Computer driven materials discovery

Gareth Conduit

Patent GB1302743.8 (2013)
Patent GB1307533.8 (2013)
Acta Materialia, 61, 3378 (2013)
Rolls-Royce Group plc invention submission NC12261 (2012)
Rolls-Royce Group plc invention submission NC13006 (2013)
Rolls-Royce Group plc invention submission NC13024 (2013)

TCM Group, Department of Physics
### Designing a new alloy – what is required?

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost</td>
<td>11.7 $lb^{-1}</td>
</tr>
<tr>
<td>Density</td>
<td>8.3 gcm$^{-3}$</td>
</tr>
<tr>
<td>Resistivity</td>
<td>8.9 $\mu\Omega$cm</td>
</tr>
<tr>
<td>$\gamma'$ fraction</td>
<td>40%</td>
</tr>
<tr>
<td>Stability</td>
<td>93%</td>
</tr>
<tr>
<td>Yield stress</td>
<td>1049 MPa</td>
</tr>
<tr>
<td>UTS</td>
<td>1437 MPa</td>
</tr>
<tr>
<td>Oxidation index</td>
<td>20</td>
</tr>
<tr>
<td>Stress rupture</td>
<td>1138 MPa</td>
</tr>
<tr>
<td>Entropy</td>
<td>14.5 Jmol$^{-1}$K$^{-1}$</td>
</tr>
</tbody>
</table>
Steps to commercialize

Composition (wt%) & variables
- Cr: 15.33
- W: 6.00
- Al: 4.26
- Mn: 0.00
- B: 0.22
- N: 0.00
- Hf: 0.00
- Co: 8.43
- Ta: 0.06
- Ti: 3.37
- Si: 1.08
- Zr: 0.09
- P: 0.00
- Ni: 52.70
- Mo: 1.88
- Nb: 1.99
- Fe: 4.25
- C: 0.00
- Cu: 0.00
- V: 0.36
- HT1Temp C: 14.32
- HT1time hr: 50.00
- HT2Temp C: 1156.67
- HT2time hr: 63.38

Properties
- Cost $/lb: 14.96
- Density g/cm3: 7.94
- Stress Rupture MPa: 1163.81
- UTS MPa: 1859.41
- Yield Stress MPa: 1372.94
- Gamma' fraction: 40.74
- Gamma + Gamma' fract: 98.12
- Resistivity uOhm cm: 8.96
- Oxidation index: 16.56
- Entropy J/molk: 13.04
- Probability of success: 0.974
Steps to commercialize
Benefits – materials selection
Benefits – materials selection
Benefits – materials selection

65Be-32Al-1Si-2Ag, Starmet Corp.
Benefits – materials characterization
Alloys designed

**Mo-Hf forging alloy**
Patent GB1307533.8 (2013)

**Ni disc alloy**
Rolls-Royce invention
NC12261 (2012)

**Mo-Nb forging alloy**
Rolls-Royce invention
NC13024 (2013)

**RR1000 grain growth**
Acta Materialia, 61, 3378 (2013)

**Ni combustor liner**
Rolls-Royce invention
NC13006 (2013)

**High entropy alloy**
Intellectual property

• “A system for the characterisation and optimisation of alloys”, Patent GB1302743.8 (2013)
• Reduce likelihood of patent infringement by not distributing source code, only compiled program when sold
Initial markets & business model

- Sell through existing materials suite – paid per sale / fixed total price
- Approach companies that make materials – paid per discovery / code
- Offer materials optimization service – paid per discovery
Designing a new alloy – what is required?

- Ni superalloy: Rolls-Royce Group plc invention submission NC12261 (2012)
- Ni combustor: Rolls-Royce Group plc invention submission NC13006 (2013)
- Mo-Nb forging: Rolls-Royce Group plc invention submission NC13024 (2013)
### SWOT matrix

<table>
<thead>
<tr>
<th>S</th>
<th>W</th>
</tr>
</thead>
</table>
| Study and discover new materials  
Account for heat treatments  
Rapid calculation & optimization | Require pre-existing experimental data  
Uncertainty in results |
| Demand for new materials  
Rise of eco-materials  
Genome Initiative | Development of a complete and rapid first principles calculation  
Patent theft |
## Business plan

<table>
<thead>
<tr>
<th></th>
<th>Year 1</th>
<th>Year 2</th>
<th>Year 3</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Revenue</strong></td>
<td>60000</td>
<td>100000</td>
<td>140000</td>
</tr>
<tr>
<td><strong>Gross margin</strong></td>
<td>54000</td>
<td>90000</td>
<td>126000</td>
</tr>
<tr>
<td><strong>Net profit</strong></td>
<td>10400</td>
<td>29600</td>
<td>48800</td>
</tr>
<tr>
<td><strong>License via suite</strong></td>
<td>0 %</td>
<td>30 %</td>
<td>50 %</td>
</tr>
<tr>
<td><strong>Optimization service</strong></td>
<td>50 %</td>
<td>30 %</td>
<td>20 %</td>
</tr>
<tr>
<td><strong>Direct sales</strong></td>
<td>50 %</td>
<td>40 %</td>
<td>30 %</td>
</tr>
</tbody>
</table>
Selected industries

- Materials producers
- Government & academic research
- Pharmaceutical & chemical
- Aerospace & defense
- Energy & nuclear
- Automotive
- Electronics
- Industrial & consumer
- Oil & Gas
- Education

£170 bn