intellegens

Machine learning for materials design

Gareth Conduit

Alchemite™ optimized design process

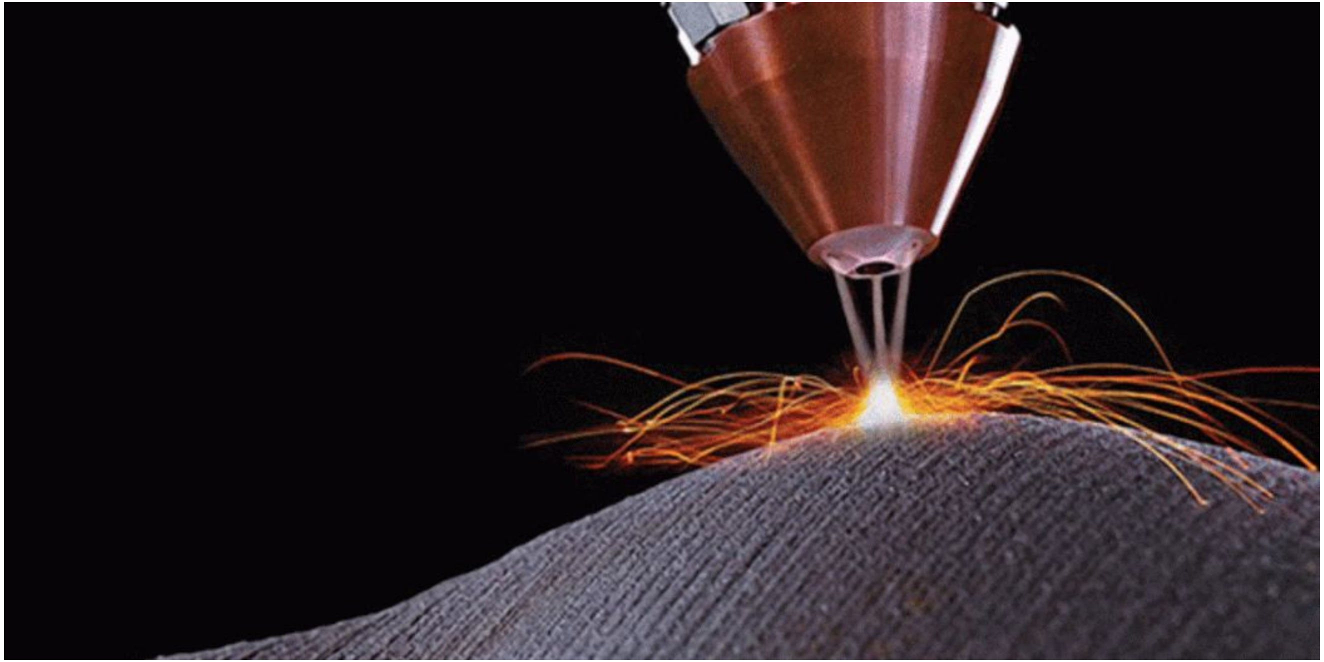
Machine learning software to aid experimental design developed at University of Cambridge, commercialized by Intellegens

Alchemite™ predicts from all **available** inputs

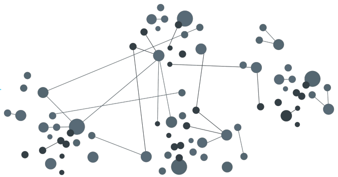
Reduce costs - 90% reduction in experiments and fewer measurements for expensive quantities

Accelerate discovery and validation to 2 years

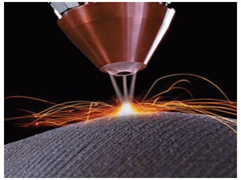
Additive manufacturing requires new alloys



Machine learning



Processability



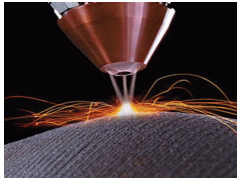
Fatigue life

Cost

Machine learning

Machine learning

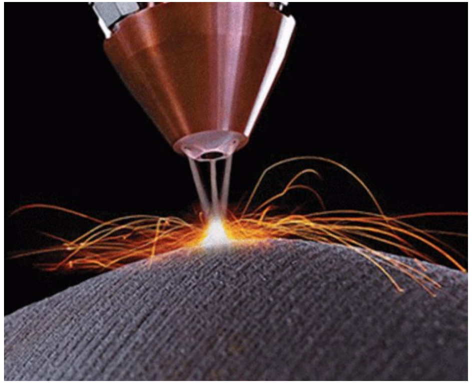
Processability



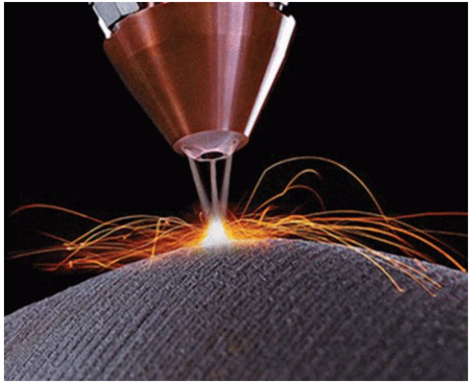
Fatigue life

Cost

Case study: alloy for direct laser deposition



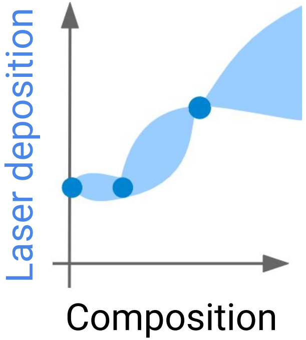
Direct laser deposition is similar to welding



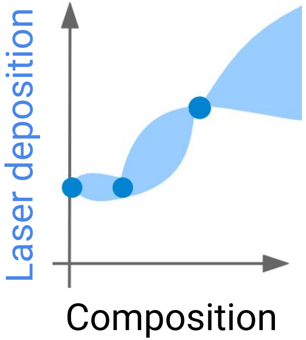
Direct laser deposition

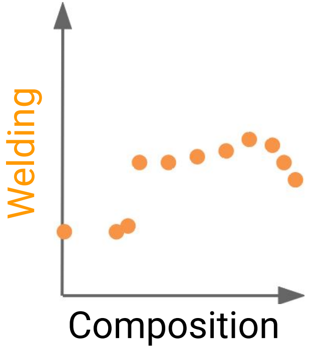
Welding

Lack of data for laser deposition

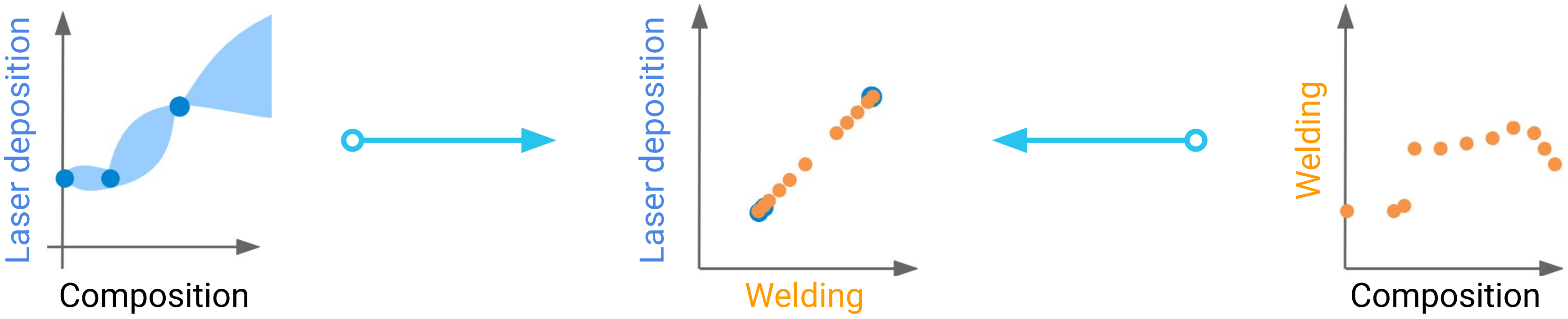


Large amount of welding data

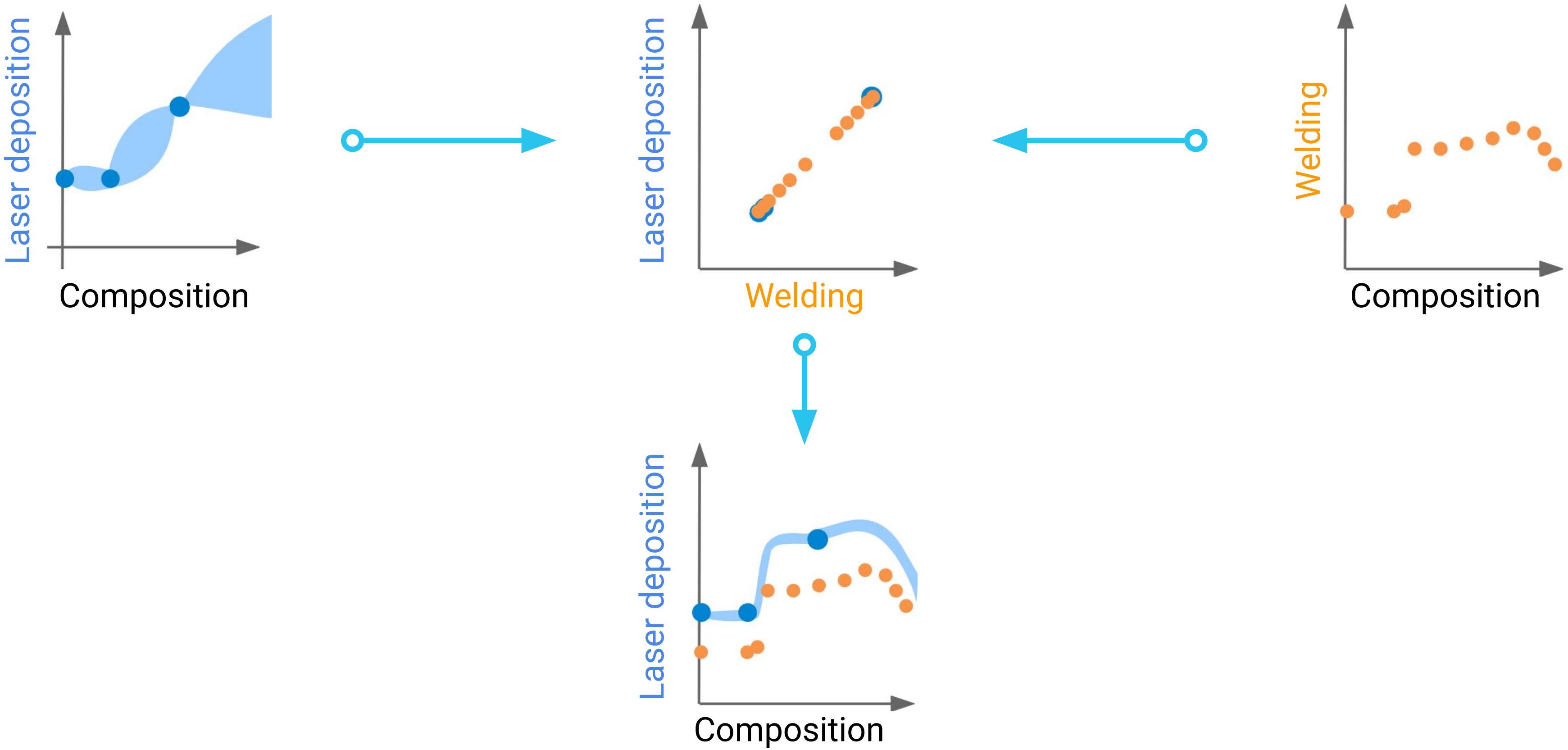




Simple welding-deposition relationship



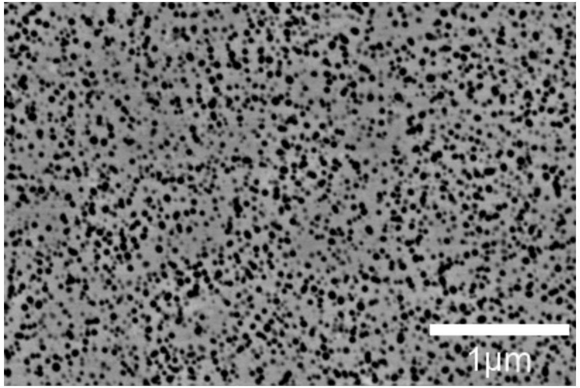
Welding data guides extrapolation



Targets for direct laser deposition alloy

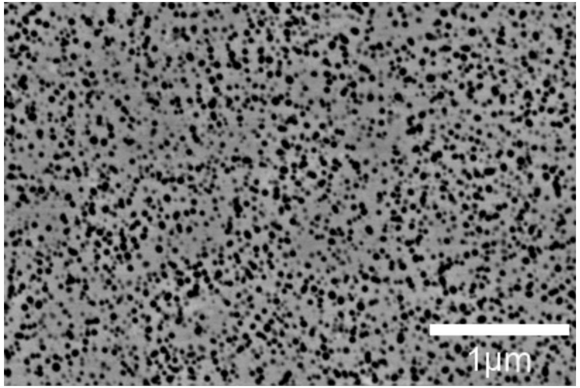
Elemental cost	$< 25\ \$\mathrm{kg}^{-1}$
Density	$< 8500\ \mathrm{kgm}^{-3}$
γ’ content	< 25 wt%
Oxidation resistance	$< 0.3\ \mathrm{mgcm}^{-2}$
Processability	$< 0.15\%$ defects
Phase stability	> 99.0 wt%
γ’ solvus	$> 1000^{\circ}\mathrm{C}$
Thermal resistance	$> 0.04\ \mathrm{K}\Omega^{-1}\mathrm{m}^{-3}$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

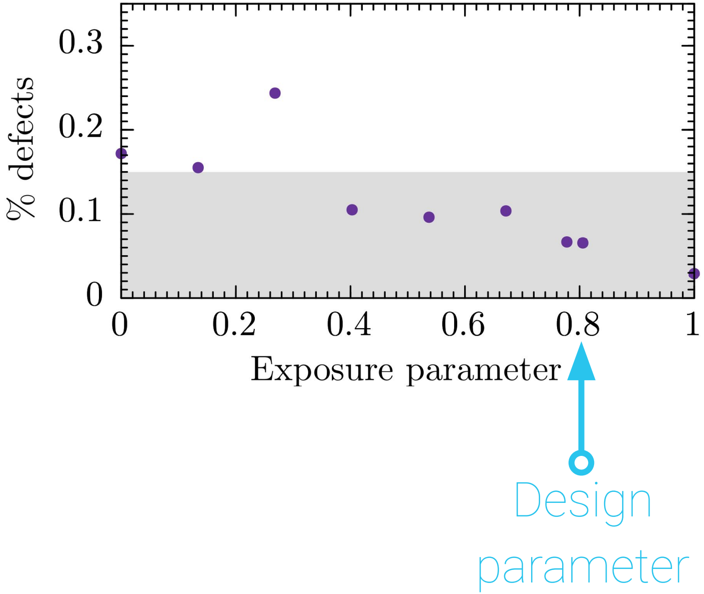
Experimental validation: microstructure



Materials & Design 168, 107644 (2019)

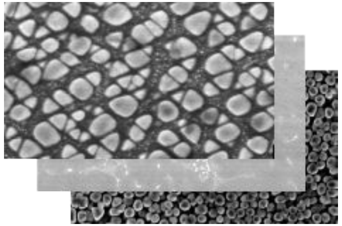
Experimental validation: defects





Materials & Design 168, 107644 (2019)

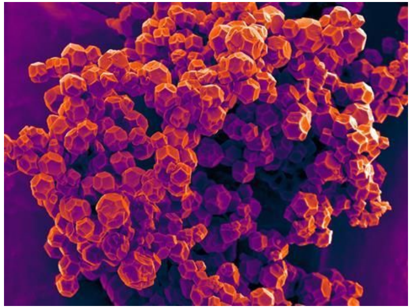
Further materials and drug design



Nickel & moly alloys

Batteries

Steels for welding



Metal-organic framework

Concrete

Drug design

OPTiMaDe, an API for materials data

OPTiMaDe consortium developed **common API** to access electronic structure databases: AFLOW, COD, TCOD, Materials Cloud, Materials Mine, MPDS, Materials Project, NoMaD, Open Materials Database, OQMD

Funding from CECAM to extend to **molecular dynamics** data

Next workshop at CECAM: 8-12 June 2020

https://www.optimade.org/

Interest in technical committee

Curation, dissemination, and exploitation of materials data

Knowledge of application of machine learning to materials data

Contact	gareth@intellegens.ai
Website	https://intellegens.ai
Demo	https://app.intellegens.ai/steel_optimise
Papers	https://intellegens.ai/article-type/papers/