Advanced material design using deep learning
**Alchemite™ optimized design process**

Machine learning software to aid experimental design developed at University of Cambridge

Alchemite™ predicts from *available* inputs

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

**Accelerate** discovery and validation to 2 years
Case study: alloy for direct laser deposition
Case study: additive manufacturing
Additive manufacturing requires new alloys
Machine learning

Processability

Fatigue life

Cost
Machine learning

Processability

Fatigue life

Cost
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

<table>
<thead>
<tr>
<th>Property</th>
<th>Target Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elemental cost</td>
<td>&lt; 25 $kg(^{-1})</td>
</tr>
<tr>
<td>Density</td>
<td>&lt; 8500 kgm(^{-3})</td>
</tr>
<tr>
<td>(\gamma)' content</td>
<td>&lt; 25 wt%</td>
</tr>
<tr>
<td>Oxidation resistance</td>
<td>&lt; 0.3 mgcm(^{-2})</td>
</tr>
<tr>
<td>Processability</td>
<td>&lt; 0.15% defects</td>
</tr>
<tr>
<td>Phase stability</td>
<td>&gt; 99.0 wt%</td>
</tr>
<tr>
<td>(\gamma)' solvus</td>
<td>&gt; 1000 °C</td>
</tr>
<tr>
<td>Thermal resistance</td>
<td>&gt; 0.04 KΩ(^{-1})m(^{-3})</td>
</tr>
<tr>
<td>Yield stress at 900 °C</td>
<td>&gt; 200 MPa</td>
</tr>
<tr>
<td>Tensile strength at 900 °C</td>
<td>&gt; 300 MPa</td>
</tr>
<tr>
<td>Tensile elongation at 700 °C</td>
<td>&gt; 8%</td>
</tr>
<tr>
<td>1000hr stress rupture at 800 °C</td>
<td>&gt; 100 MPa</td>
</tr>
<tr>
<td>Fatigue life at 500 MPa, 700 °C</td>
<td>&gt; 10(^5) cycles</td>
</tr>
</tbody>
</table>
Composition of alloy for direct laser deposition

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^\circ C
Experimental validation: microstructure
Experimental validation: defects

Experimental validation: oxidation resistance

Further materials and drug design

- Nickel & moly alloys
- Batteries
- Steels for welding
- Metal-organic framework
- Concrete
- Drug design
Future opportunities: Integrated software

1. Load data
2. Training
3. Predict & design
Summary of future opportunities of Alchemite™

Alchemite™, a full stack machine learning solution to merge sparse data

Designed and experimentally verified material for thermometry, and other alloys and drugs

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Papers  https://www.intellegens.ai/paper.html