The modern-day blacksmith

Bryce Conduit, Trevor Illston, Divya Vadegadde Duggappa, Scarlett Baker, Stephen Harding, Howard Stone & Gareth Conduit

Theory of Condensed Matter group
Neural network algorithm to

Train from **sparse** datasets

**Merge** simulations, physical laws, and experimental data

**Reduce** the need for expensive experimental development

**Accelerate** materials 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

Composition

Properties
  Process
  Fatigue
  Welding
Neural networks for materials design

Composition

Properties

Process

Fatigue

Welding
Neural networks for materials design

Composition

Properties
- Process
- Fatigue
- Welding
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
Neural networks for materials design

Composition

Properties
- Process
- Fatigue
- Welding
Neural networks for materials design

Composition

Properties

Process

Fatigue

Welding

Composition

Properties

Process

Fatigue

Welding
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: $>1000^\circ C$
- Thermal resistance: $>0.04 KΩ^{−1}m^{−3}$
- Yield stress at $900^\circ C$: $>200 MPa$
- Tensile strength at $900^\circ C$: $>300 MPa$
- Tensile elongation at $700^\circ C$: $>8\%$
- 1000hr stress rupture at $800^\circ C$: $>100 MPa$
- Fatigue life at $500 MPa$, $700^\circ C$: $>10^5$ cycles
# Composition

<table>
<thead>
<tr>
<th>Element</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cr</td>
<td>19%</td>
</tr>
<tr>
<td>Co</td>
<td>4%</td>
</tr>
<tr>
<td>Mo</td>
<td>4.9%</td>
</tr>
<tr>
<td>W</td>
<td>1.2%</td>
</tr>
<tr>
<td>Zr</td>
<td>0.05%</td>
</tr>
<tr>
<td>Nb</td>
<td>3%</td>
</tr>
<tr>
<td>Al</td>
<td>2.9%</td>
</tr>
<tr>
<td>C</td>
<td>0.04%</td>
</tr>
<tr>
<td>B</td>
<td>0.01%</td>
</tr>
<tr>
<td>Ni</td>
<td></td>
</tr>
<tr>
<td>Expose</td>
<td>0.8</td>
</tr>
<tr>
<td>$T_{HT}$</td>
<td>1230°C</td>
</tr>
</tbody>
</table>
Microstructure
Testing the processability

% defects

Exposure parameter

Design parameter
Testing the yield stress

![Graph showing yield stress versus HT temperature](image)

- **Yield stress / MPa**
- **$T_{HT}/^\circ C$**

Markers at 780°C and 900°C highlight specific points of interest.

**Solidus**

**Design parameter**
Testing the oxidation resistance

![Graph showing mass gain over time for C263 and AlloyDLD. The graph indicates that C263 has a higher mass gain compared to AlloyDLD, suggesting lower oxidation resistance for C263.]
Materials designed

Nickel and molybdenum

Experiment and DFT for batteries

Steel for welding
More materials

Quantum and experiment for thermometry

Lubricants with molecular dynamics and experiments

Drug design
Summary

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

Designed and experimentally verified alloy for direct laser deposition

Apply technology to other materials and drug design

Commercialized by startup Intellegens