

# Computer driven materials discovery

## Gareth Conduit

Patent GB1302743.8 (2013)

Patent GB1307533.8 (2013)

Acta Materialia, **61**, 3378 (2013)

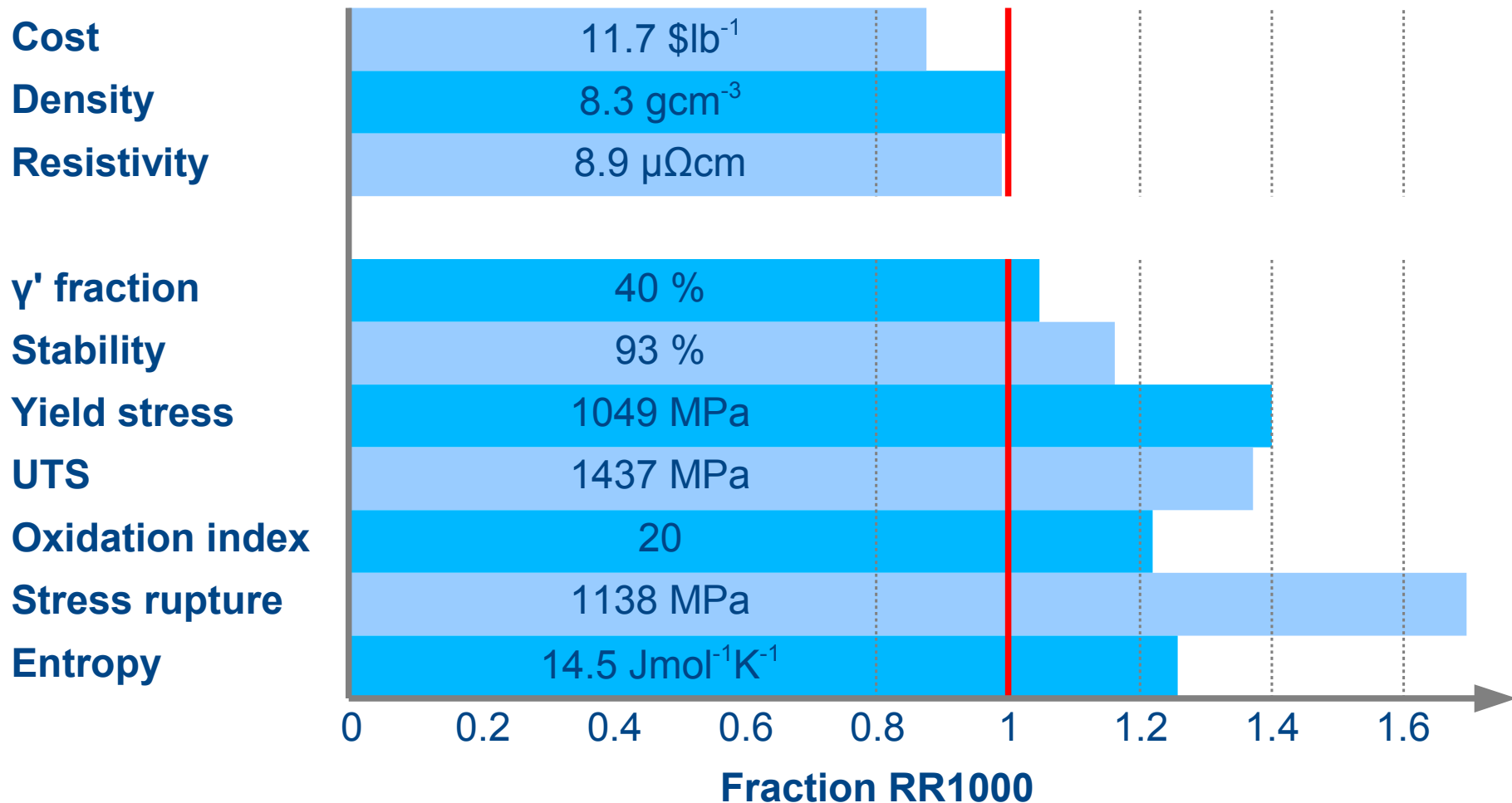
Rolls-Royce Group plc invention submission NC12261 (2012)

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 ?



# Steps to commercialize

The screenshot shows a gedit editor window with two panes. The left pane displays a list of material properties with their units and values. The right pane displays the composition (wt%) and variables for the material, along with a comparison of current values against target values and a probability of success.

Property	Unit	Value
Cost \$/lb	T F -1	15.0
Density g/cm3	T F -1	8.000
Stress Rupture MPa	T F 1	750.0
UTS MPa	T F 1	1700.0
Yield Stress MPa	T F 1	1050.0
Gamma' fraction	T F 1	35.
Gamma + Gamma' fract	T F 1	95.0
Resistivity uOhm cm	T F -1	9.0
Oxidation index	T F 1	16.5
Entropy J/molK	T F 1	13.0
alpha UTS MPa	F F 1	830.0

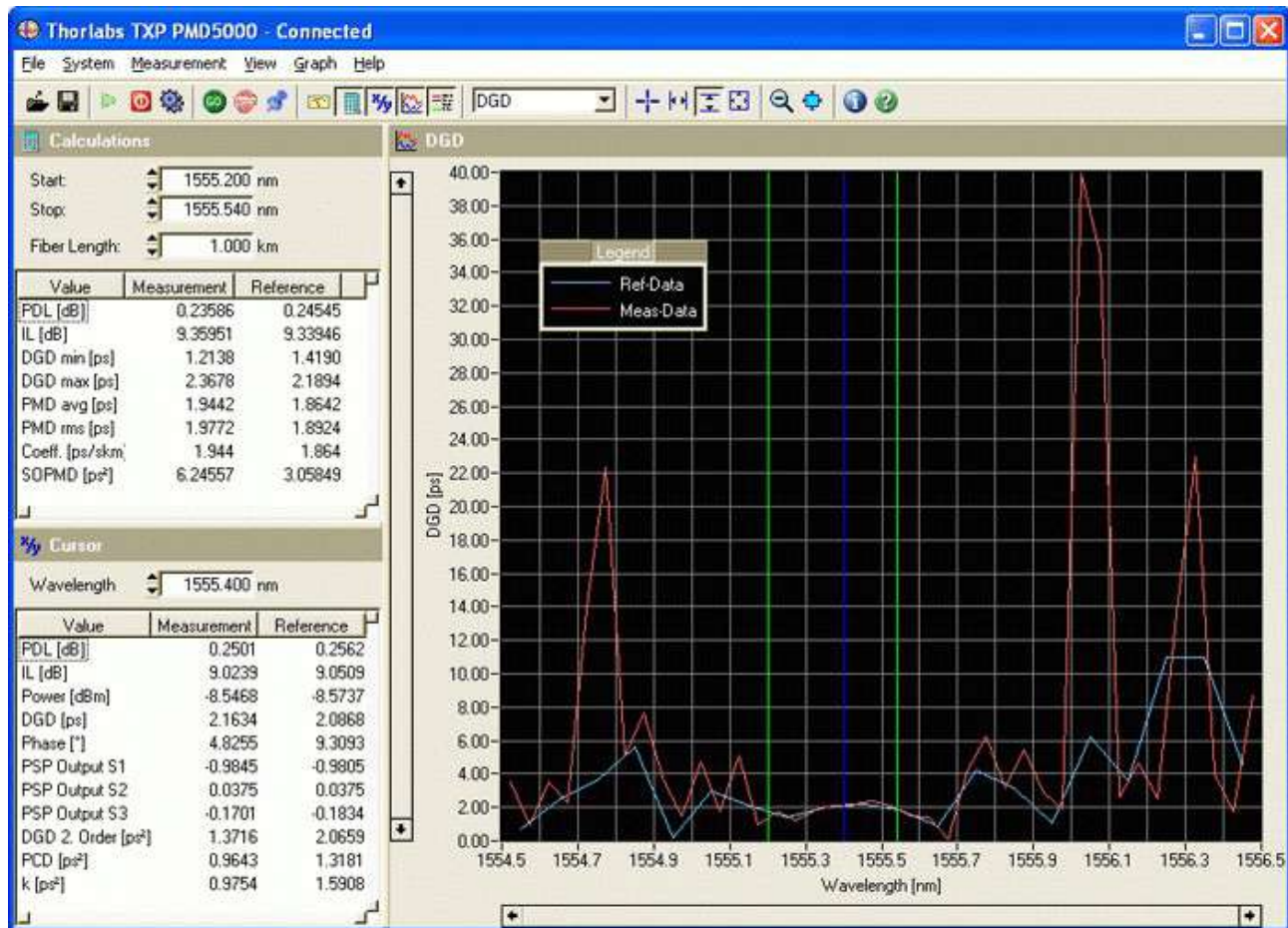
  

Element	Value	Element	Value	Element	Value
Cr	15.33	Co	8.43	Mo	1.88
W	6.00	Ta	0.06	Nb	1.99
Al	4.26	Ti	3.37	Fe	4.25
Mn	0.00	Si	1.08	C	0.00
B	0.22	Zr	0.09	Cu	0.00
N	0.00	P	0.00	V	0.36
Hf	0.00	Ni	52.70	HT1Temp C	14.32
HT1time hr	50.00	HT2Temp C	1156.67	HT2time hr	63.38

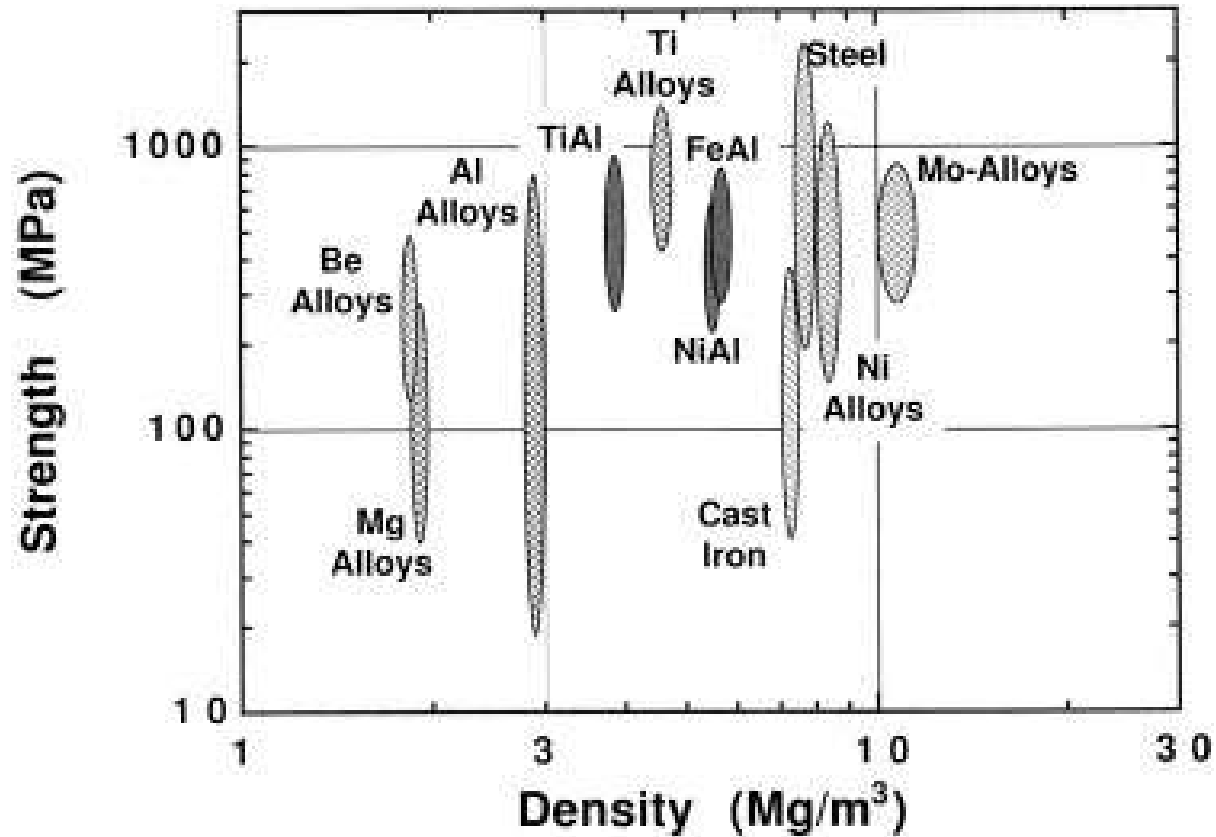
  

Property	Current Value	Target	Comparison	Probability
Cost \$/lb	14.96 +- 0.01	target < 15.00	<	Y
Density g/cm3	7.94 +- 0.01	target < 8.00	<	Y
Stress Rupture MPa	1163.81 +- 194.55	target > 750.00	>	Y
UTS MPa	1859.41 +- 40.77	target > 1700.00	>	Y
Yield Stress MPa	1372.94 +- 134.43	target > 1050.00	>	Y
Gamma' fraction	40.74 +- 1.65	target > 35.00	>	Y
Gamma + Gamma' fract	98.12 +- 0.95	target > 95.00	>	Y
Resistivity uOhm cm	8.96 +- 0.01	target < 9.00	<	Y
Oxidation index	16.56 +- 0.01	target > 16.50	>	Y
Entropy J/molK	13.04 +- 0.01	target > 13.00	>	Y
Probability of success	0.974			

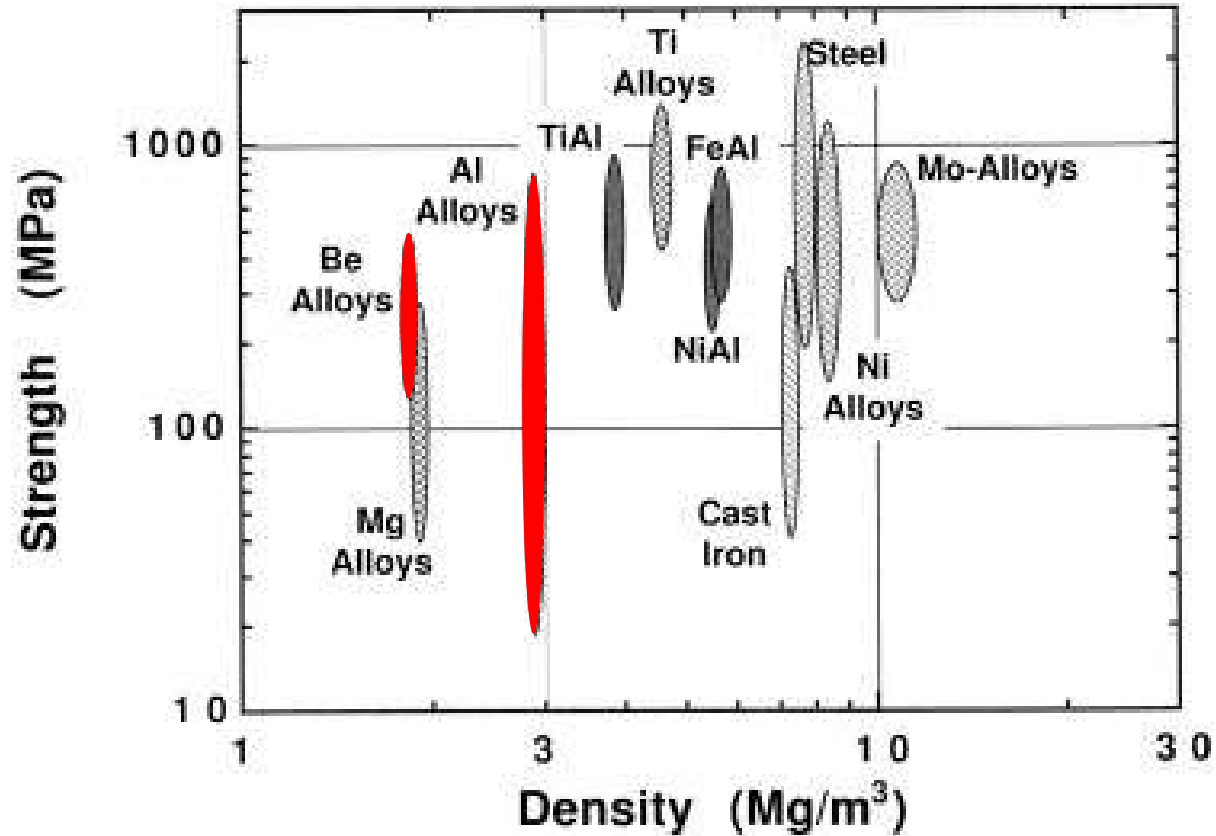
# Steps to commercialize



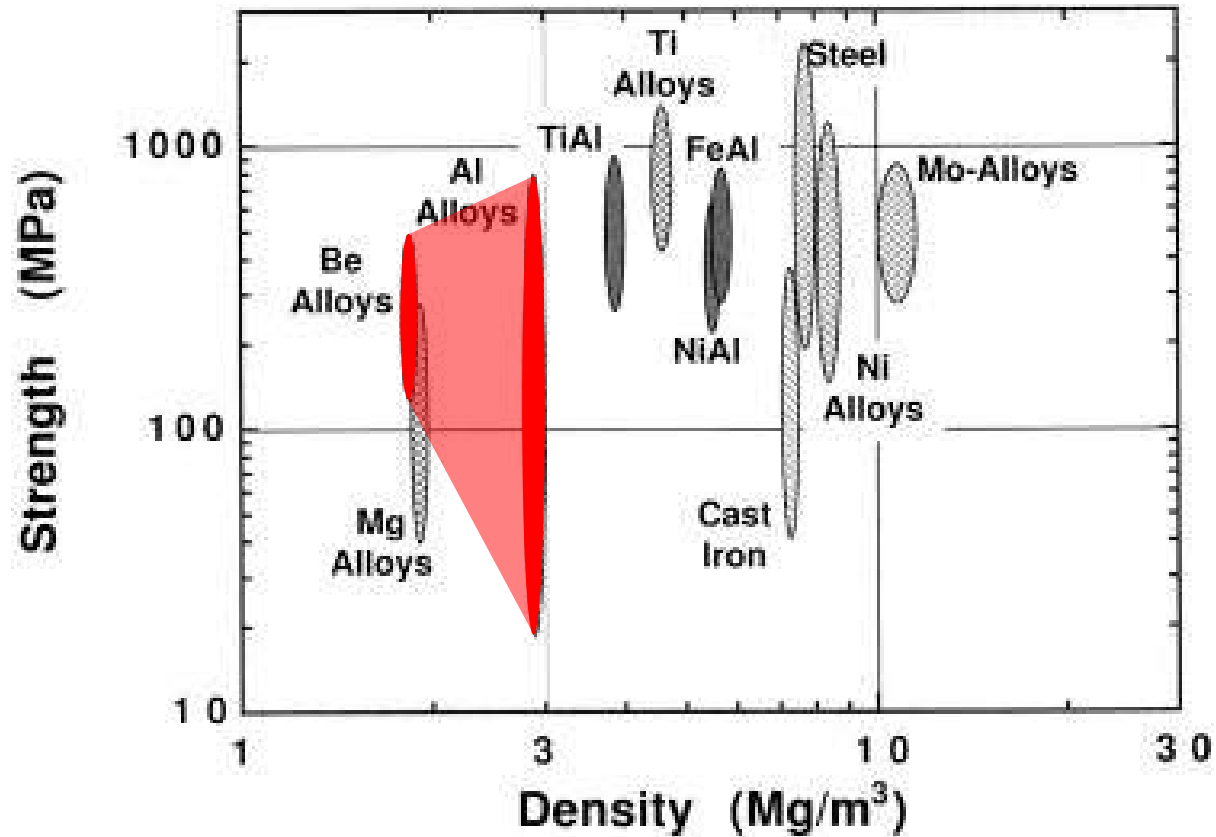
# Benefits – materials selection



# Benefits – materials selection

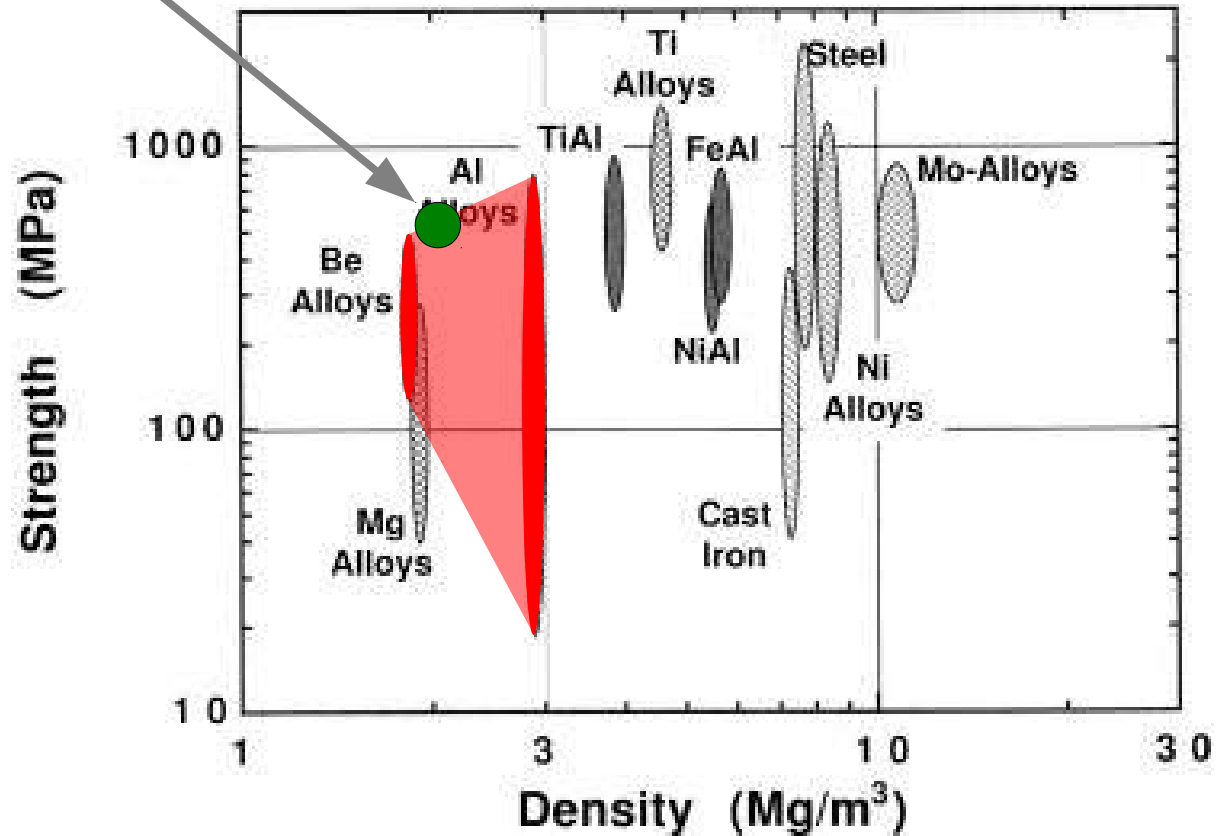


# Benefits – materials selection



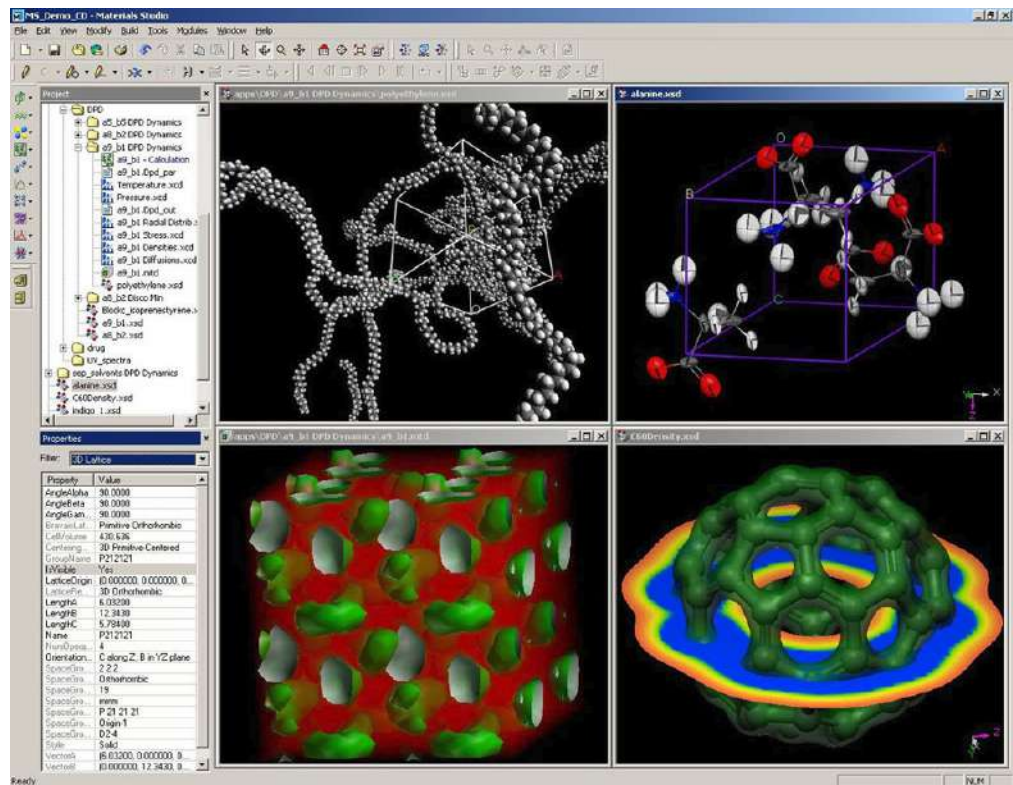
# Benefits – materials selection

65Be-32Al-1Si-2Ag, Starmet Corp.





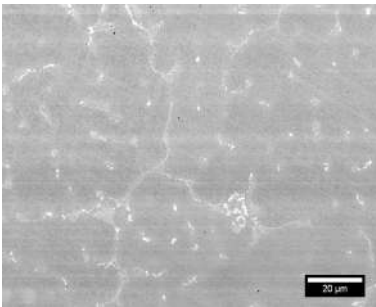
# Benefits – materials characterization



# Alloys designed

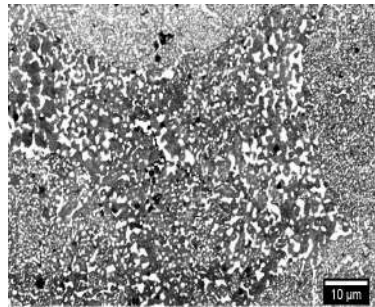
## Mo-Hf forging alloy

Patent GB1307533.8 (2013)



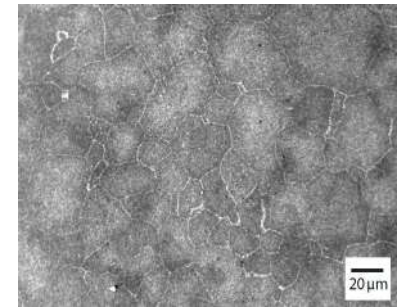
## Mo-Nb forging alloy

Rolls-Royce invention  
NC13024 (2013)



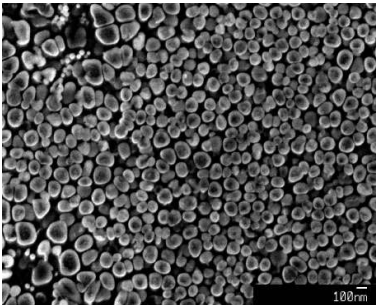
## RR1000 grain growth

Acta Materialia, **61**,  
3378 (2013)



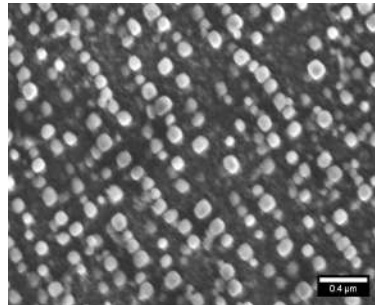
## Ni disc alloy

Rolls-Royce invention  
NC12261 (2012)

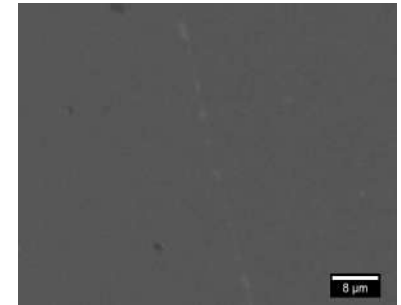


## Ni combustor liner

Rolls-Royce invention  
NC13006 (2013)



## High entropy alloy



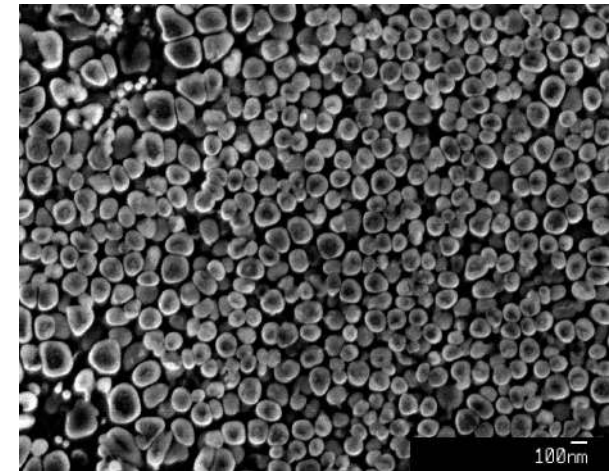
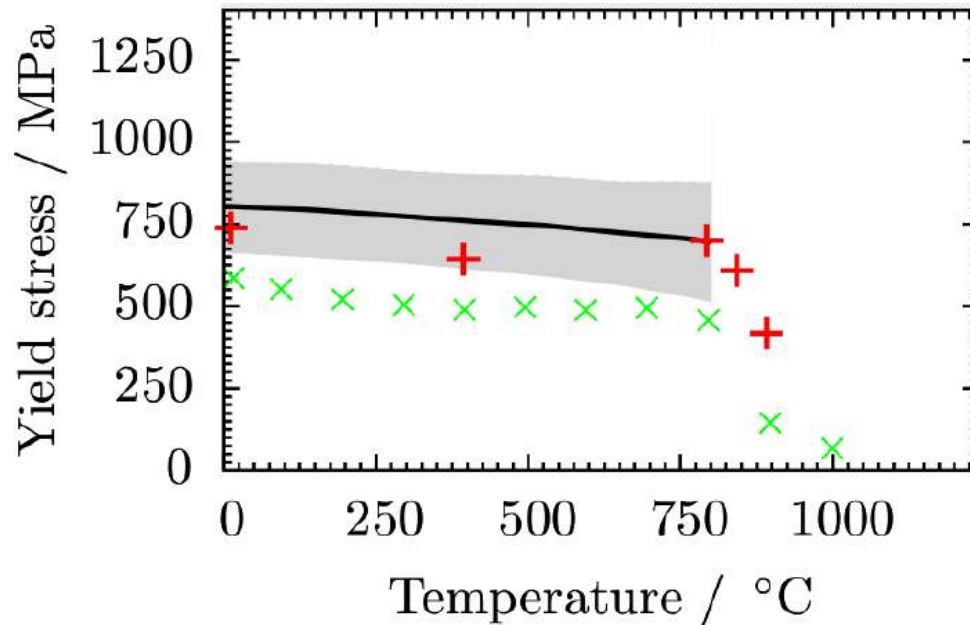
# Intellectual property

- “*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 ?



**Mo-Hf forging**

Patent GB1307533.8 (2013)

**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)

**RR1000 grains**

Acta Materialia, **61**, 3378 (2013)

# SWOT matrix

**S**  
Study and discover new materials  
Account for heat treatments  
Rapid calculation & optimization

**W**  
Require pre-existing experimental data  
Uncertainty in results

**O**  
Demand for new materials  
Rise of eco-materials  
Genome Initiative

**T**  
Development of a complete and rapid first principles calculation  
Patent theft

# Business plan

	<b>Year 1</b>	<b>Year 2</b>	<b>Year 3</b>
<b>Revenue</b>	60000	100000	140000
<b>Gross margin</b>	54000	90000	126000
<b>Net profit</b>	10400	29600	48800
<b>License via suite</b>	0 %	30 %	50 %
<b>Optimization service</b>	50 %	30 %	20 %
<b>Direct sales</b>	50 %	40 %	30 %

# Selected industries

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



£170 bn