Intellegens

Design of an alloy for direct laser deposition using neural networks

About

Deep learning software for materials design

Aggregate all sources of data

Predictive models reduce costs by 80%

Accelerates materials discovery to 1 year

Traditional materials design

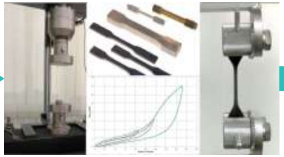
Current process is expert driven and iterative

Highly specialist alloys can cost > $10m and take 20 years to finalize and approve

Traditional materials design

Composition

Fabrication



Testing

DLD ability

Properties

Weldability

Standard deep learning

Composition

DLD ability

Properties

Weldability

Standard deep learning: train

Composition

DLD ability

Properties

Weldability

Standard deep learning: predict

Composition

DLD ability

Properties

Weldability

Alchemite™ deep learning

Composition

DLD ability

Properties

Weldability

Composition

DLD ability

Properties

Weldability

Optimized materials design

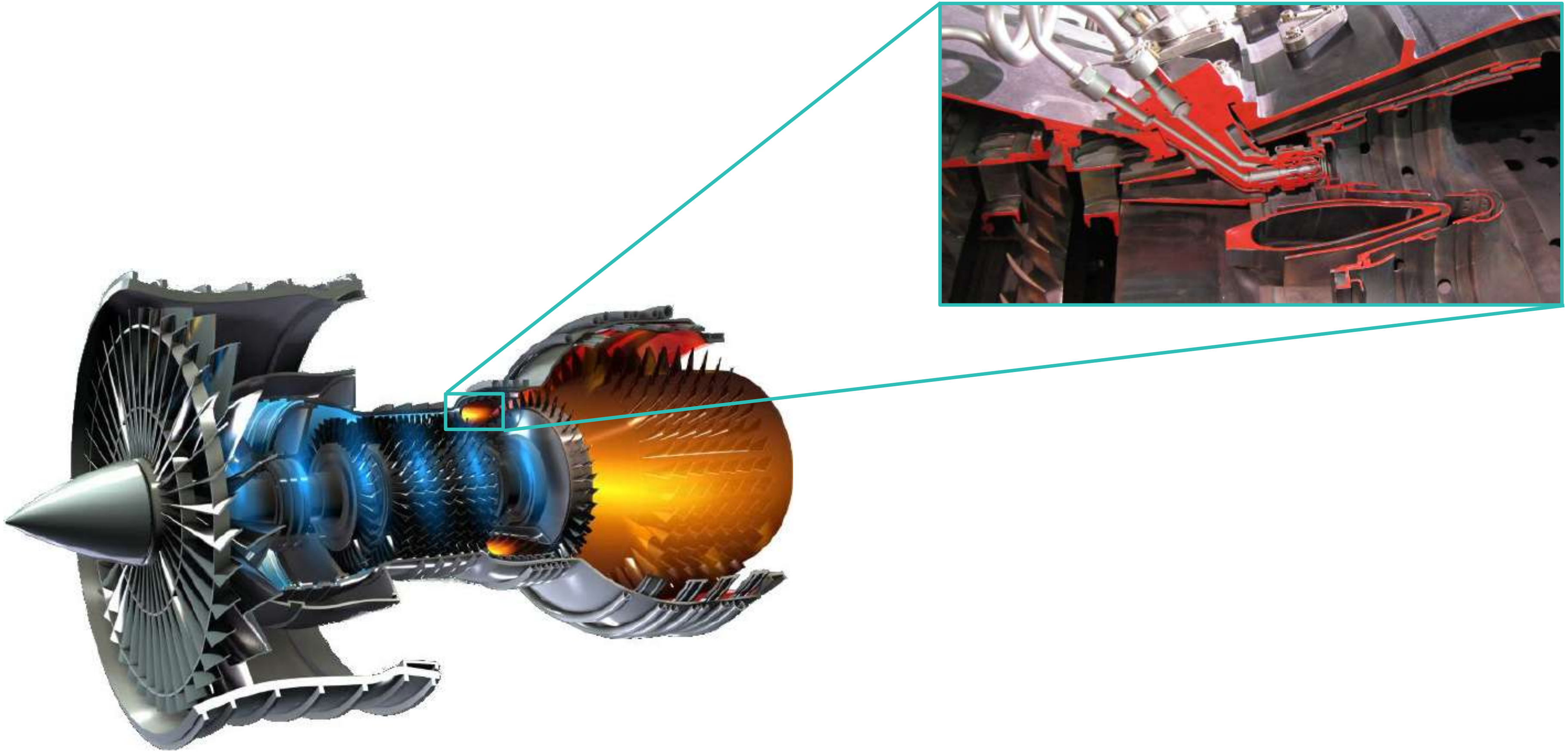
Reduce expensive experimental costs by 80%

Design new alloy in 1 year

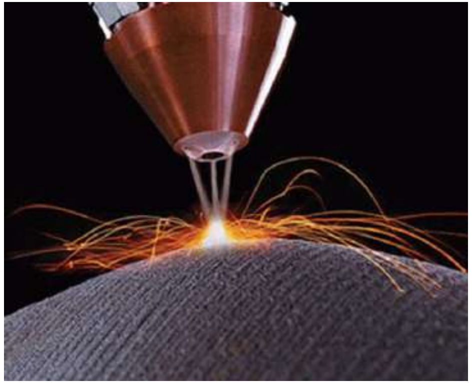
Improve target property optimization

Standardize design process across company

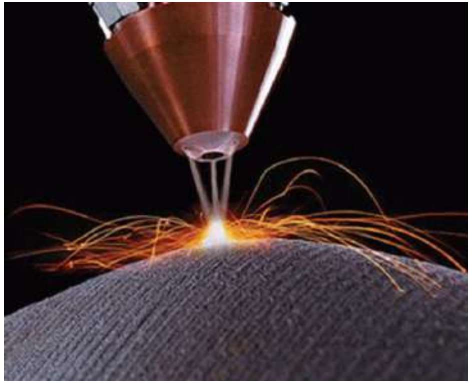
Case study: jet engine



Direct laser deposition requires new alloys



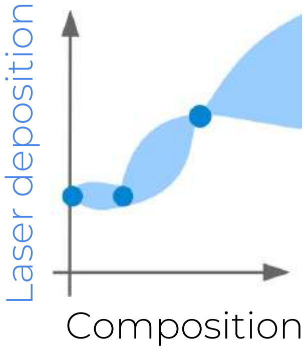
Direct laser deposition is similar to welding



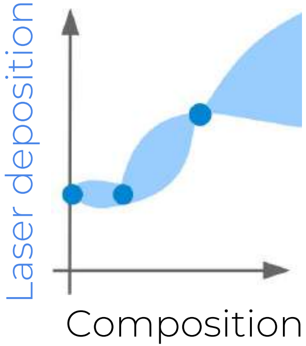
Direct laser deposition

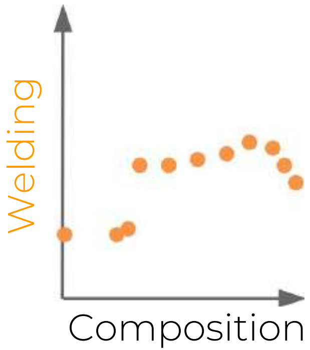
Welding

Lack of data for laser deposition

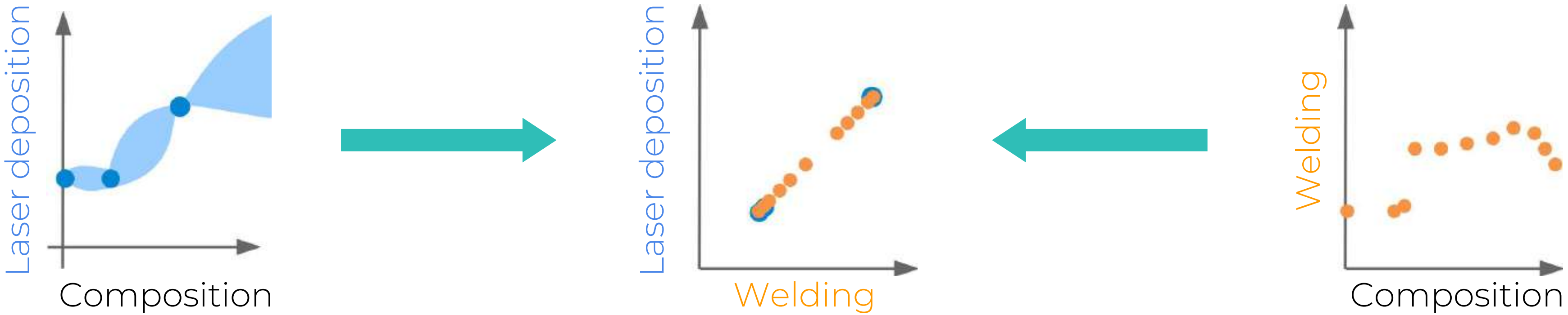


Large amount of welding data

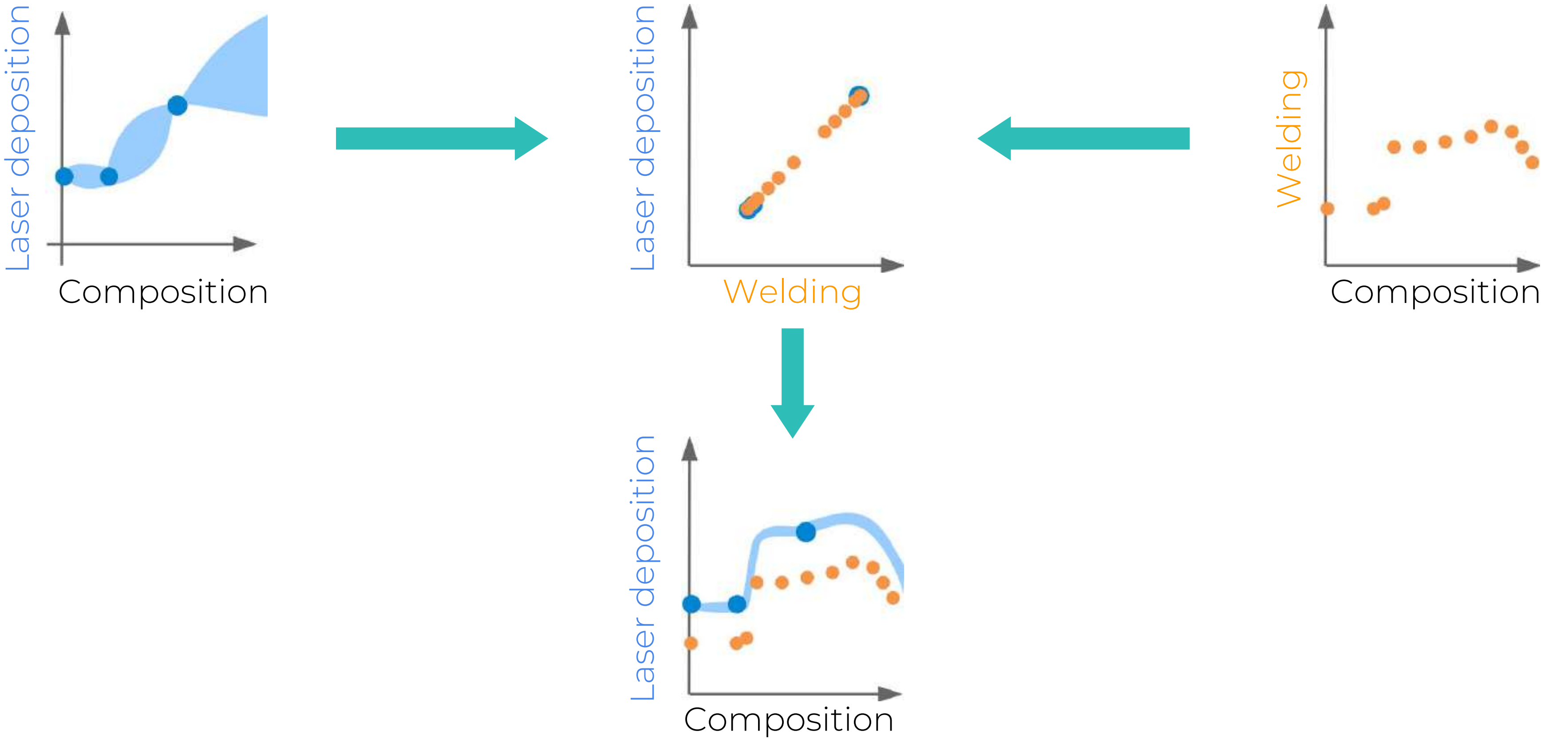




Simple welding-deposition relationship



Welding data guides extrapolation



Targets for direct laser deposition alloy

Elemental cost	$< 25\ \$\mathrm{kg}^{-1}$
Density	$< 8500\ \mathrm{kgm}^{-3}$
γ’ content	< 25 wt%
Oxidation resistance	$< 0.3\ \mathrm{mgcm}^{-2}$
Processability	< 0.15% defects
Phase stability	> 99.0 wt%
γ’ solvus	> 1000 ˚C
Thermal resistance	$> 0.04\ \mathrm{K\Omega^{-1}m^{-3}}$
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

Targets for direct laser deposition alloy

Cr 19%

Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%

Al 2.9%

C 0.04%

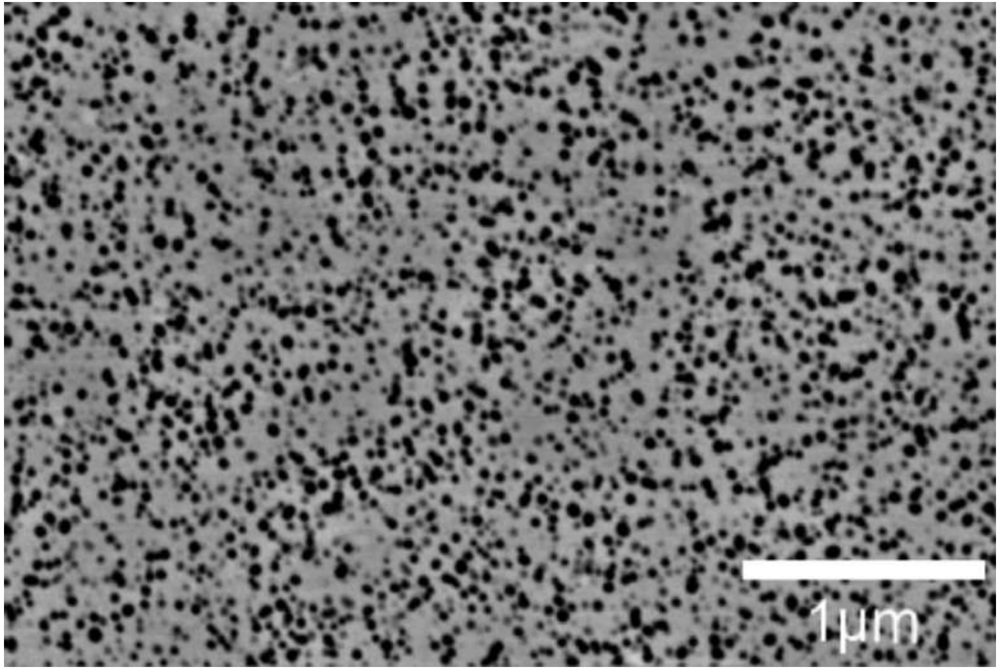
B 0.01%

Ni balance

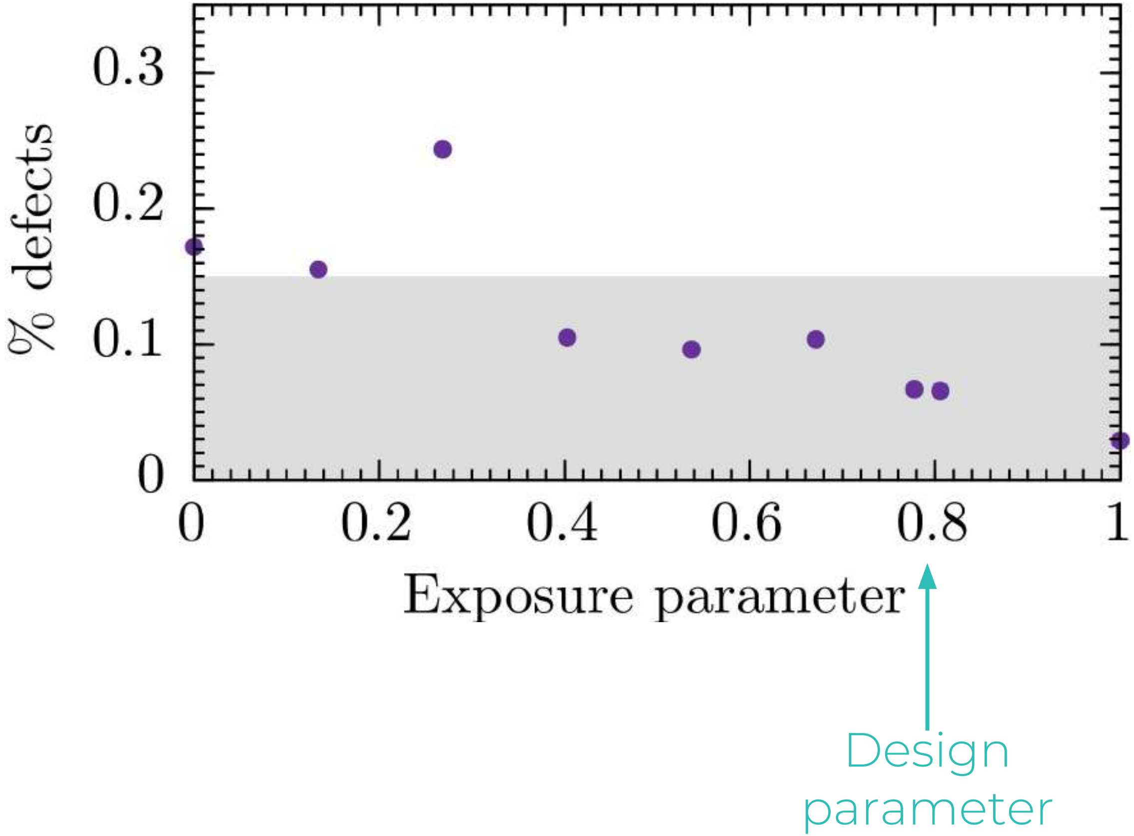
Exposure 0.8

T_{HT} 1230°C

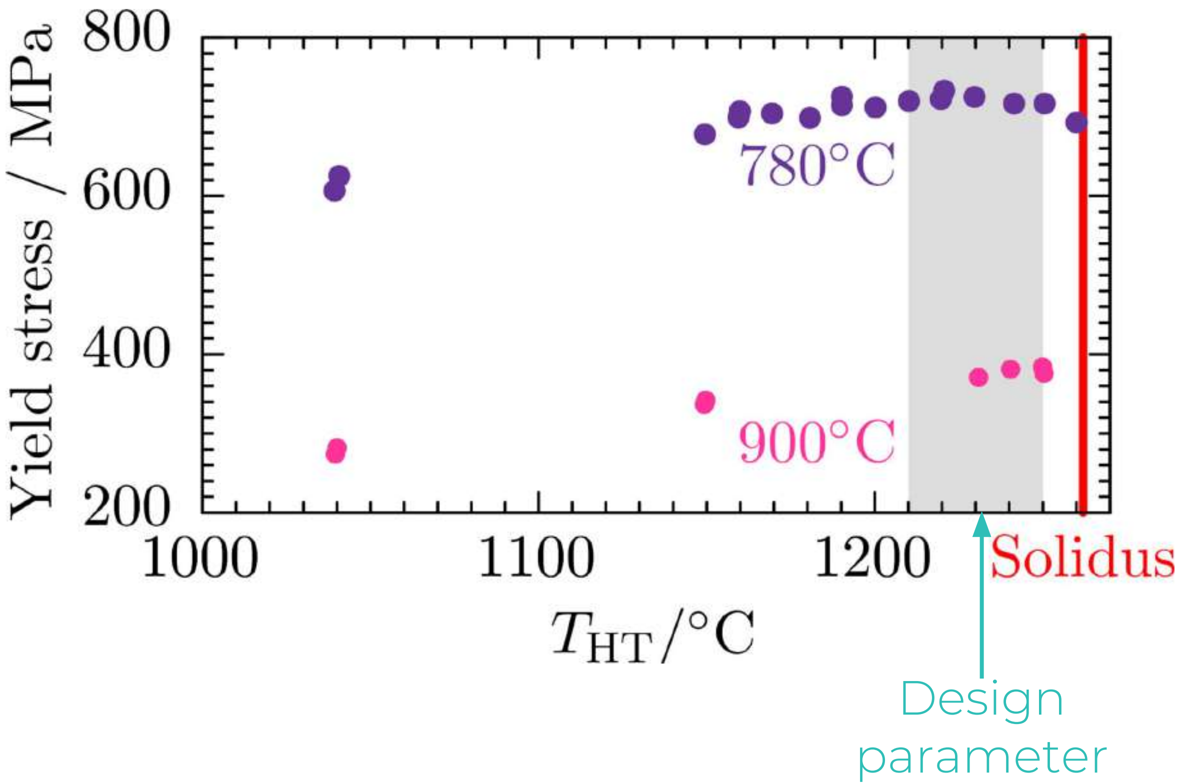
Microstructure



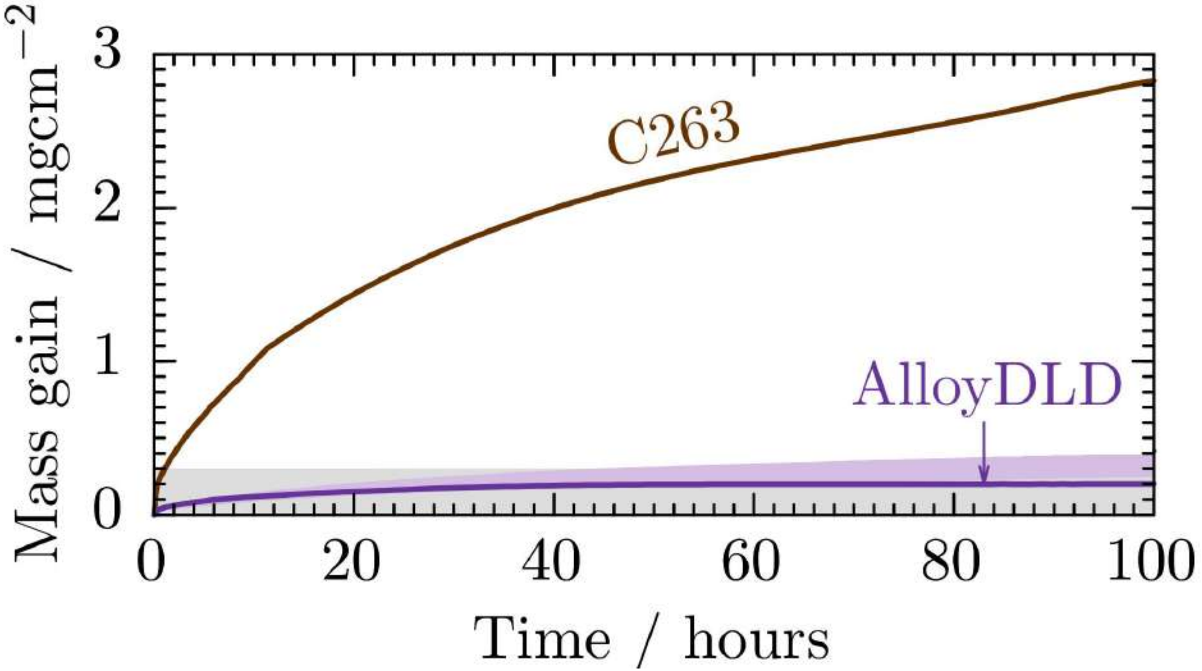
Testing the processability: horizontal printing



Testing the yield stress



Test the oxidation resistance



Printing components for the engine

Alchemite™ materials design

Merged welding, heat capacity, thermal expansivity, phase behavior to predict ability for direct laser deposition

Proposed and tested alloy for direct laser deposition within 1 year

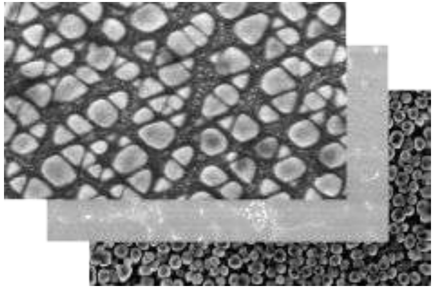
Experimentally verified properties of alloy

Designed a steel welding consumable

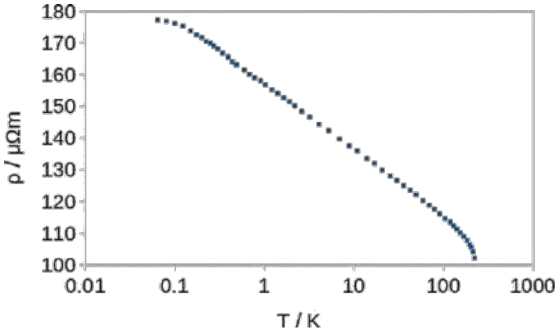
Materials & Design 168, 107644 (2019), Computational Materials Science 147, 176 (2018)

More materials design

Nickel and molybdenum-base alloys for jet engines



Material for thermometry



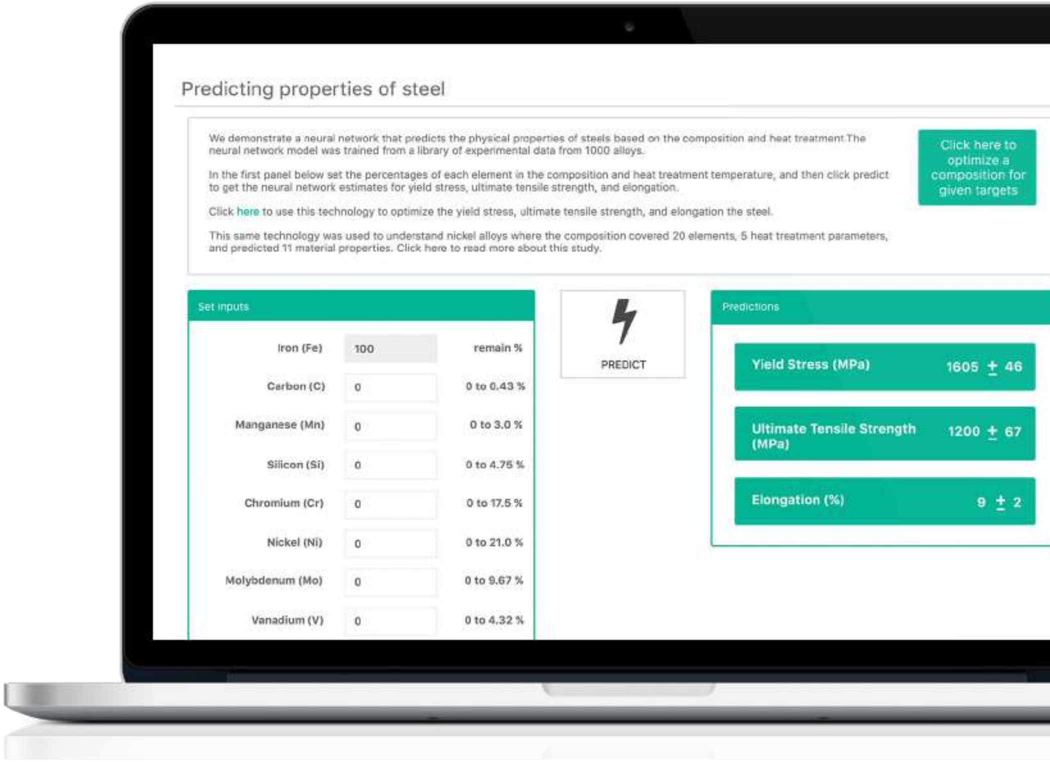
Scripta Materialia 146, 82 (2018), Materials & Design 131, 358 (2017)

Integrated software

1 Data load

2 Training

3 Design & predict



Summary

Alchemite™ exploits all available information for materials design

Proposed and verified new alloy for direct laser deposition in 1 year

Additional design of steel, nickel, molybdenum, and thermometry materials

Information

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Inventor https://www.tcm.phy.cam.ac.uk/~gjc29/index.html

Papers

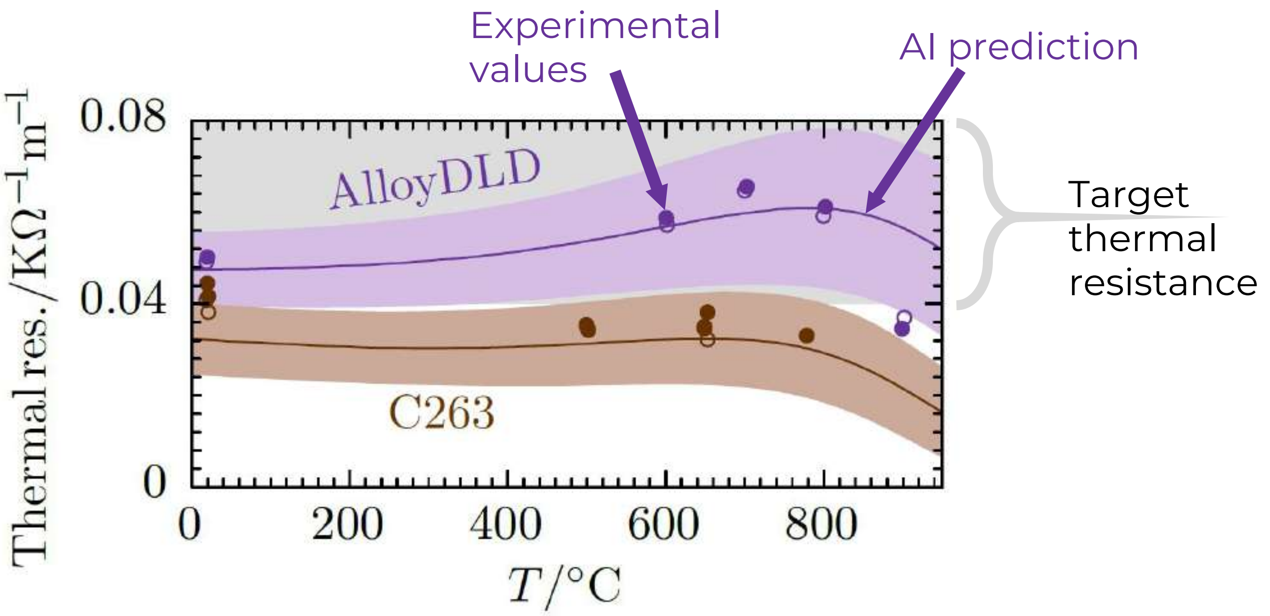
https://www.intellegens.ai/downloads/Probabilistic_neural_network_identification_of_an_alloy_for_direct_laser_deposition.pdf
https://www.intellegens.ai/downloads/Materials_data_validation_and_imputation_with_an_artificial_neural_network.pdf
https://www.intellegens.ai/downloads/Materials_data_validation_and_imputation_with_an_artificial_neural_network.pdf
https://www.intellegens.ai/downloads/ConduitJonesStoneConduit17ii.pdf
https://www.intellegens.ai/downloads/Whitehead19.pdf

Steels demonstrator

https://app.intellegens.ai/steel_search
https://app.intellegens.ai/steel_optimise

Appendix

Case study: direct laser deposition



B.D. Conduit et al., *Probabilistic neural network identification of an alloy for direct laser deposition*, under peer review.

Alchemite™ Materials design

Historical materials data - composition, treatment processes and resultant properties - is abundant but sparse.

	COMPOSITION			PROPERTIES			PROCESS
	Iron	Carbon	Nickel	Melt	Hard	Density	Temperature
Steel 1	10	0.3	22	1538	608		832
Steel 2	12		21	1085		8.96	1100
Steel 3		0.2	15		188	19.3	
Steel 4	11	0.6	0.6	660		2.7	1000

Tens of properties

Thousands of materials

Alchemite™ Materials design

Traditional AI - model 1 property at a time on compete data.

Information lost

	COMPOSITION			PROPERTIES			PROCESS
	Iron	Carbon	Nickel	Melt	Hard	Density	Temperature
Steel 1	10	0.3	22	1538	~~608~~		~~832~~
Steel 2	~~12~~		~~21~~	~~1085~~		~~8.96~~	~~1100~~
Steel 3		~~0.2~~	~~15~~		~~188~~	~~19.3~~	
Steel 4	11	0.6	0.6	660		~~2.7~~	~~1000~~

Tens of properties

Thousands of materials

Alchemite™ Materials design

Predict all values, supplying probability distributions for each.
Likelihoods can help inform ‘safest’ predictions to achieve targets or most ‘risky’ predictions

	COMPOSITION			PROPERTIES			PROCESS
	Iron	Carbon	Nickel	Melt	Hard	Density	Temperature
Steel 1	10	0.3	22	1538	608	**12.2** ∓1.1	832
Steel 2	12	**0.4** ∓0.1	21	1085	**440**∓2.1	8.96	1100
Steel 3	**11.5** ∓0.6	0.2	15	**740** ∓11	188	19.3	**990** ∓23
Steel 4	11	0.6	0.6	660	**220** ∓0.6	2.7	1000

Tens of properties

Thousands of materials

Alchemite™ Materials design

Steel 5 - design for desired targets - predictive mode

	COMPOSITION			PROPERTIES			PROCESS
	Iron	Carbon	Nickel	Melt	Hard	Density	Temperature
Steel 1	10	0.3	22	1538	608	12.2 ∓1.1	832
Steel 2	12	0.4 ∓0.1	21	1085	440∓2.1	8.96	1100
Steel 3	11.5 ∓0.6	0.2	15	740 ∓11	188	19.3	990 ∓23
Steel 4	11	0.6	0.6	660	220 ∓0.6	2.7	1000
Steel 5			**1.2**	**300**	**400**		

Tens of properties

Thousands of materials

Alchemite™ Materials design

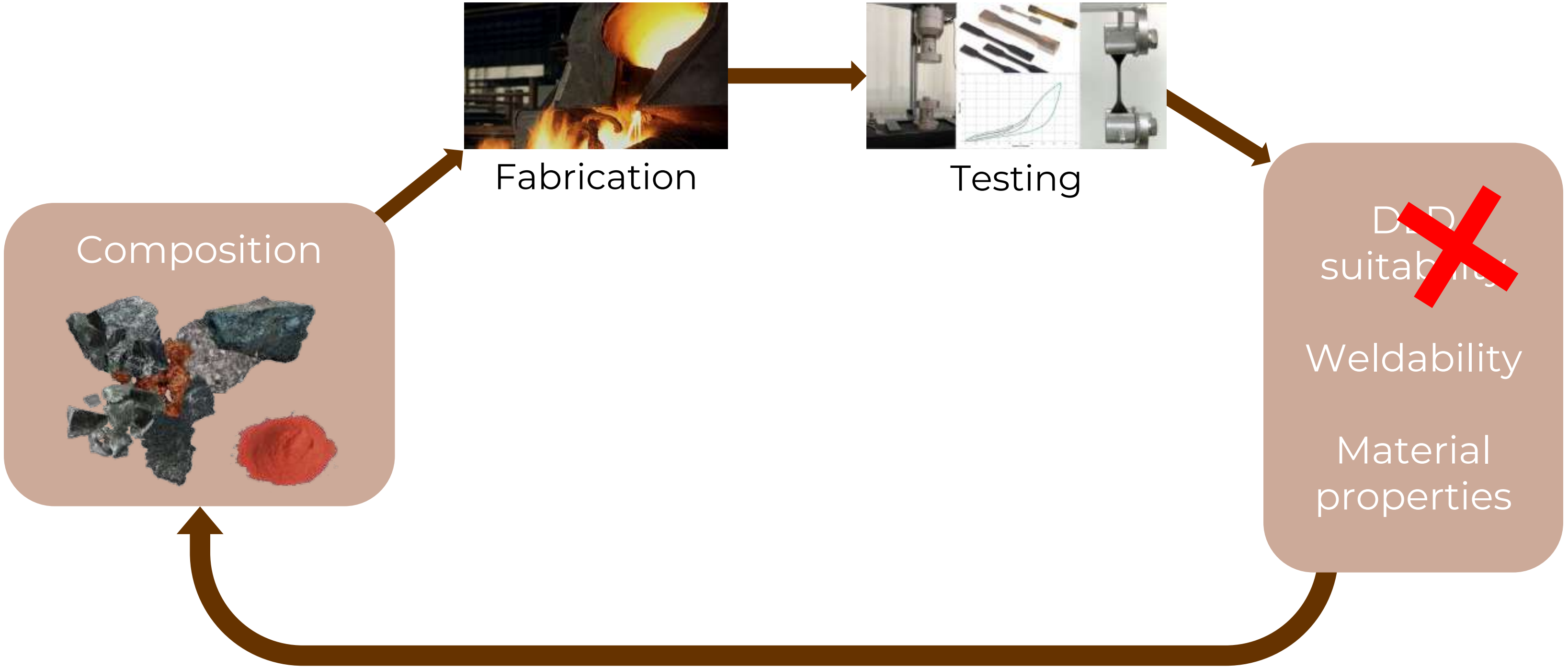
Steel 5 - design for desired targets

	COMPOSITION			PROPERTIES			PROCESS
	Iron	Carbon	Nickel	Melt	Hard	Density	Temperature
Steel 1	10	0.3	22	1538	608	12.2 ∓1.1	832
Steel 2	12	0.4 ∓0.1	21	1085	440∓2.1	8.96	1100
Steel 3	11.5 ∓0.6	0.2	15	740 ∓11	188	19.3	990 ∓23
Steel 4	11	0.6	0.6	660	220 ∓0.6	2.7	1000
Steel 5	**12 ∓0.6**	**0.3 ∓0.1**	1.2	300	400	**9.1 ∓0.2**	**780 ∓21.2**

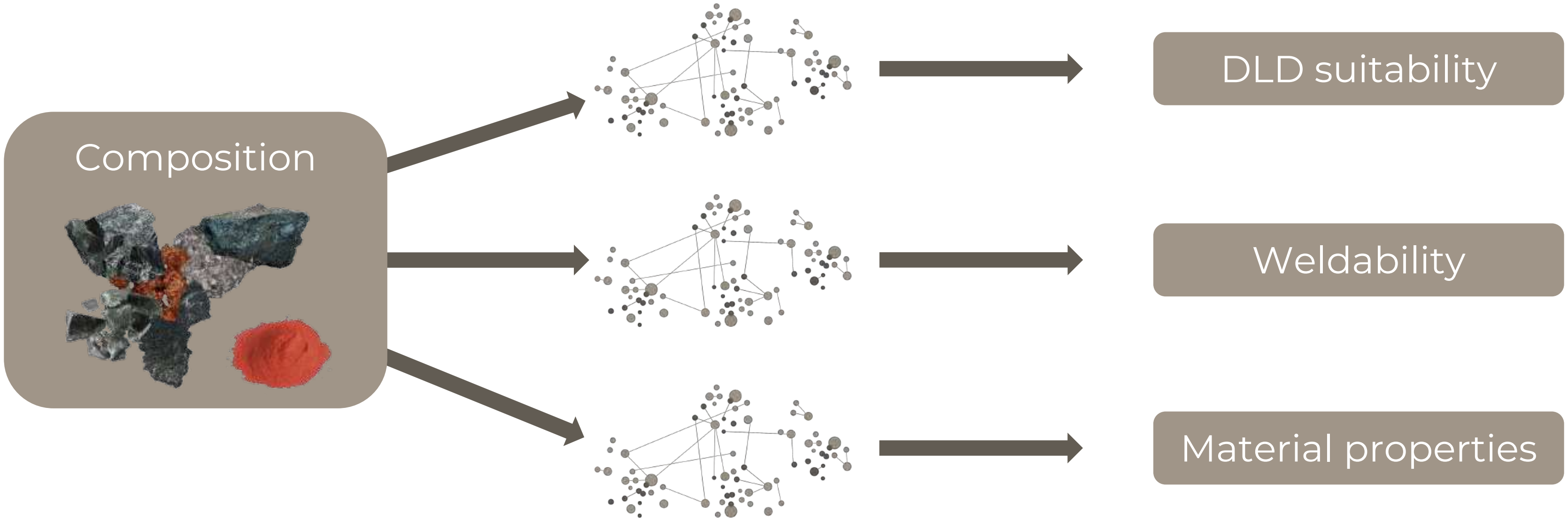
Tens of properties

Thousands of materials

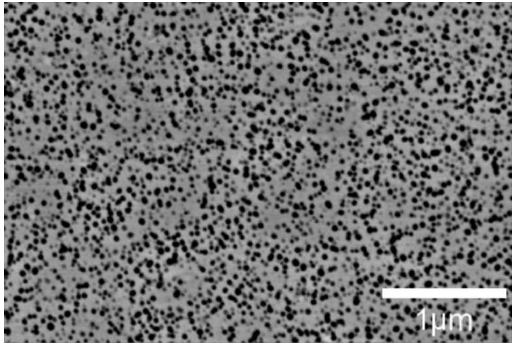
Traditional materials design

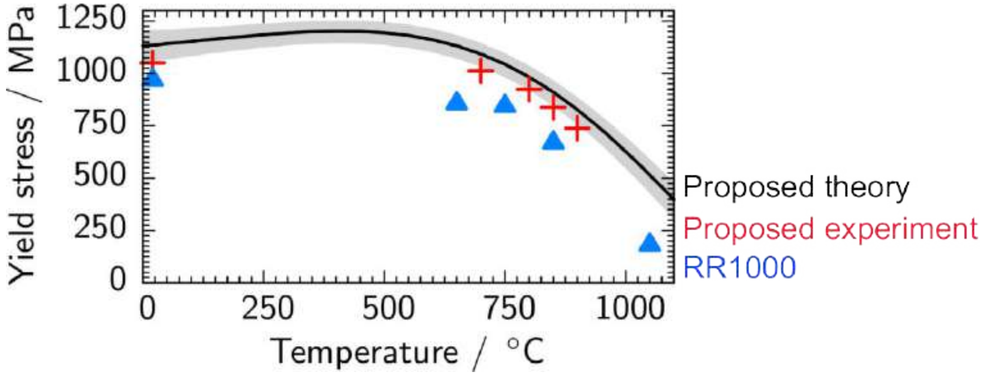


Conventional AI materials design



Validation





Designed alloy satisfies 14 target properties, experimentally verified and patented. Reduced development time by 18 years, saving £10m

Scripta Materialia 146, 82 (2018), Materials & Design 131, 358 (2017)
EP14157622, US2013/0052077A2, EP14153898, US2014/177578, EP14161255, US2014/223465

Alchemite™ for drug discovery

Improving compound protein interaction database by a factor of 400, enabling saving experimental costs

	DESCRIPTORS			PROTEINS						
	SlogP	SMR	TPSA	P1	P2	P3	P4	P5	P6	P7
Drug 1	3.6	157	133		**A**			**A**		**I**
Drug 2	4.2	192	102		**A**			**A**		
Drug 3	3.9	110	112						**I**	

Millions of molecules

Thousands of proteins

2,000,000 compounds with 6000 proteins → 12,000,000,000 possible values

Data only 0.05% complete → 6,000,000 values

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Alchemite™ Other applications

Predictive maintenance.

Given a network of assets, we can merge datasets to optimise cleaning schedules, reducing costs and preventing critical failures

Asset	Weather	Geology	Simulation	History

Patient analytics

Use all available data, patient profiles, multiple treatment plans and multiple outcomes, to model and suggest likelihoods of outcomes when specific therapeutic plans are applied to a presenting patient

Patient	History	Treatments	Outcomes