UNIVERSITY OF CAMBRIDGE

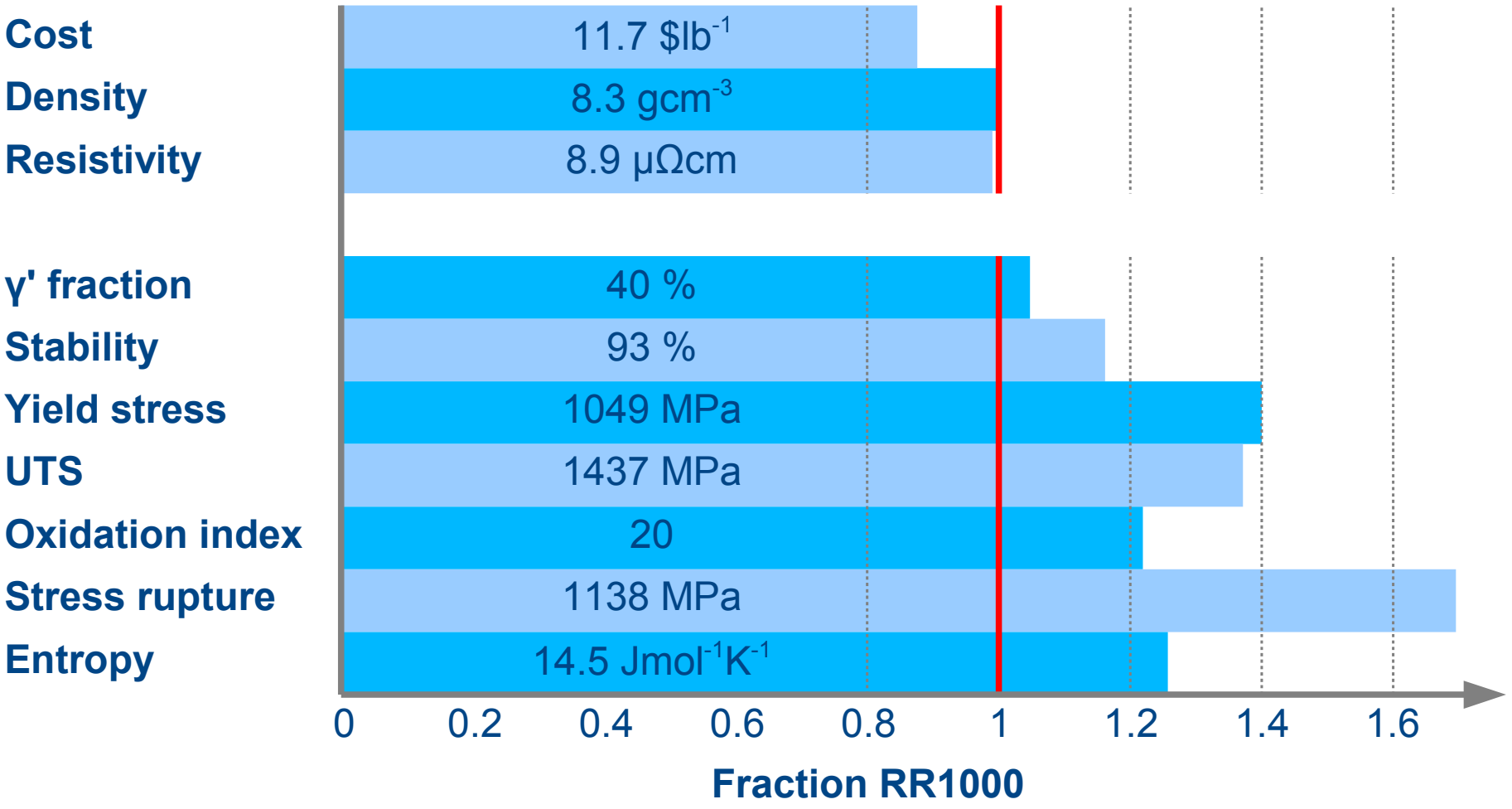
Computer driven materials discovery

Gareth Conduit

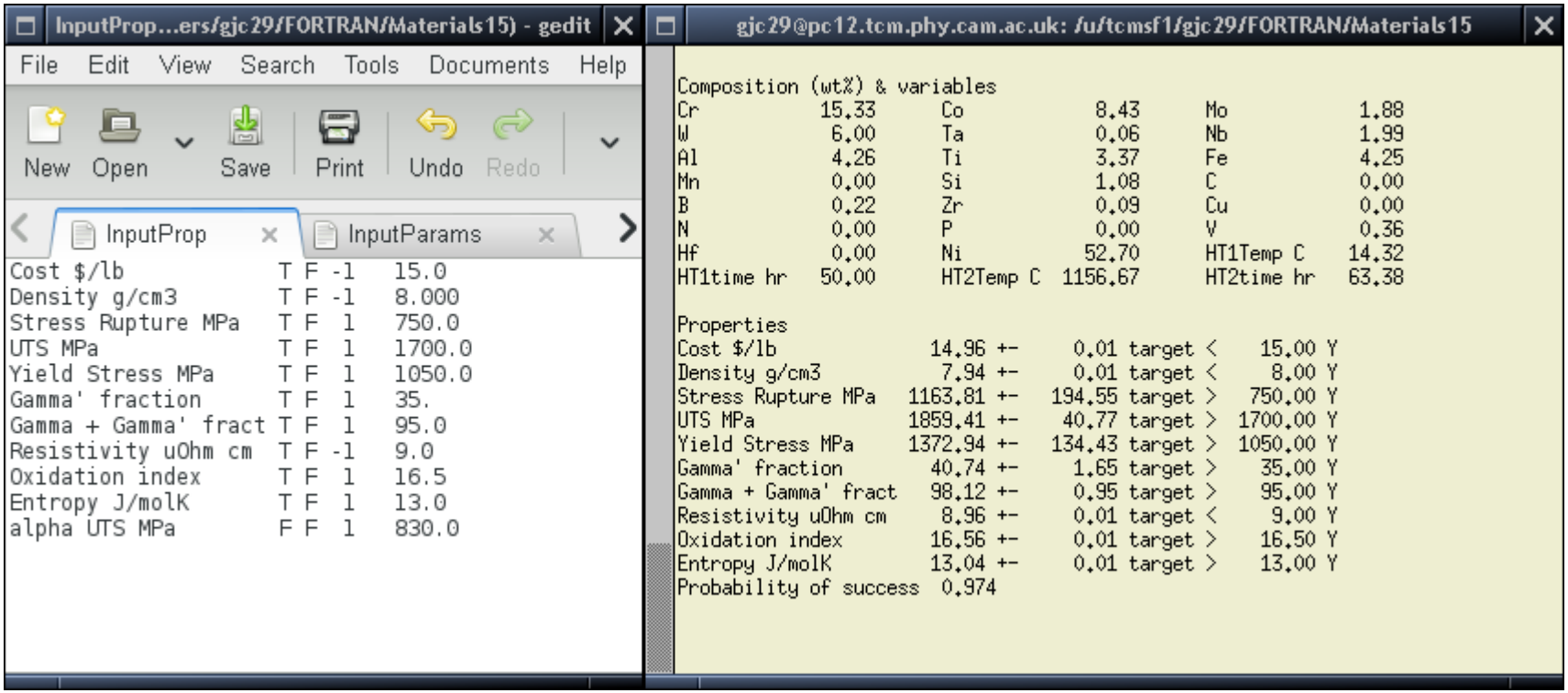
Patent GB1302743.8 (2013)
Patent GB1307533.8 (2013)
Acta Materialia, **61**, 3378 (2013)
Rolls-Royce Group plc invention submission NC12261 (2012)
Rolls-Royce Group plc invention submission NC13006 (2013)
Rolls-Royce Group plc invention submission NC13024 (2013)

TCM Group, Department of Physics

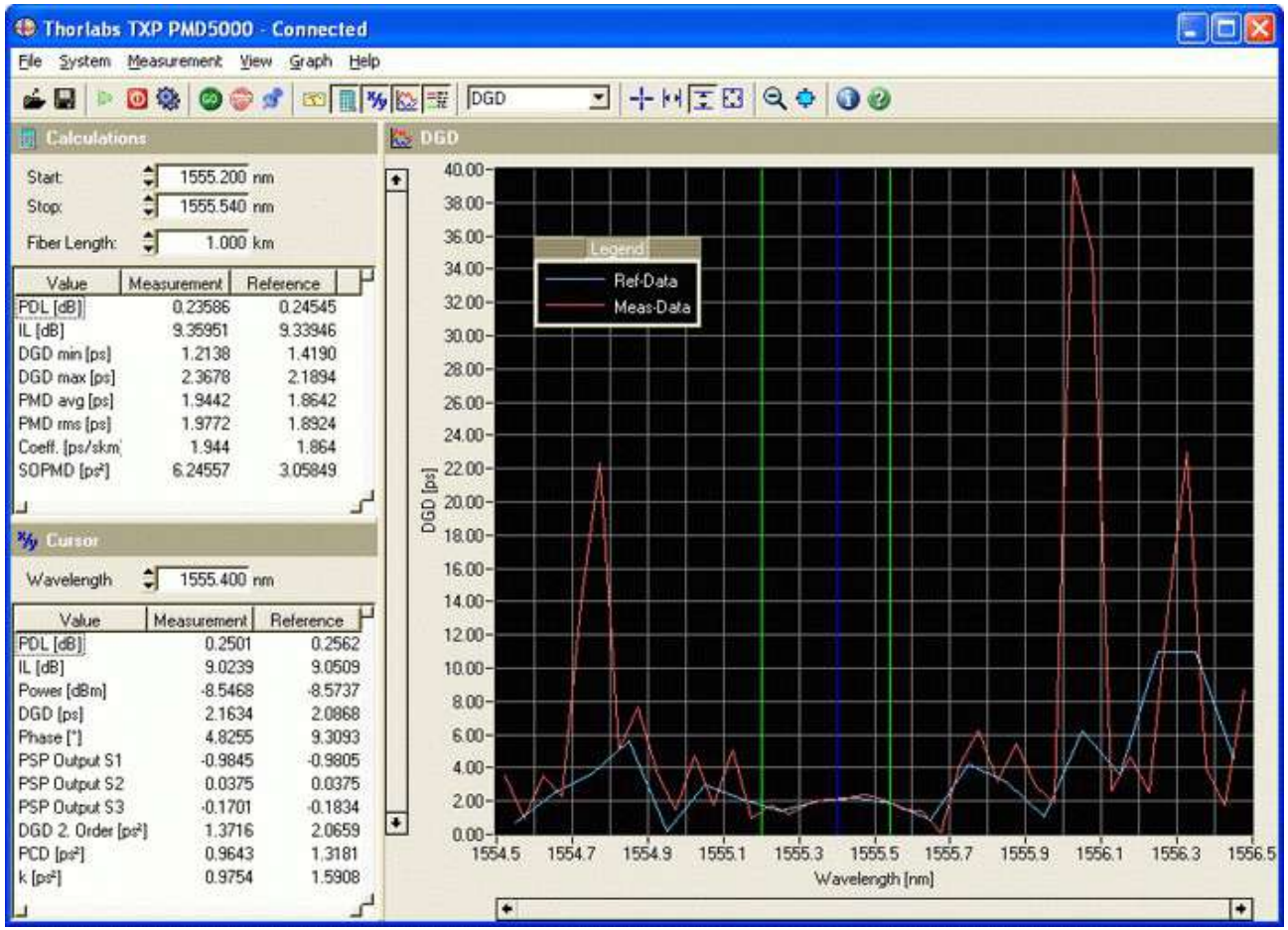
Designing a new alloy – what is required ?



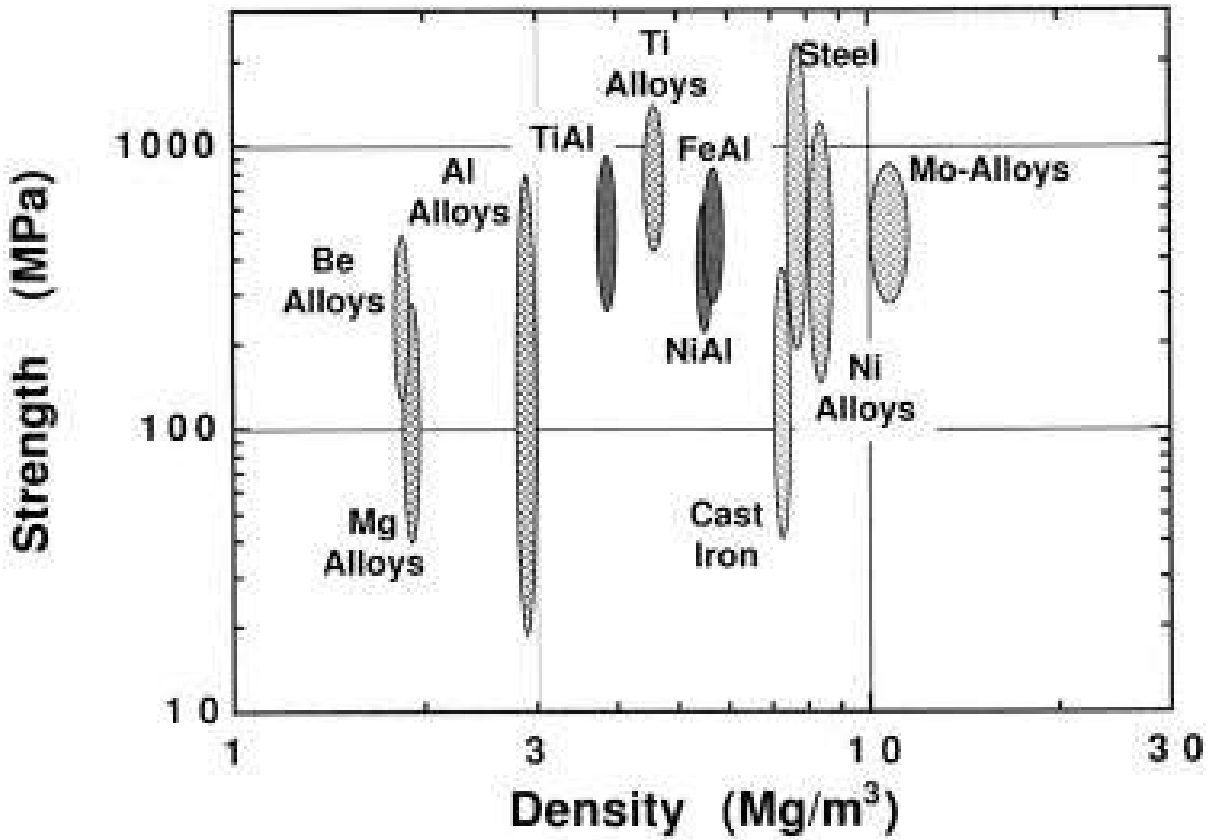
Steps to commercialize



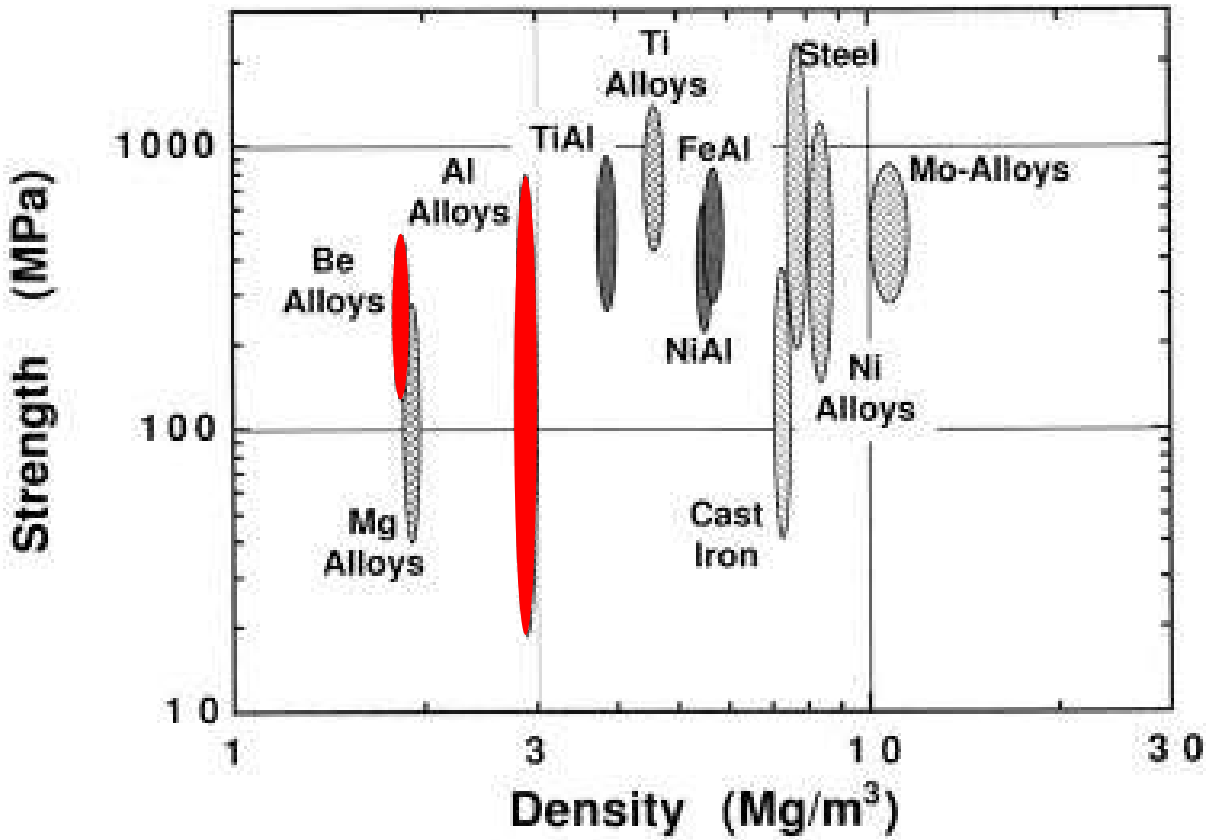
Steps to commercialize



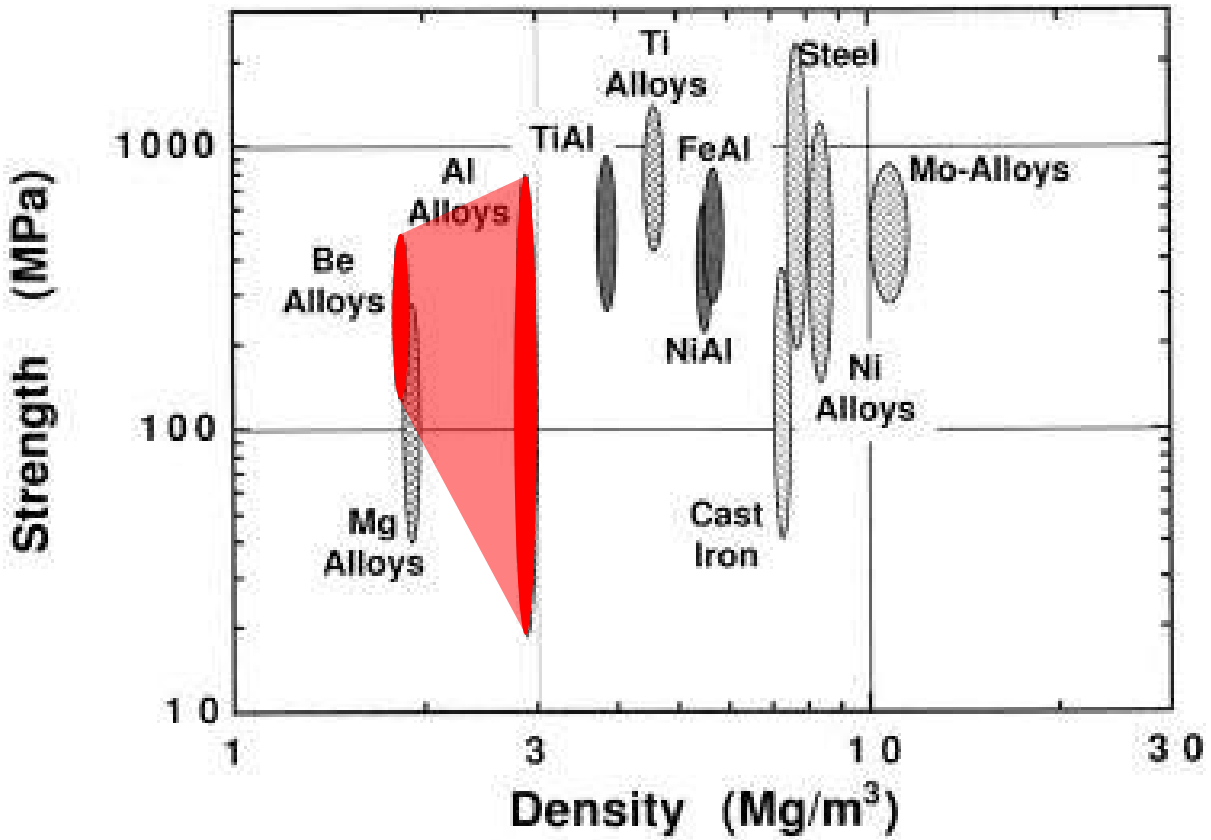
Benefits – materials selection



Benefits – materials selection

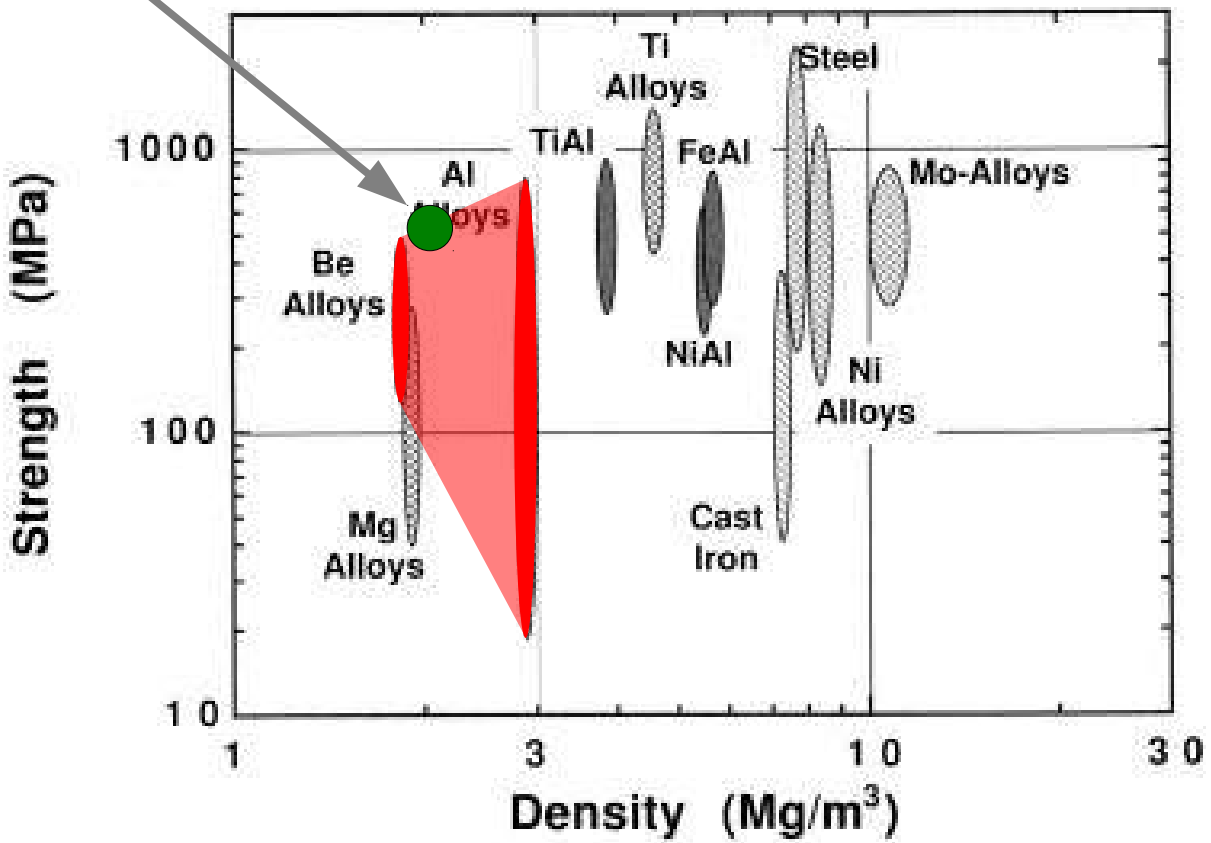


Benefits – materials selection

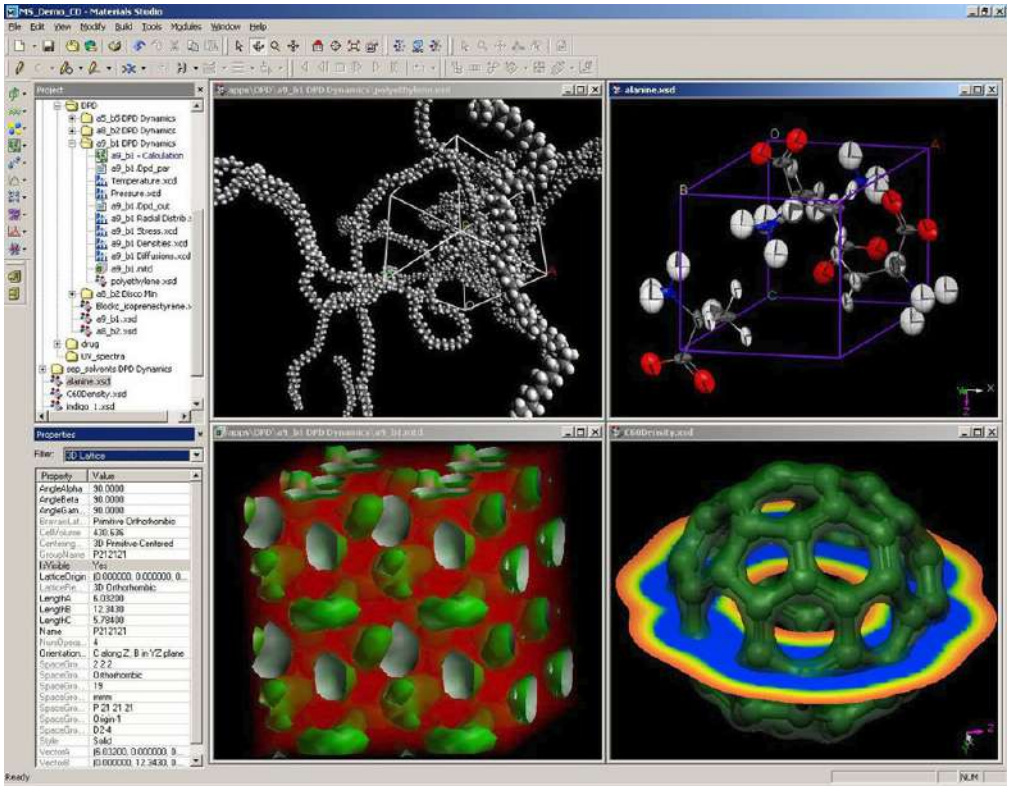


Benefits – materials selection

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

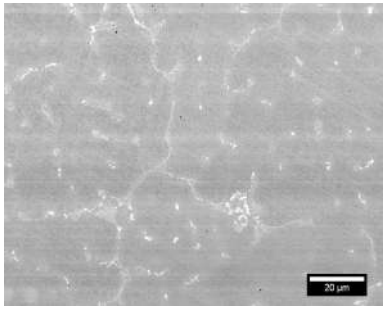


Benefits – materials characterization

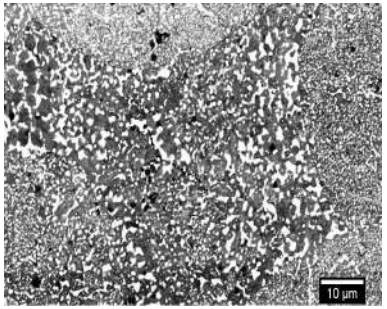


Alloys designed

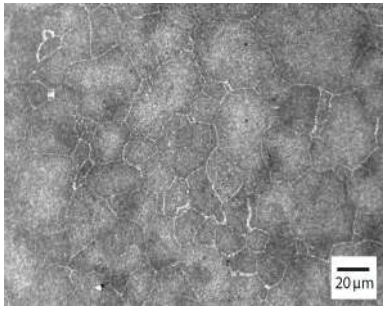
Mo-Hf forging alloy
Patent GB1307533.8 (2013)



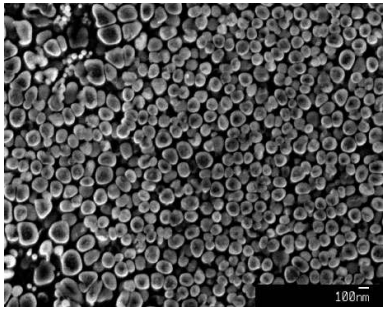
Mo-Nb forging alloy
Rolls-Royce invention
NC13024 (2013)



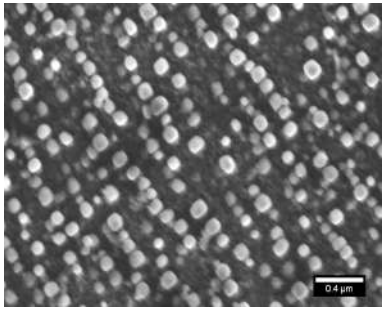
RR1000 grain growth
Acta Materialia, **61**, 3378 (2013)



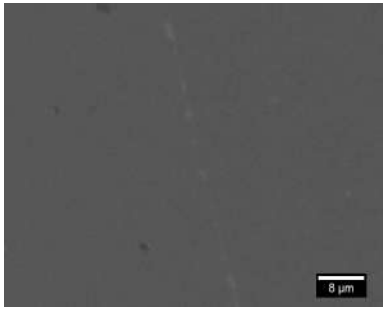
Ni disc alloy
Rolls-Royce invention
NC12261 (2012)



Ni combustor liner
Rolls-Royce invention
NC13006 (2013)



High entropy alloy



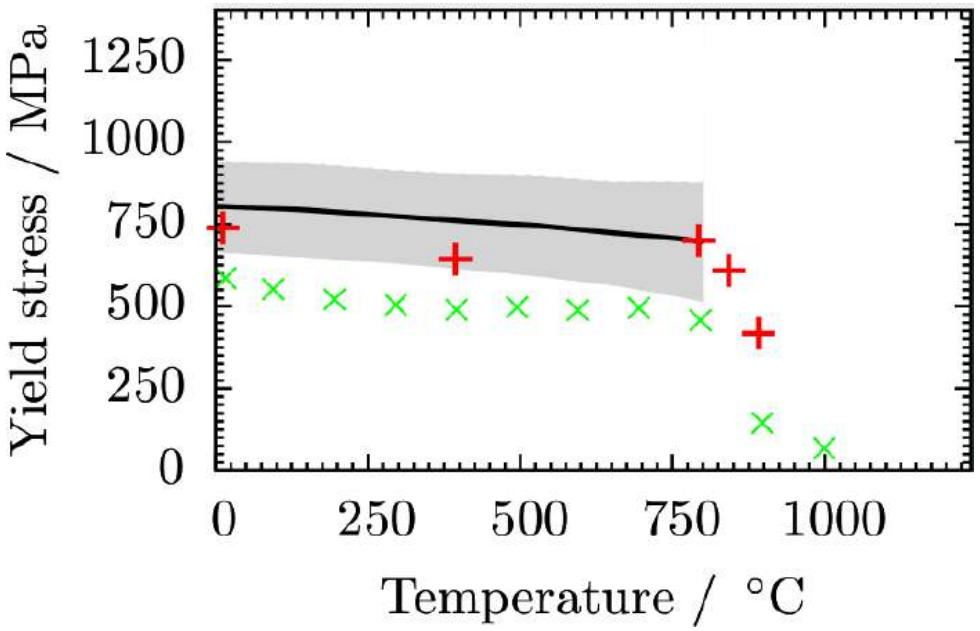
Intellectual property

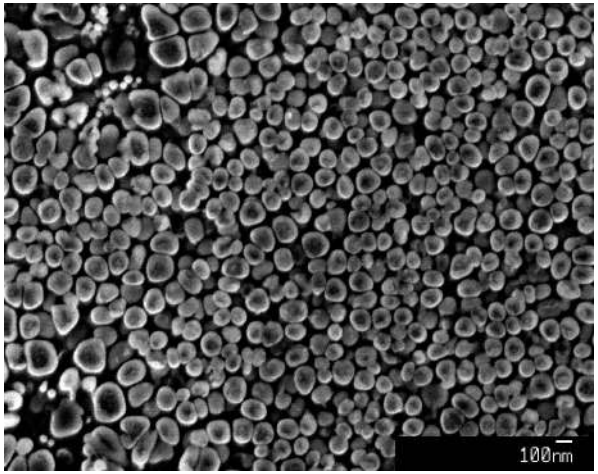
- "*A system for the characterisation and optimisation of alloys*", Patent GB1302743.8 (2013)
- Reduce likelihood of patent infringement by not distributing source code, only compiled program when sold

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

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

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

Selected industries

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