Concurrent materials design

Gareth Conduit

Patent GB1302743.8 (2013)
Patent GB1307533.8 (2013)
Patent GB1307535.3 (2013)
Acta Materialia, 61, 3378 (2013)
Intermetallics, advanced online publication (2013)

Theory of Condensed Matter Group, Department of Physics
Four new tools

- Experimental databases
- Physically based
- Computational
- Materials characterization
Four new tools

- Experimental databases
- Neural network fitting
- Physically based
- Computational
- Recursive learning
- Property correlations
- Materials optimization
Neural network fitting & optimization

Yield stress

Aluminium

Target
Recursive learning

1. Calculate material property
2. Generate neural network models
3. Search for optimal solution

![Graph showing Recursive learning process with Aluminium and Precipitate axes]
Recursive learning

- Calculate material property
- Generate neural network models
- Search for optimal solution

Precipitate

Target

Aluminium
Probability

Probability of alloy satisfying all properties

Yield stress
Cycle fatigue
Cost
Oxidation resistance

Patent GB1302743.8 (2013)
<table>
<thead>
<tr>
<th>Property</th>
<th>Method</th>
<th>Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost</td>
<td>Physically based</td>
<td></td>
</tr>
<tr>
<td>Density</td>
<td>Physically based</td>
<td></td>
</tr>
<tr>
<td>Precipitate content</td>
<td>CALPHAD (Thermocalc)</td>
<td></td>
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<tr>
<td>Phase stability</td>
<td>CALPHAD (Thermocalc)</td>
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</tr>
<tr>
<td>Solvus temperature</td>
<td>CALPHAD (Thermocalc)</td>
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<tr>
<td>Yield stress</td>
<td>Neural net over database</td>
<td>6939</td>
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<tr>
<td>Ultimate tensile strength</td>
<td>Neural net over database</td>
<td>6127</td>
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<tr>
<td>300hr stress rupture</td>
<td>Neural net over database</td>
<td>10860</td>
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<tr>
<td>Cr activity (oxidation resis.)</td>
<td>Neural net over database</td>
<td>915</td>
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<tr>
<td>Tensile elongation</td>
<td>Neural net over database</td>
<td>2248</td>
</tr>
<tr>
<td>Fatigue life</td>
<td>Neural net over database</td>
<td>15105</td>
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Ni-base superalloy

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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<tbody>
<tr>
<td>Cost</td>
<td>32.1 $/lb^{-1}</td>
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<tr>
<td>Density</td>
<td>8240 kg/m^{-3}</td>
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<tr>
<td>Precipitate content</td>
<td>48 %</td>
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<tr>
<td>Phase stability</td>
<td>99.5 %</td>
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<td>Solvus temperature</td>
<td>1080 °C</td>
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<tr>
<td>Yield stress</td>
<td>1070 MPa</td>
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<tr>
<td>Ultimate tensile strength</td>
<td>1438 MPa</td>
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<tr>
<td>300hr stress rupture</td>
<td>980 MPa</td>
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<tr>
<td>Cr activity (oxidation resis.)</td>
<td>0.157</td>
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<tr>
<td>Tensile elongation</td>
<td>15.2 %</td>
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<td>Fatigue life</td>
<td>$10^{5.2}$</td>
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</tbody>
</table>
Ni-base superalloy

Amendment to patent US 2013/0052077 A1 (2013)
Mo-base alloy

Patents GB1307533.8 (2013), GB1307535.3 (2013)
Correlations between properties

Data for Al-Mg-Si alloy from Mat. Sci and Engin. A 443, 172 (2007)
Correlations between properties

Alloy for direct laser deposition

10 points for quality of deposition

Weldability, thermal conductivity, thermal expansivity, precipitate fraction

Property correlations
Semiconductors

- Band structure: band gap, density of states, effective mass
- 100 points for band gap, luminous efficacy, efficiency
- Property correlations

Band structure: band gap, density of states, effective mass
Four new tools

- Experimental databases
- Neural network fitting
- Physically based
- Recursive learning
- Property correlations

Ni-based alloy
US 2013/0052077 A1
Mo-Hf: GB1307533.8
Mo-Nb: GB1307535.3
Ni-based alloy for direct laser deposition
InGaN-based LED
Prospects in the future

Include other experimental & computational databases

Combine further first principles approaches: DFT, molecular dynamics, phase field models

Conformance testing, retirement-for-cause

Concurrent materials design
Mo-base alloy

Mo rich → Hf rich

UTS / MPa

Cost per cycle / $