Concurrent materials design

Gareth Conduit
Trapped atoms

Theory

P.O. Bugnion, J. Lofthouse & GJC, PRL 111, 045301 (2013)
P.O. Bugnion & GJC, PRA 87, 060502(R) (2013)

Experiment

Electron gas

Theory

Experiment
S. Lausberg et al. PRL 109, 216402 (2012)
Huxley group, in preparation (2013)
Concurrent materials design
Phase equilibrium
Properties: $\gamma'$ fraction

Calculate grid of

$$F_{(\gamma, \gamma')}(n_{ni}, n_{Al}, n_{Cr}, n_{Co}, n_{Mo}, n_{Ti})$$
Calculate grid of

\[ F_{(\gamma, \gamma')} (n_{\text{ni}}, n_{\text{Al}}, n_{\text{Cr}}, n_{\text{Co}}, n_{\text{Mo}}, n_{\text{Ti}}) \]

generate neural network model and uncertainty
Properties: $\gamma'$ fraction

Calculate grid of

$$F_{(\gamma, \gamma')}(n_{ni}, n_{Al}, n_{Cr}, n_{Co}, n_{Mo}, n_{Ti})$$

Generate neural network model and uncertainty

Calculate phase equilibrium and uncertainty
Calculate grid of $F_{(\gamma, \gamma')} (n_{ni}, n_{Al}, n_{Cr}, n_{Co}, n_{Mo}, n_{Ti})$

Generate neural network model and uncertainty

Calculate phase equilibrium and uncertainty

Large uncertainty
Designing a new material – what is required?

- Cost
- Density
- Fatigue
- Creep
- Oxidation
- Corrosion
- Processibility
- Conductivity
- Weldability
- Yield
- Stability
- Cost
- Density
- Fatigue
- Creep
- Oxidation
- Corrosion
- Processibility
- Conductivity
- Weldability
- Yield
- Stability

Overall probability
Concurrent materials design

Disc alloy
Case study: RR1000

<table>
<thead>
<tr>
<th>Element</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Ni</td>
<td>52</td>
</tr>
<tr>
<td>Cr</td>
<td>15</td>
</tr>
<tr>
<td>Co</td>
<td>19</td>
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<tr>
<td>Mo</td>
<td>5</td>
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<tr>
<td>Ti</td>
<td>3.6</td>
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<tr>
<td>Al</td>
<td>3</td>
</tr>
<tr>
<td>Ta</td>
<td>2</td>
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<tr>
<td>Hf</td>
<td>0.5</td>
</tr>
<tr>
<td>C</td>
<td>0.1</td>
</tr>
<tr>
<td>T</td>
<td>800</td>
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<tr>
<td>t</td>
<td>8</td>
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Case study: improved disc alloy

<table>
<thead>
<tr>
<th>Element</th>
<th>%</th>
<th></th>
<th>Element</th>
<th>%</th>
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<th>Element</th>
<th>%</th>
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<tbody>
<tr>
<td>Ni</td>
<td>56</td>
<td></td>
<td>Cr</td>
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<td>Mo</td>
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<td>C</td>
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<td>T</td>
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<tr>
<td>W</td>
<td>6.0</td>
<td></td>
<td>Mn</td>
<td>0.1</td>
<td></td>
<td>B</td>
<td>0.1</td>
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<tr>
<td>Zr</td>
<td>0.2</td>
<td></td>
<td>Nb</td>
<td>5.6</td>
<td></td>
<td>Fe</td>
<td>3.4</td>
</tr>
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</table>

The table shows the weight percent of various elements in the improved disc alloy.
<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost</td>
<td>11.7 $/lb$^{-1}</td>
</tr>
<tr>
<td>Density</td>
<td>8.3 g/cm$^3$</td>
</tr>
<tr>
<td>Resistivity</td>
<td>8.9 $\mu\Omega$cm</td>
</tr>
<tr>
<td>$\gamma'$ precipitate</td>
<td>40 %</td>
</tr>
<tr>
<td>Phase stability</td>
<td>99 %</td>
</tr>
<tr>
<td>Solvus</td>
<td>1095°C</td>
</tr>
<tr>
<td>Yield stress</td>
<td>1049 MPa</td>
</tr>
<tr>
<td>UTS</td>
<td>1437 MPa</td>
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<tr>
<td>Stress rupture</td>
<td>593 hr</td>
</tr>
<tr>
<td>Low cycle fatigue</td>
<td>$10^{5.2}$</td>
</tr>
<tr>
<td>Elongation</td>
<td>15.2</td>
</tr>
<tr>
<td>Weldability</td>
<td>8.0 %</td>
</tr>
<tr>
<td>Oxidation</td>
<td>20</td>
</tr>
</tbody>
</table>
Electron micrograph
Yield stress

![Graph showing yield stress vs temperature.](image-url)
Yield stress

![Graph showing yield stress vs temperature](image-url)
Yield stress

![Graph showing yield stress vs temperature]
Oxidation

![Graph showing mass gain over time for RR1000 material.](image-url)
Oxidation

The graph illustrates the mass gain per square centimeter as a function of time in hours. Two curves are shown: one for RR1000 and another for Ni disc alloy. The mass gain is plotted on the y-axis, while time is shown on the x-axis. The RR1000 curve is represented by a green line, and the Ni disc alloy curve is shown in black with a shaded area to indicate variability or uncertainty.
Oxidation

![Graph showing oxidation mass gain over time for RR1000 and Ni disc alloy.](#)
Case study: improved disc alloy

- Cost: 11.7 $/lb⁻¹
- Density: 8.3 g/cm³
- Resistivity: 8.9 μΩ/cm
- γ' precipitate: 40%
- Phase stability: 99%
- Solvus: 1095°C
- Yield stress: 1049 MPa
- UTS: 1437 MPa
- Stress rupture: 593 hr
- Low cycle fatigue: $10^{5.2}$
- Elongation: 15.2%
- Weldability: 8.0%
- Oxidation: 20
Heat treatments

Reduce $P$ and $T$

$\alpha + \beta$ $\omega + \beta$
Heat treatments

- Reduce $T$
- Reduce $P$

Diagram showing the effect of temperature ($T$) and pressure ($P$) on the phases $\alpha + \beta$, $\beta$, $\omega + \beta$, and $\beta$. The diagrams illustrate the phase transformations under different conditions.
Concurrent materials design

Few atoms in a trap

Electron gas

Concurrent materials design