
50	10	66	37	89	02	90	1		
71	52	69	09	46	74	44	9		
01	14	04	44	97	49	48	02	Fatigue	
48	88	85	27	61	10	99	1		
20	33	32	72	19	94	99	5		
97	65	79	34	22	43	41	8		
39	40	46	70	39	60	39	3	Welding	
59	76	92	86	81	11	23	9		
37	64	13	43	94	87	34	1		
36	65	24	47	27	73	78	7		
14	42	19	81	03	26	66	10	Cost	
80	55	56	06	95	26	64	9		
98	34	43	99	48	81	09	1		

Neural networks for materials design



Neural networks for materials design

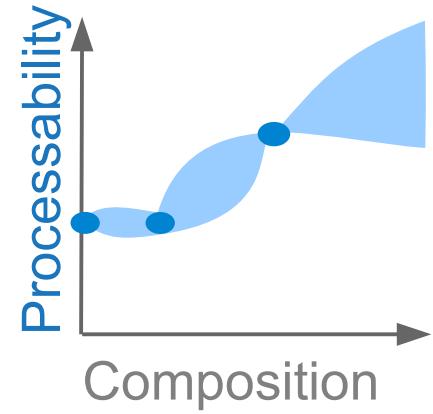


Laser

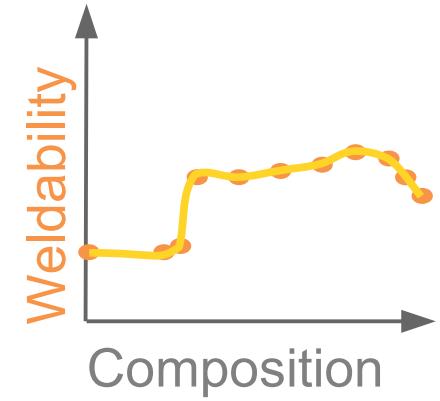
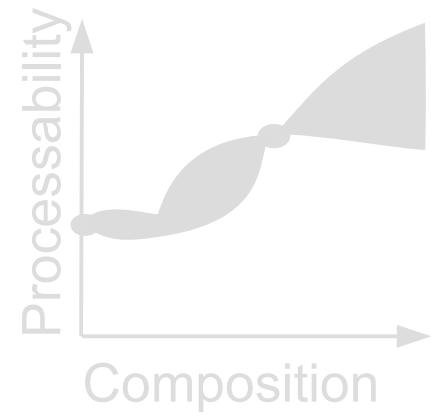


Electricity

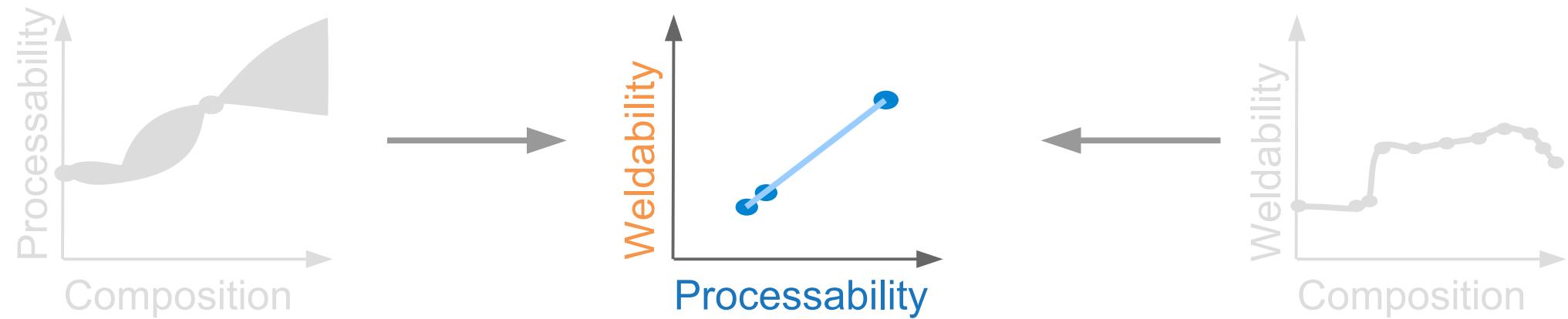
Insufficient data for processability



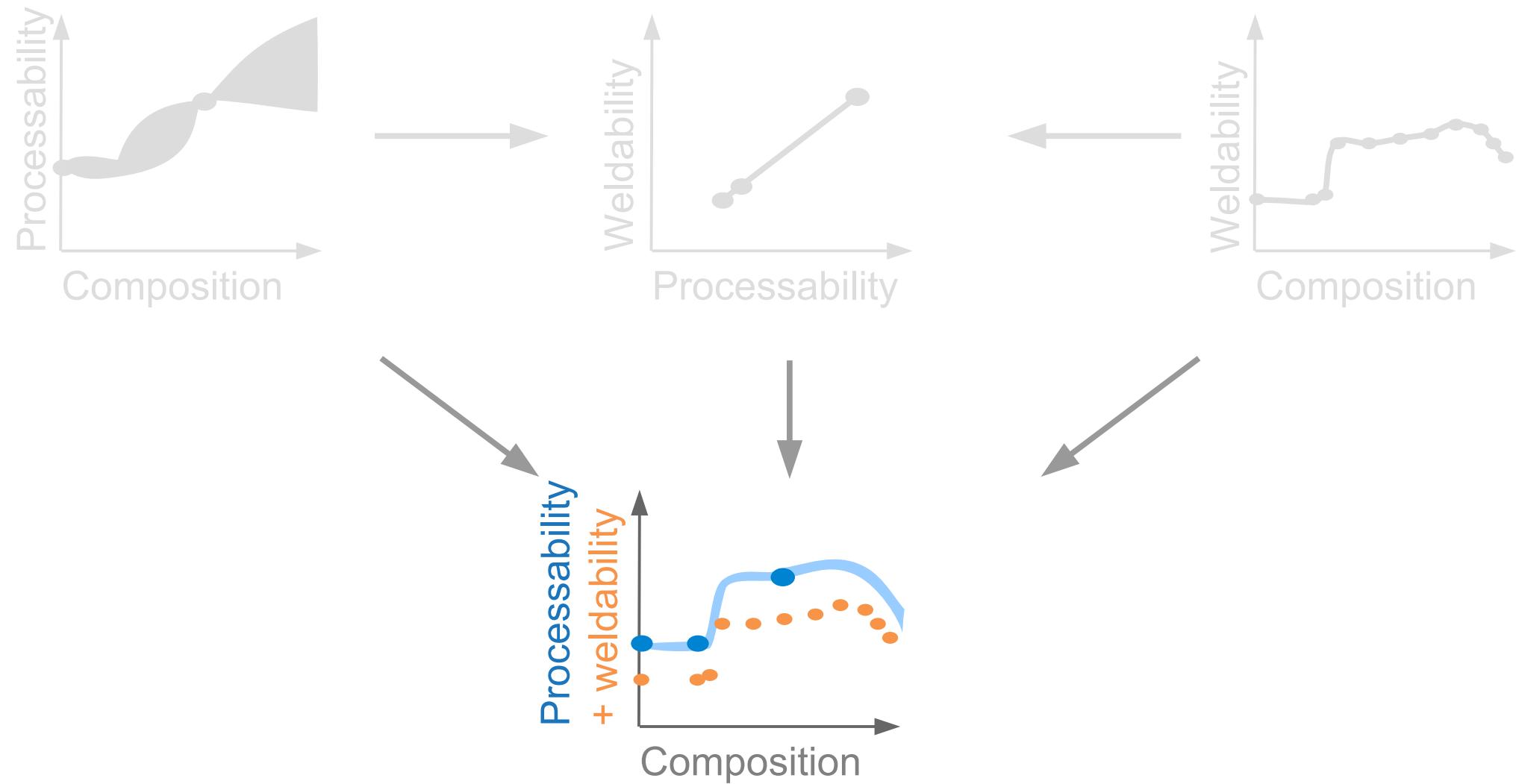
Welding is analogous to direct laser deposition



Simple processability-welding relationship



Merging properties with the neural network



Target properties

Elemental cost < 25 \$kg⁻¹

Density < 8500 kgm⁻³

γ' content < 25 wt%

Oxidation resistance < 0.3 mgcm⁻²

Processability < 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

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



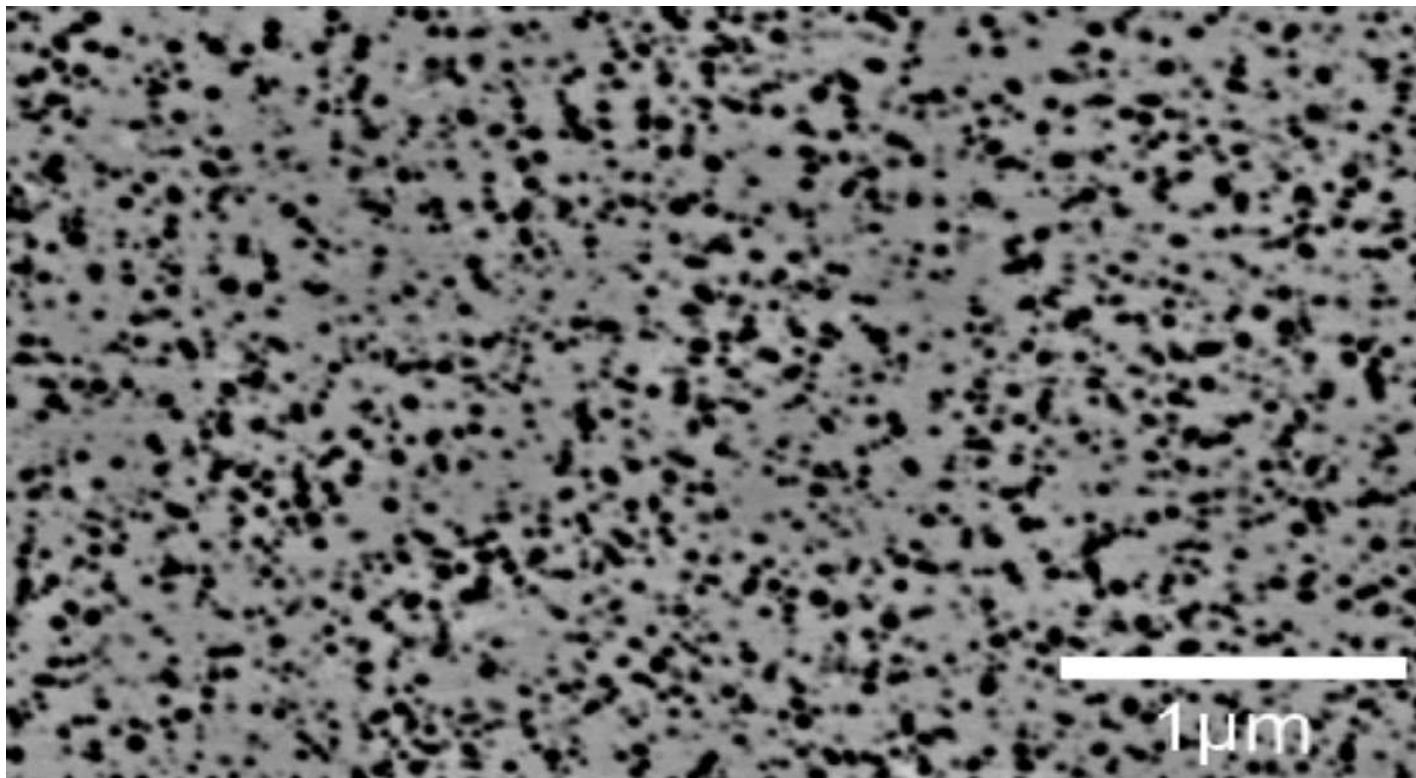
Expose 0.8



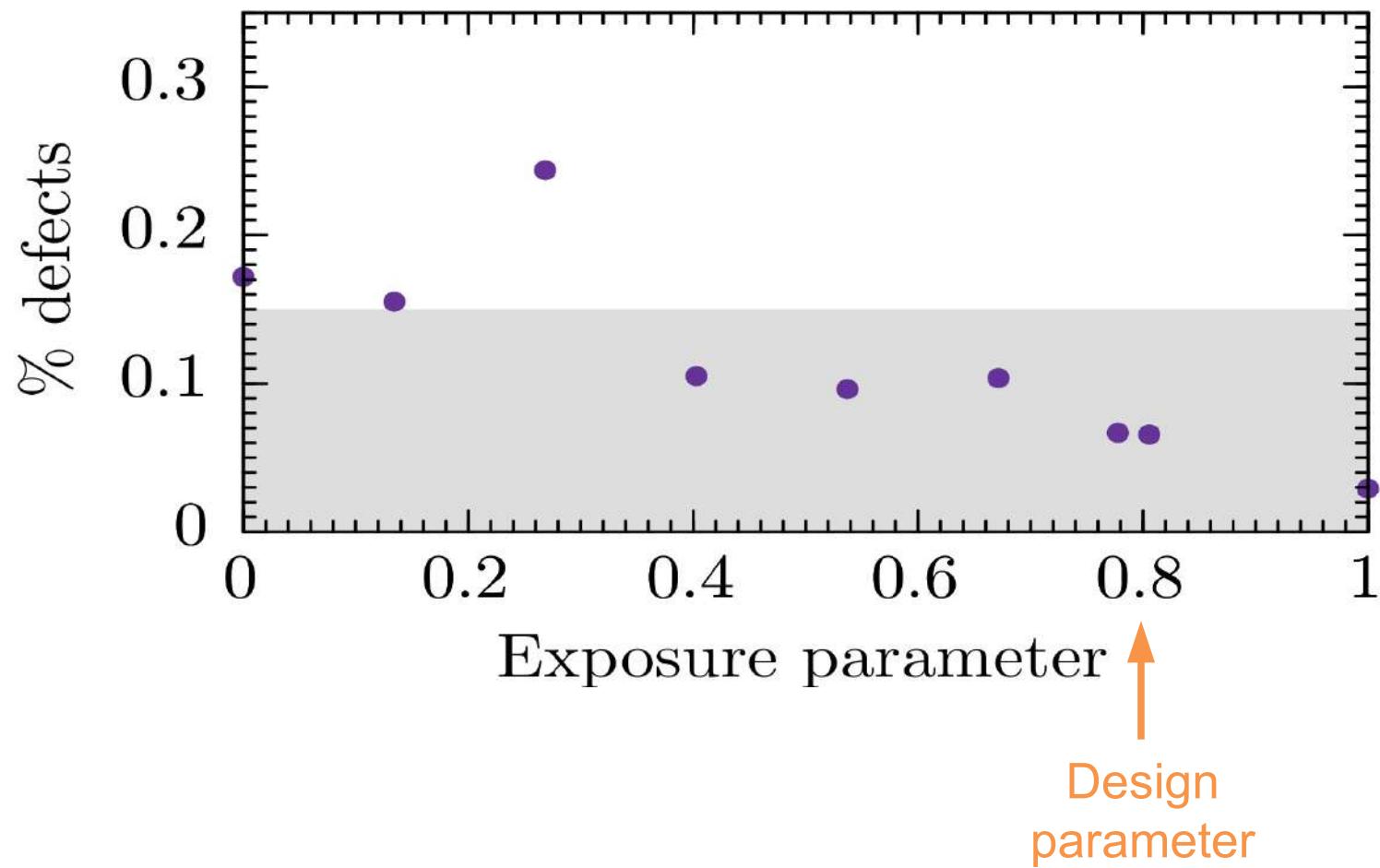
T_{HT} 1300°C



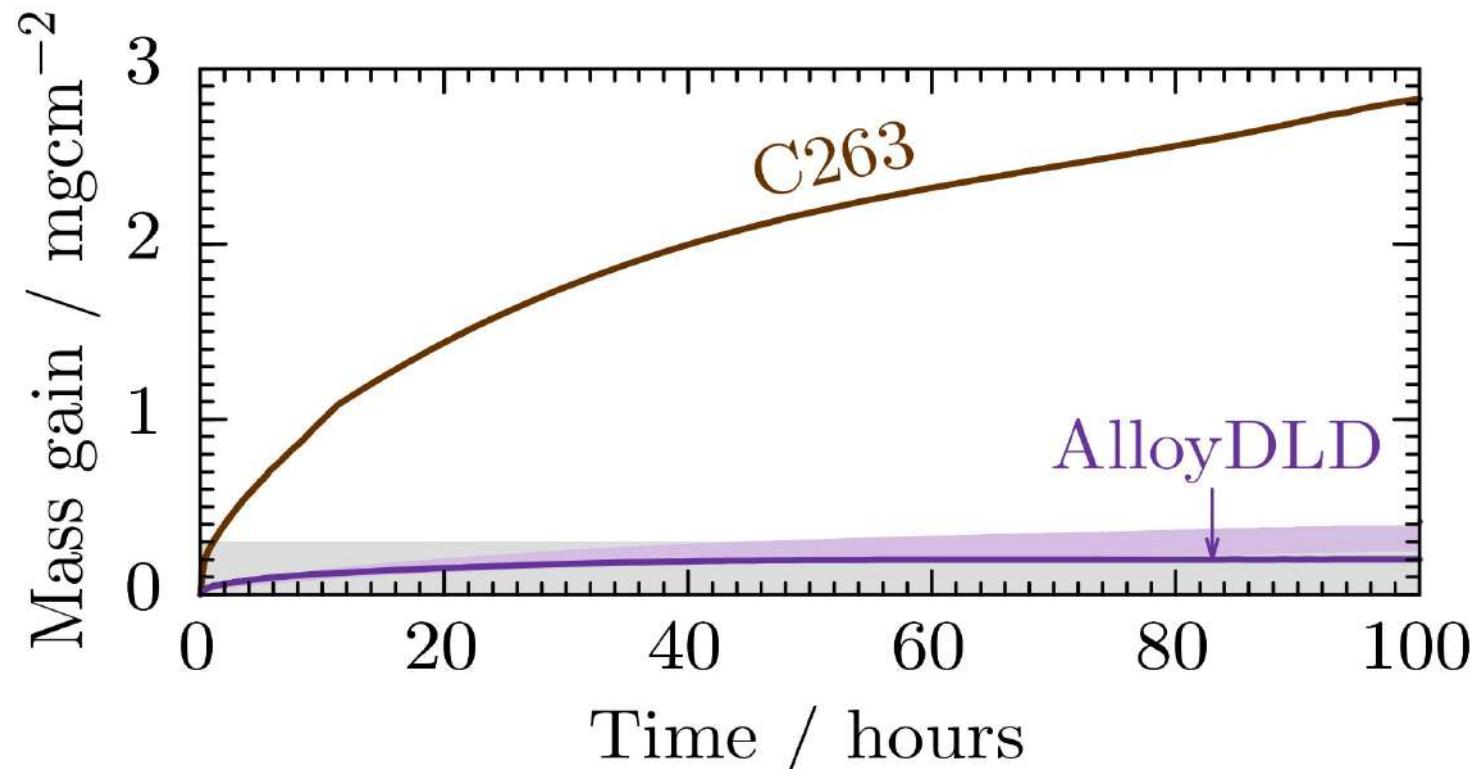
Microstructure



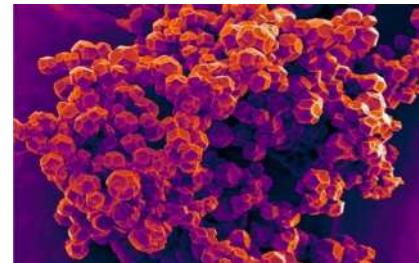
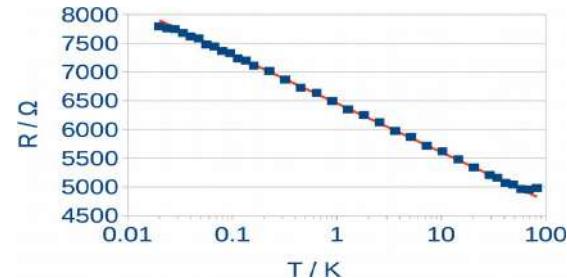
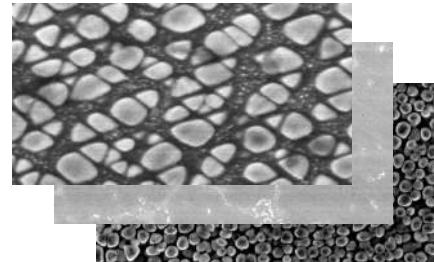
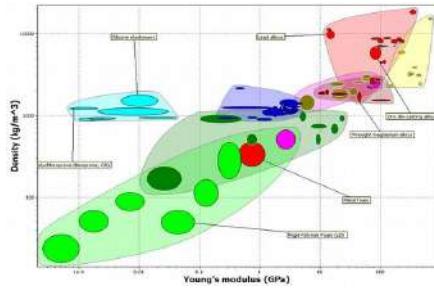
Testing the processability



Testing the oxidation resistance



Materials designed



Productizing machine learning



1 Upload data

2 Train models

3 Design materials

A tablet device displays a web-based application titled "Predicting properties of steel". The app interface includes a descriptive text box, input fields for element percentages, a "PREDICT" button, and a results section showing predicted physical properties.

Predicting properties of steel

We demonstrate a neural network that predicts the physical properties of steels based on the composition and heat treatment. The neural network model was trained from a library of experimental data from 1000 alloys.

In the first panel below set the percentages of each element in the composition and heat treatment temperature, and then click predict to get the neural network estimates for yield stress, ultimate tensile strength, and elongation.

Click [here](#) to use this technology to optimize the yield stress, ultimate tensile strength, and elongation of the steel.

This same technology was used to understand nickel alloys where the composition covered 20 elements, 5 heat treatment parameters, and predicted 11 material properties. Click [here](#) to read more about this study.

Set inputs

Iron (Fe)	100	remain %
Carbon (C)	0	0 to 0.43 %
Manganese (Mn)	0	0 to 3.0 %
Silicon (Si)	0	0 to 4.75 %
Chromium (Cr)	0	0 to 17.5 %
Nickel (Ni)	0	0 to 21.0 %
Molybdenum (Mo)	0	0 to 9.67 %
Vanadium (V)	0	0 to 4.32 %

PREDICT

Predictions

Yield Stress (MPa)	1605 ± 46
Ultimate Tensile Strength (MPa)	1200 ± 67
Elongation (%)	9 ± 2

[Click here to optimize a composition for given targets](#)

Summary

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

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

Designed many other materials, marketed by **Intellegens**