

# The modern day blacksmith

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Neural network algorithm to



**Reduce** development costs

Accelerate materials discovery

Merge simulations, physical laws, and experimental data

**Generic** with **proven** applications in multiple material domains

## A black box





## Train with complete data





## Predict with complete data



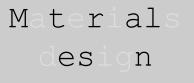


## Train with fragmented data









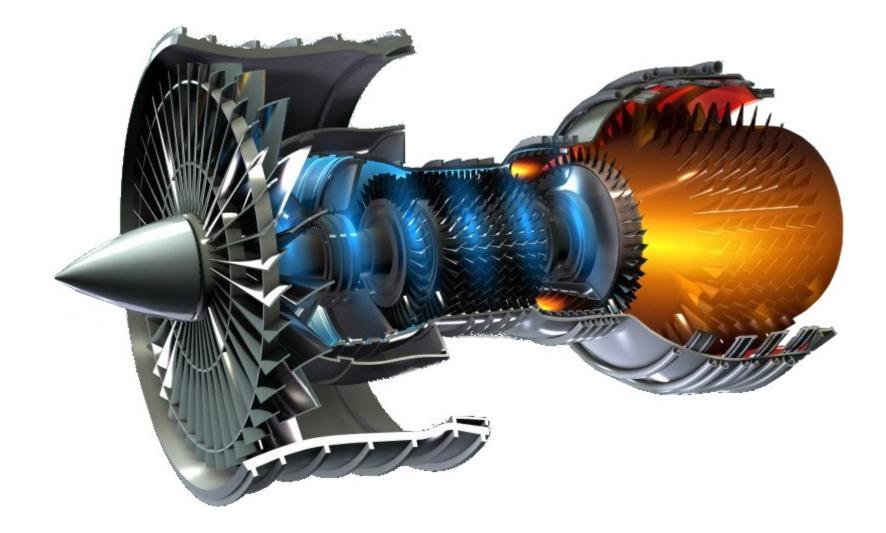
## Predict with fragmented data





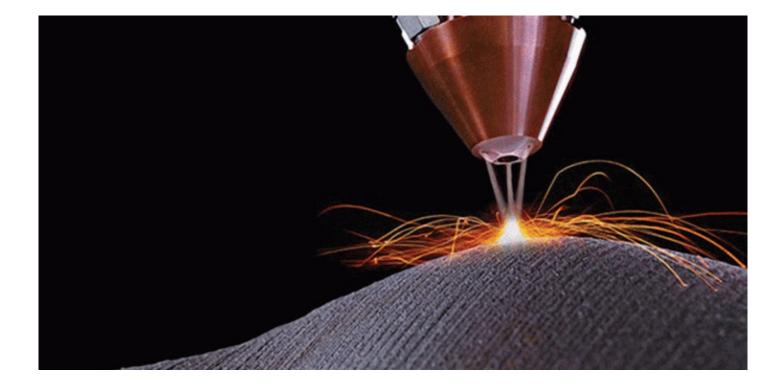
## Schematic of a jet engine





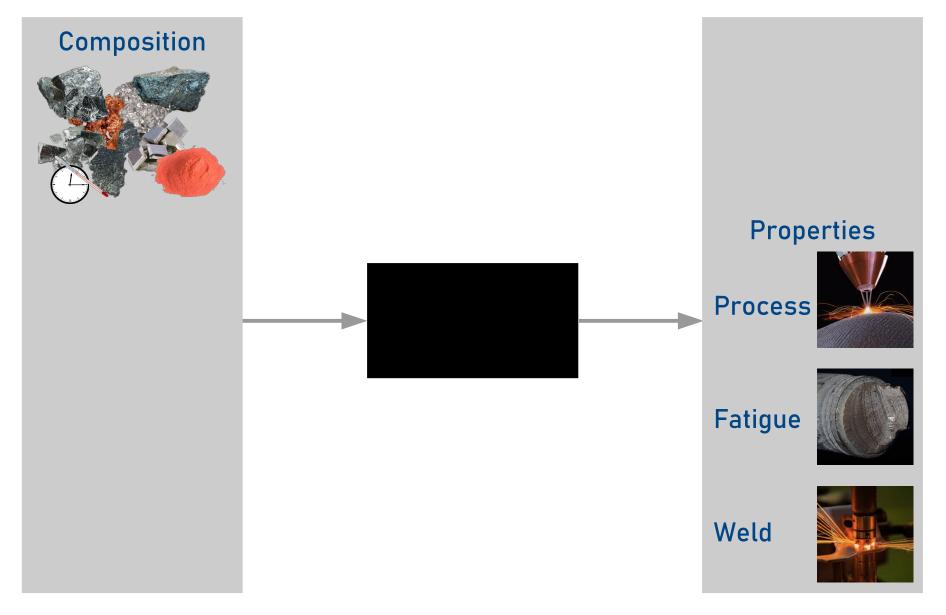
## Direct laser deposition requires new alloys





## Neural network for materials design





## Train the network



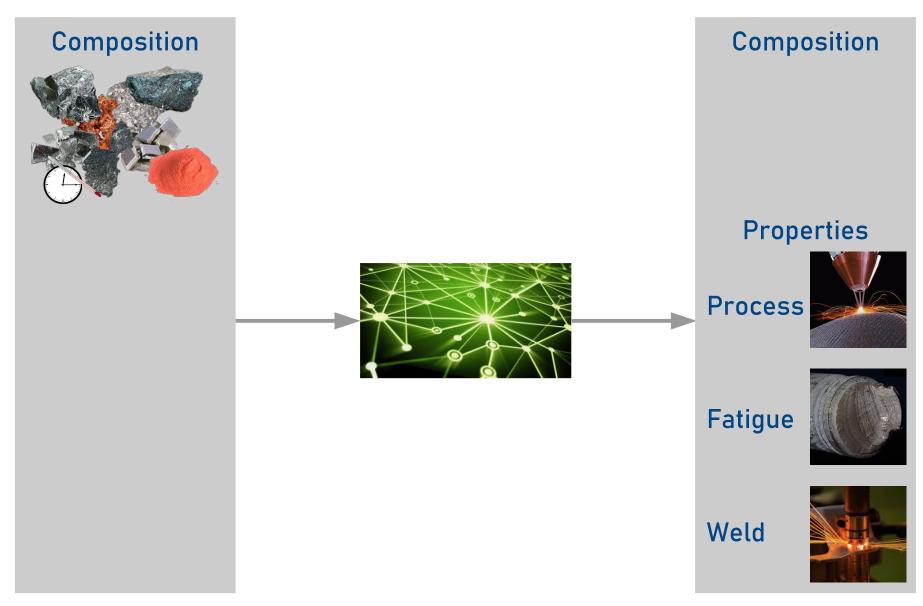




#### Composition

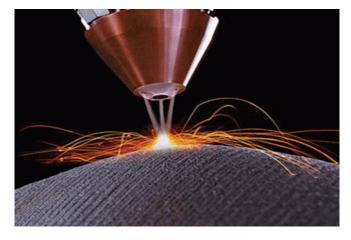
## Predict and design new materials



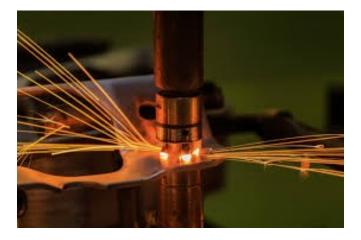


## Direct laser deposition and melting





Laser

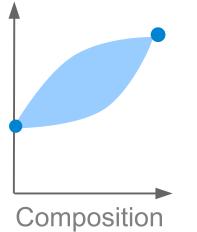


### Electricity

Direct laser deposition is analogous to welding

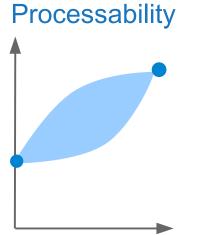




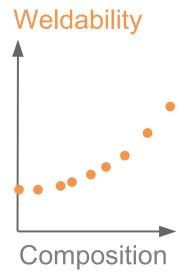


Merge properties with a neural network

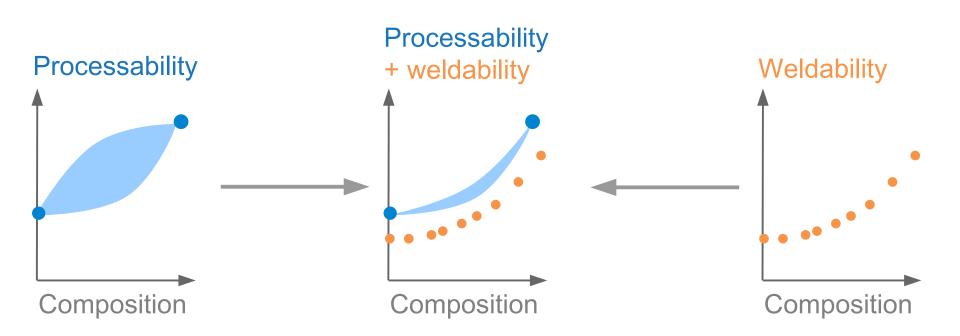




Composition



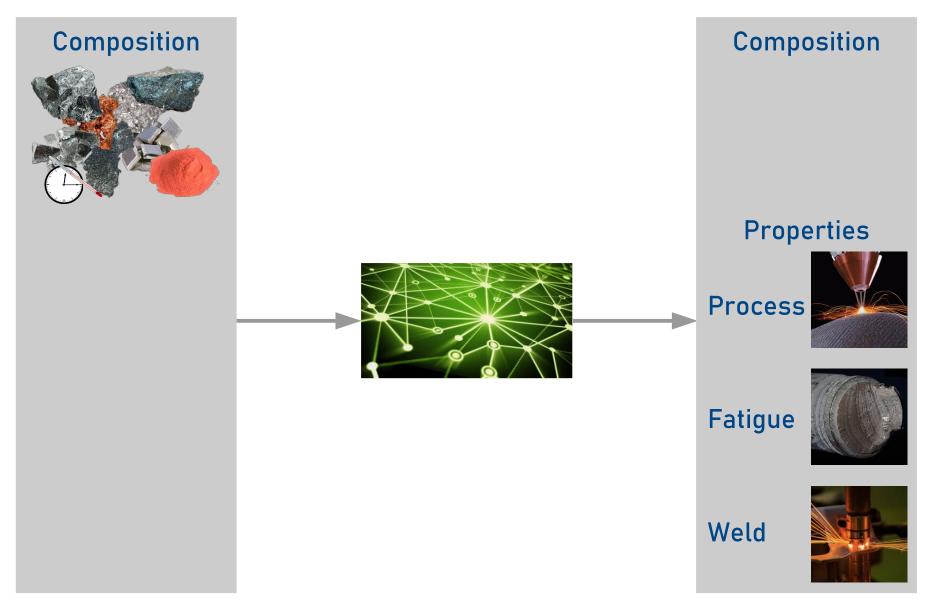
Merge properties with a neural network





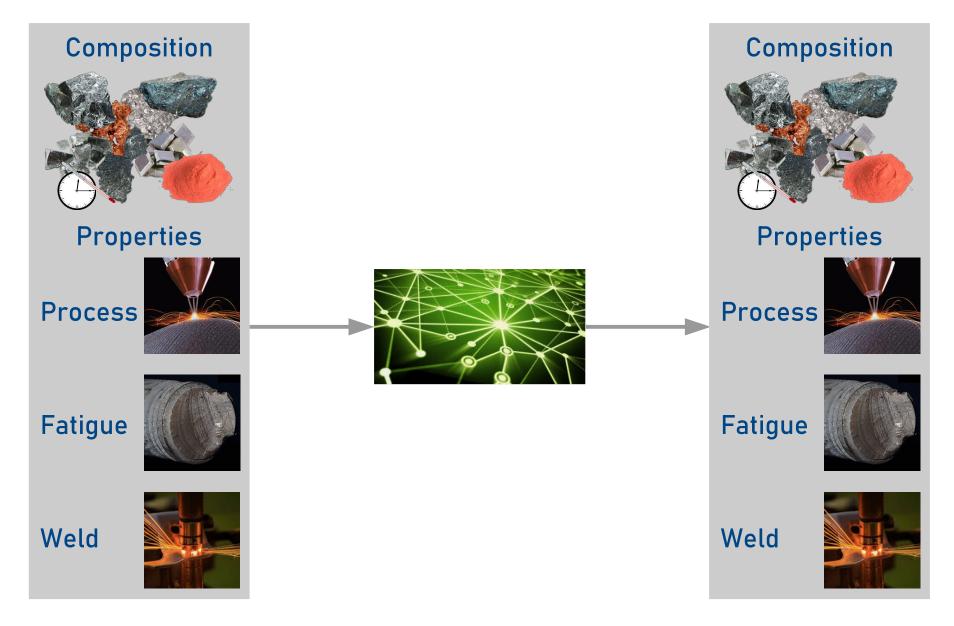
## Standard neural network





## Neural network learns property-property link





## **Target properties**

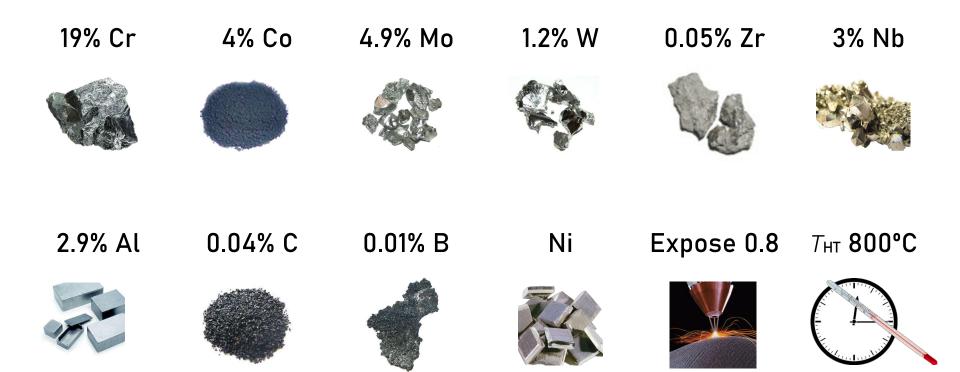


Elemental cost	< 25 \$kg⁻¹
Density	< 8500 kgm⁻³
gamma' content	< 25 wt%
Oxidation resistance	< 0.3 mgcm <sup>-2</sup>
Processability	< 0.15% defects
Phase stability	> 99.0 wt%
gamma' solvus	> 1000°C
Thermal resistance	> 0.04 KΩ⁻¹m⁻³
Yield stress at 900°C	> 200 MPa
Tensile strength at 900°C	> 300 MPa
Tensile elongation at 700°C	> 8%
1000hr stress rupture at 800°C	> 100 MPa

Fatigue life at 500 MPa. 700°C > 10<sup>5</sup> cycles

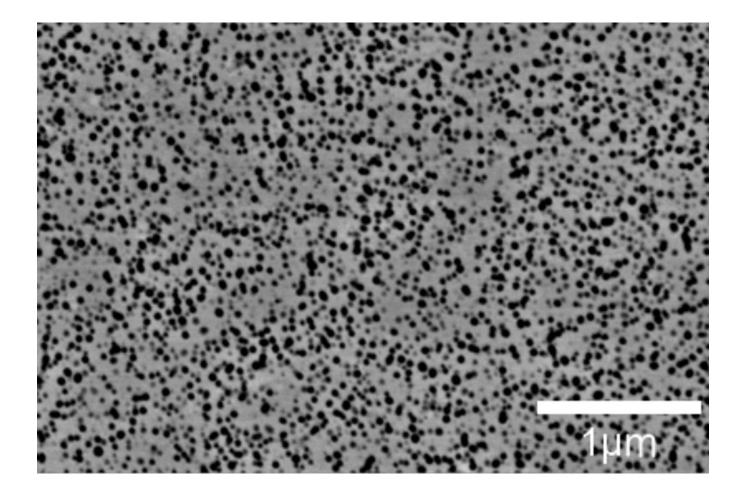
## Material designed





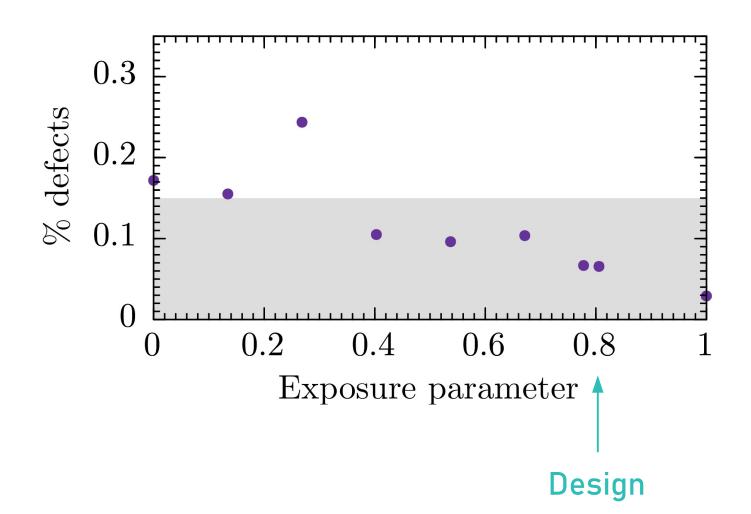
## **Microstructure**



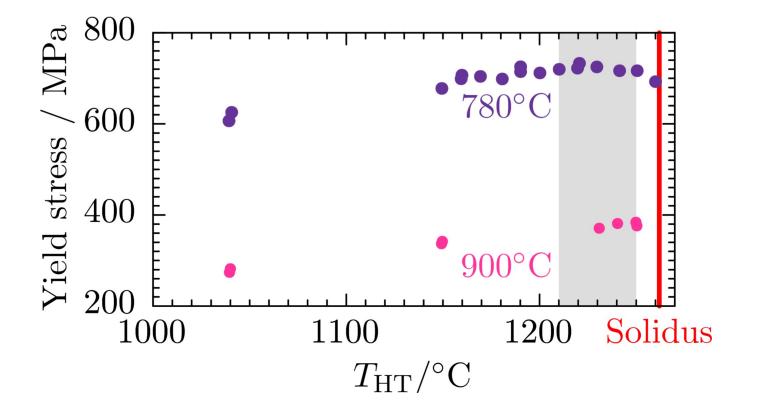


## Testing the processability



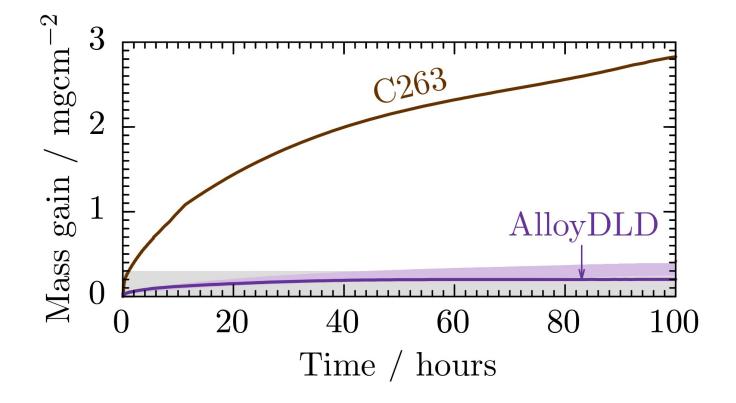


## Verifying the yield stress





## Verifying the oxidation resistance



## Printing a component

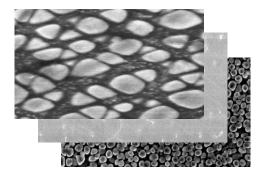




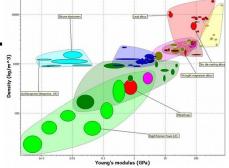
## Materials designed

### Nickel and molybdenum alloys

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



### Identified and corrected errors in material database Computational Materials Science 147, 176 (2018)





## Merging data



Linked the ability for direct laser deposition to weldability

Can also link experimental data to computational simulations

Merge quality with quantity

Materials designed with simulations

Lubricants with experiments and molecular dynamics simulations



Batteries with experiments and Density Functional Theory



## Integrated software by Intellegens



Data load and transform

Train the neural network

Use model to design new materials

neural network model was trained from a library of experimental data from 1000 al     In the first panel below set the percentages of each element in the composition ar     to get the neural network estimates for yield stress, ultimate tensile strength, and     Click here to use this technology to optimize the yield stress, ultimate tensile strength, and     Click here to use this technology to optimize the yield stress, ultimate tensile strength, and     Click here to use this technology to optimize the yield stress, ultimate tensile strength, and     Set inputs     Set inputs     Iron (Fe)   100     Ranganese (Mn)   0     0   0 to 0.43 %     Silicon (Si)   0     0   0 to 17.5 %     Nickel (Ni)   0   0 to 9.67 %     Vanadium (V)   0   0 to 4.32 %
Click here to use this technology to optimize the yield stress, ultimate tensile street This same technology was used to understand nickel alloys where the composition 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 %
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Iron (Fe)     100     remain %     PRE       Carbon (C)     0     0 to 0.43 %     PRE       Manganese (Mn)     0     0 to 3.0 %     Silicon (Si)     0     0 to 4.75 %       Silicon (Si)     0     0 to 17.5 %     Nickel (Ni)     0     0 to 21.0 %       Molybdenum (Mo)     0     0 to 9.67 %     0     0     0
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https://app.intellegens.ai/steel\_search





Designed and experimentally verified alloy for direct laser deposition

**Reduce** development costs

Accelerate materials discovery

Enable **concurrent** materials design



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