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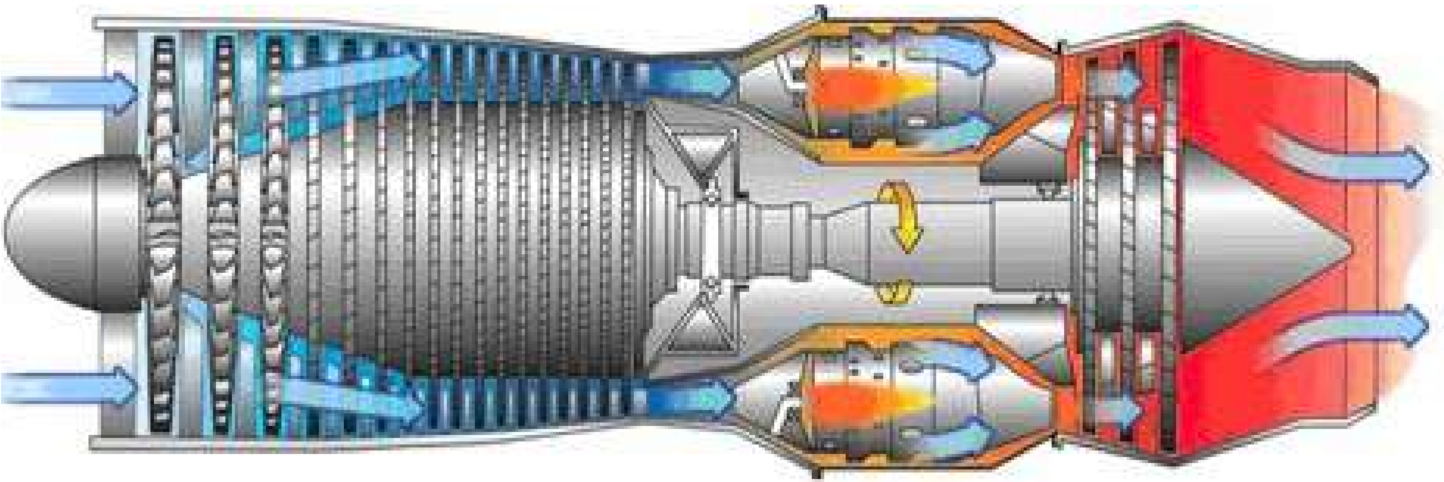
Concurrent materials design

Gareth Conduit

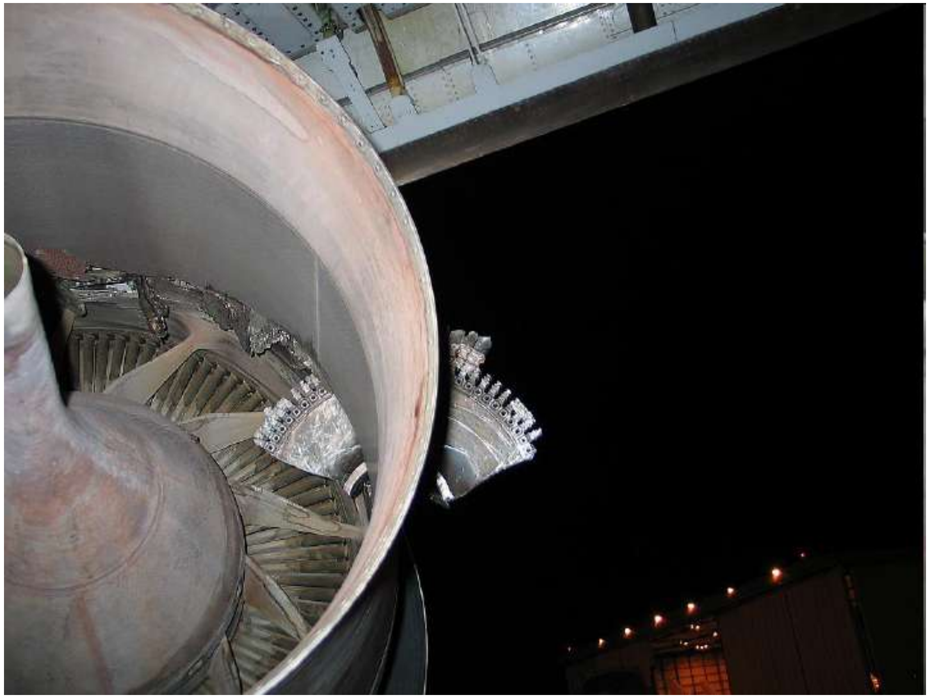
Patent GB1302743.8 (2013)
Patent GB1307533.8 (2013)
Patent GB1307535.3 (2013)
Acta Materialia, **61**, 3378 (2013)
Rolls-Royce Group plc invention submission NC12261 (2012)
Rolls-Royce Group plc invention submission NC13006 (2013)

TCM Group, Department of Physics

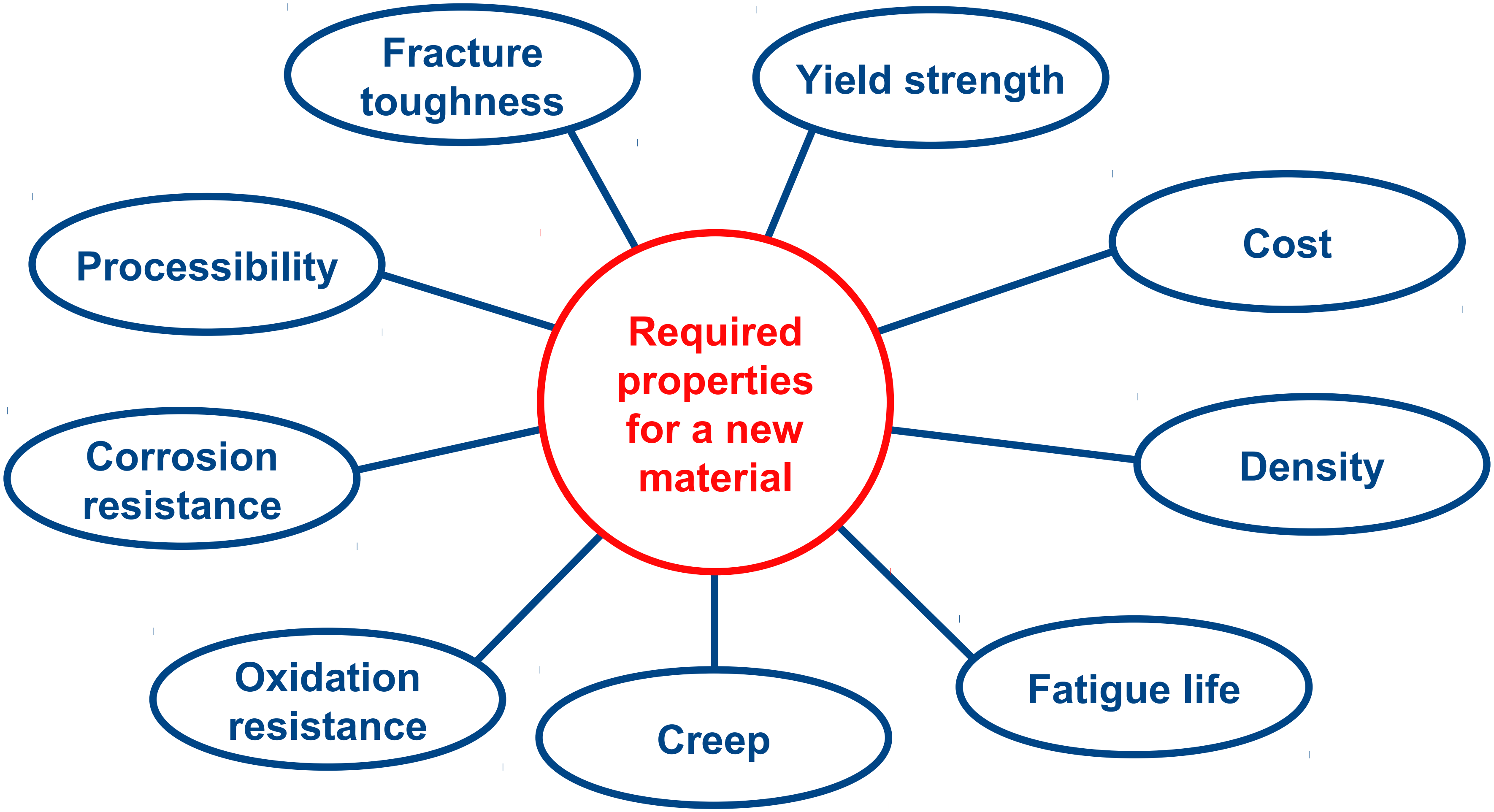
Jet engine



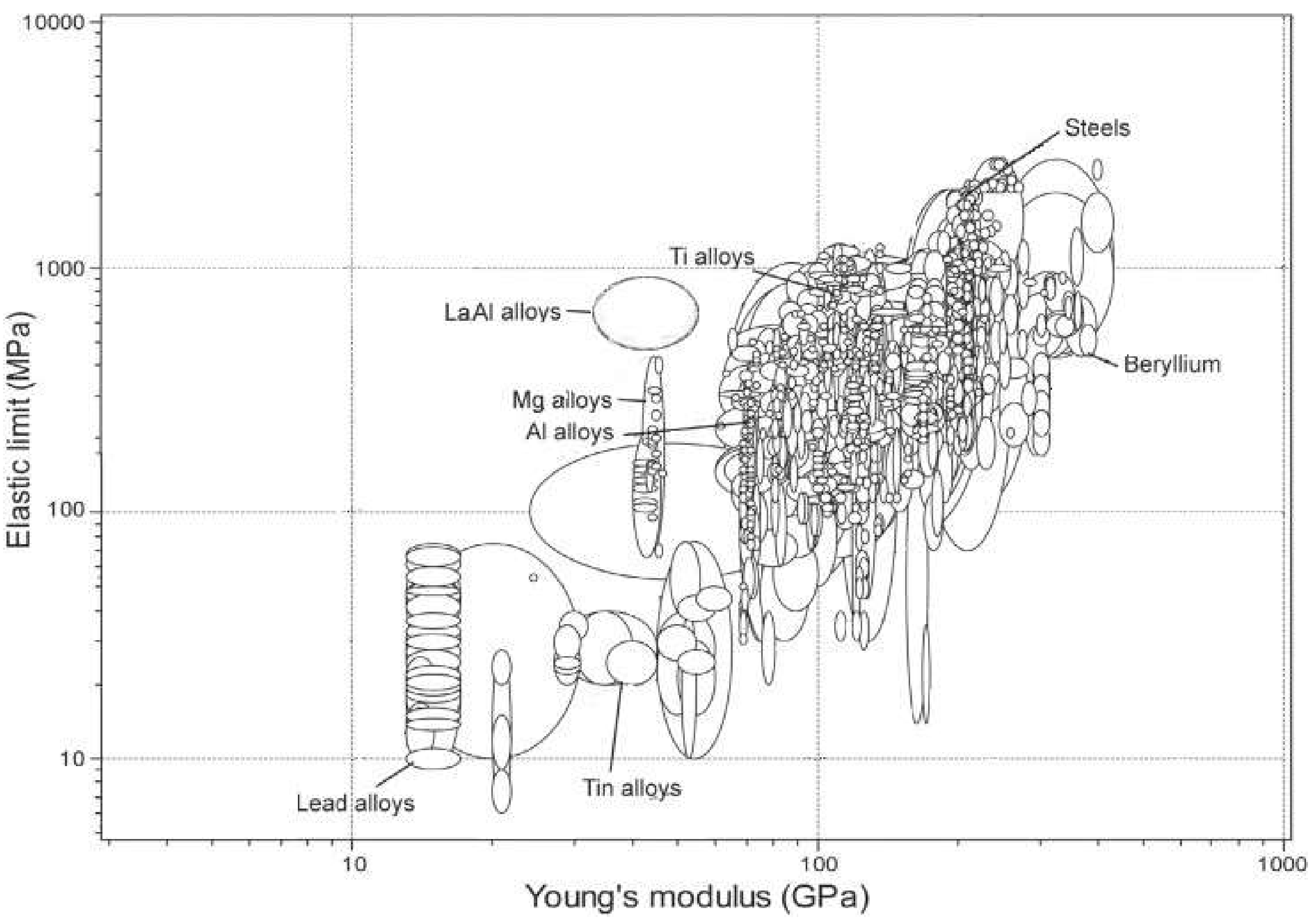
Jet engine: disc failure



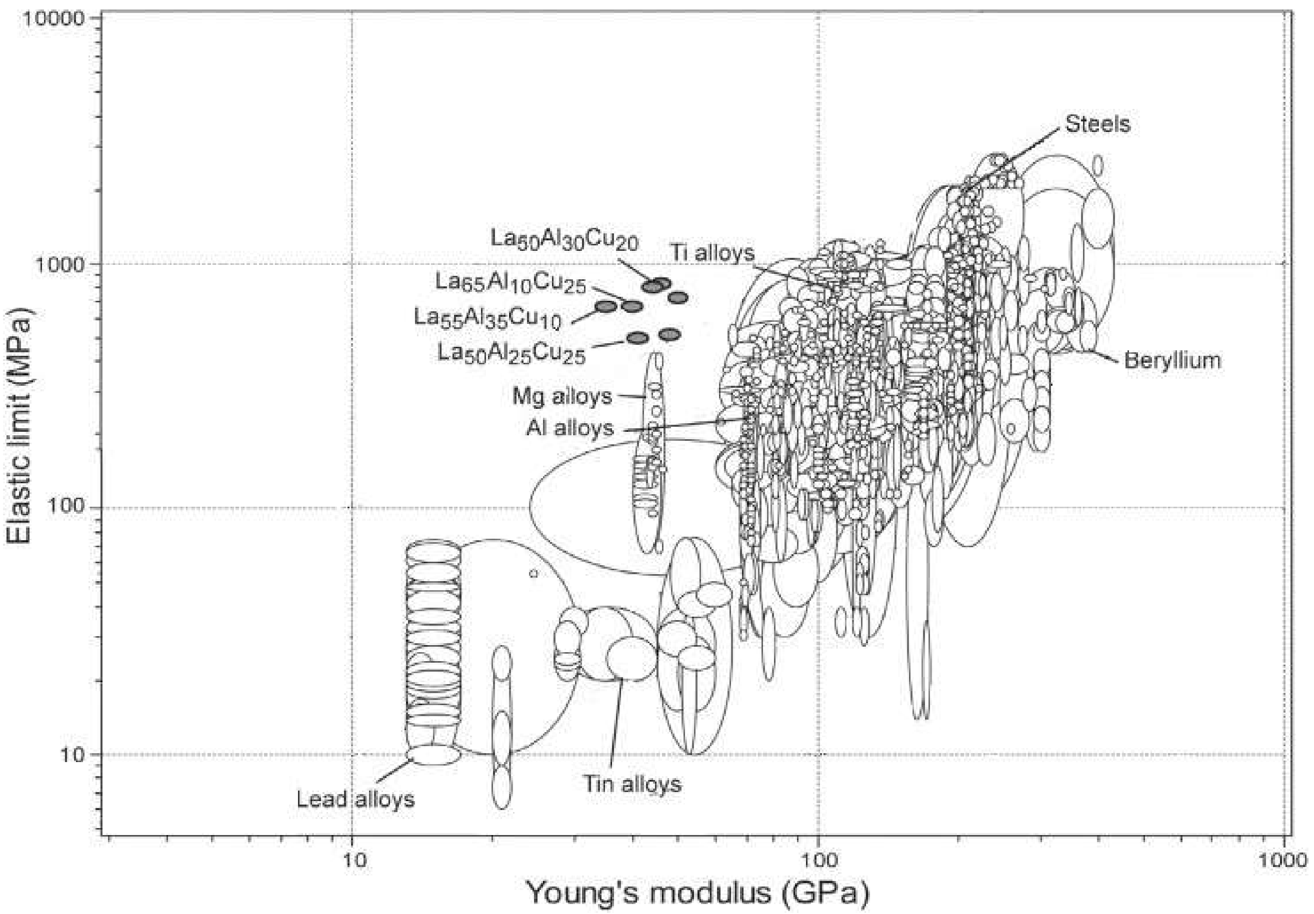
Designing a new material – what is required ?



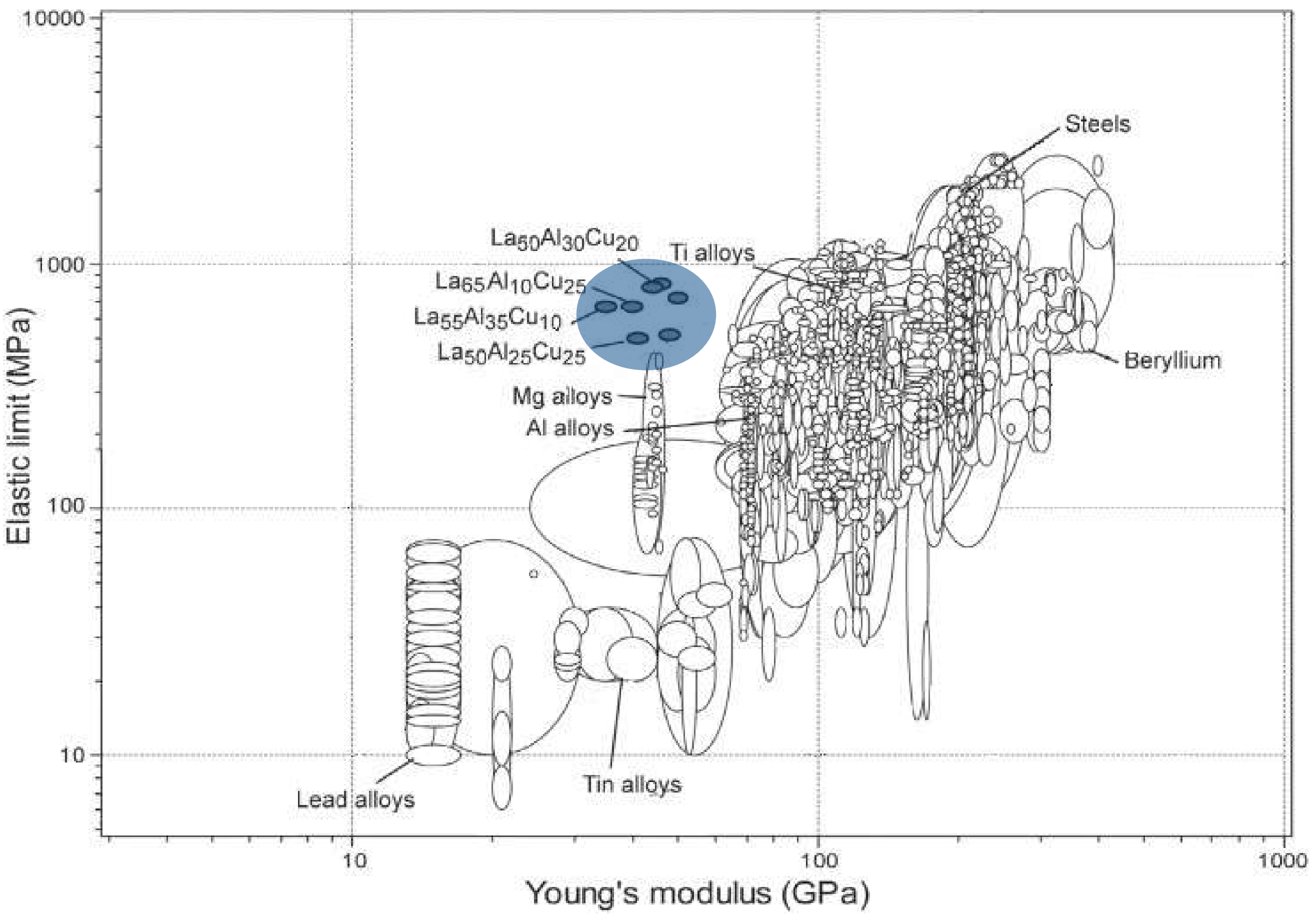
Materials selection



Materials selection



Materials selection



Materials selection

Guide the discovery of new materials

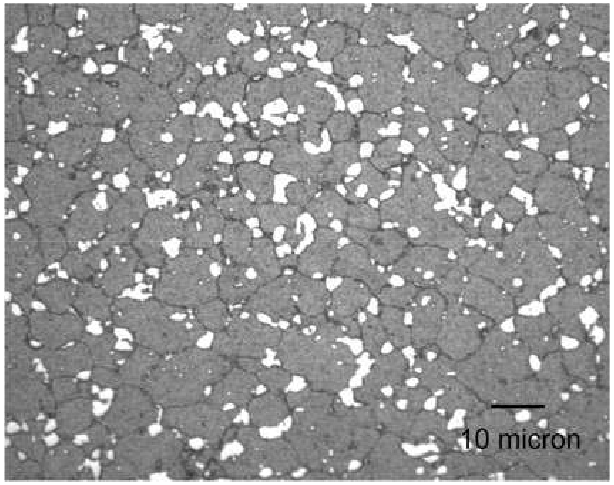
Concurrent materials design

Assess data quality

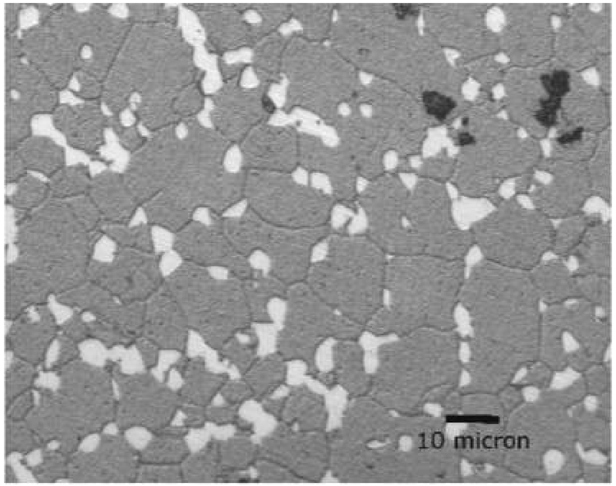
Estimate missing data

Contemporary alloys

RR1000



N18



Alloy	Firm	Ni	Cr	Co	Mo	Ti	Al	C	Hf	Ta	W	Nb
Waspaloy	UTC	58	19	13	4	3	1.4					
Rene 88	General Elec.	56.5	16	13	4	3.7	2.1	0.03			4	0.7
N18	SNECMA	58	11.1	15.4	6.4	4.3	4.3	0.02	0.5			
RR1000	Rolls Royce	52.4	15	18.5	5	3.6	3	0.03	0.5	2		

Properties

Cost $lb^{-1}
γ' fraction
Stability
Density gcm^{-3}
Yield stress MPa
UTS MPa
Oxidation index
Stress rupture MPa
Resistivity μΩcm
Entropy $Jmol^{-1}K^{-1}$
Low cycle fatigue
High cycle fatigue
Weldability
Creep model

Properties

Cost $lb^{-1}
γ' fraction
Stability
Density gcm^{-3}
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Weldability
Creep model

$$\mathrm{Cost}\left[\$/\mathrm{lb}\right] = 9.59n_{ni} + 0.94n_{Al} + 6.77n_{Cr} + 16.5n_{Co} + 19.6n_{Mo} + 5.44n_{Ti}$$

Properties

- Cost lb^{-1}
- γ' fraction
- Stability
- Density gcm^{-3}
- **Yield stress MPa**
- UTS MPa
- Oxidation index
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Collect data for yield stress from 2248 alloys

Properties

- Cost $\$lb^{-1}$
- γ' fraction
- Stability
- Density gcm^{-3}
- **Yield stress MPa**
- UTS MPa
- Oxidation index
- Stress rupture MPa
- Resistivity μΩcm
- Entropy $Jmol^{-1}K^{-1}$
- Low cycle fatigue
- High cycle fatigue
- Weldability
- Creep model

Collect data for yield stress from 2248 alloys

↓

Generate neural network model

$$\mathrm{YS}[\mathrm{MPa}] = F(n_{\mathrm{ni}}, n_{\mathrm{Al}}, n_{\mathrm{Cr}}, n_{\mathrm{Co}}, n_{\mathrm{Mo}}, n_{\mathrm{Ti}}, T_{\mathrm{HT}}, t_{\mathrm{HT}})$$

Properties

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γ' fraction
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Collect data for yield stress from 2248 alloys

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Generate neural network model

$$YS[MPa] = F(n_{ni}, n_{Al}, n_{Cr}, n_{Co}, n_{Mo}, n_{Ti}, T_{HT}, t_{HT})$$

↓

Calculate uncertainty in neural network model

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Cost $\$lb^{-1}$
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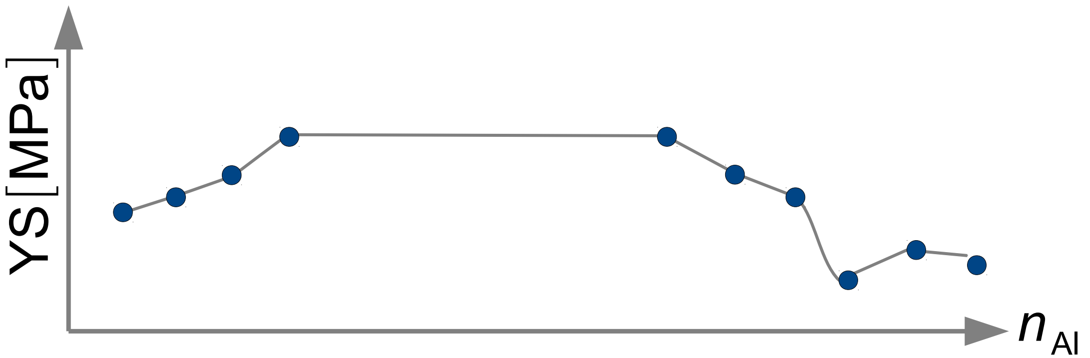

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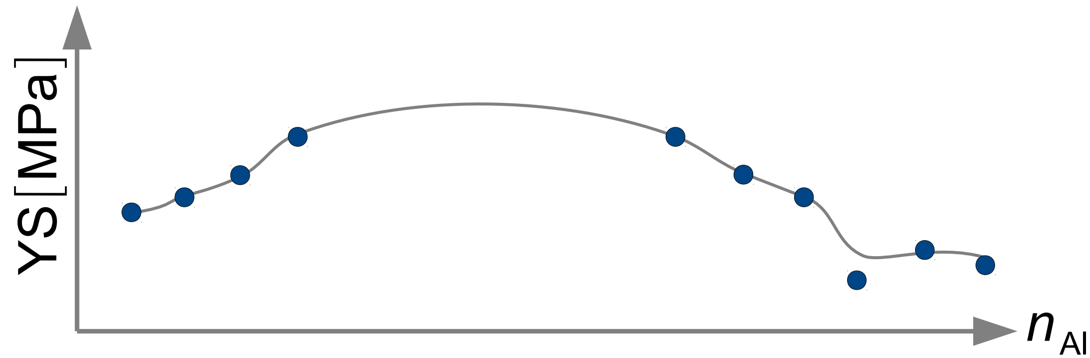

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Collect data for yield stress from 2248 alloys

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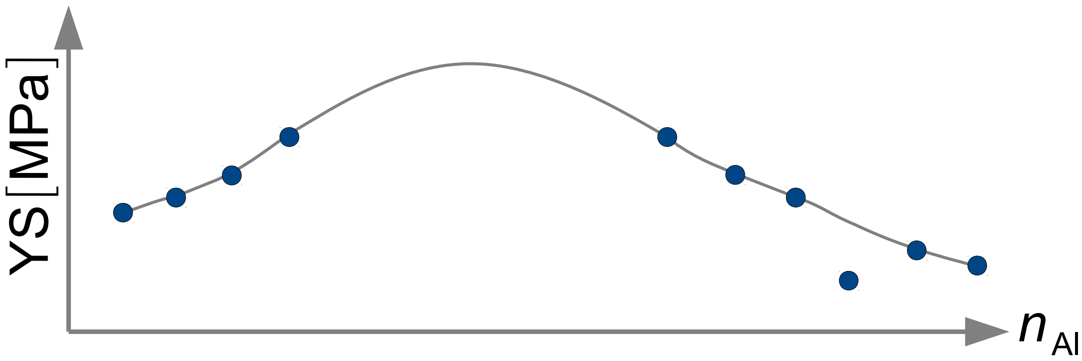
Calculate uncertainty in neural network model



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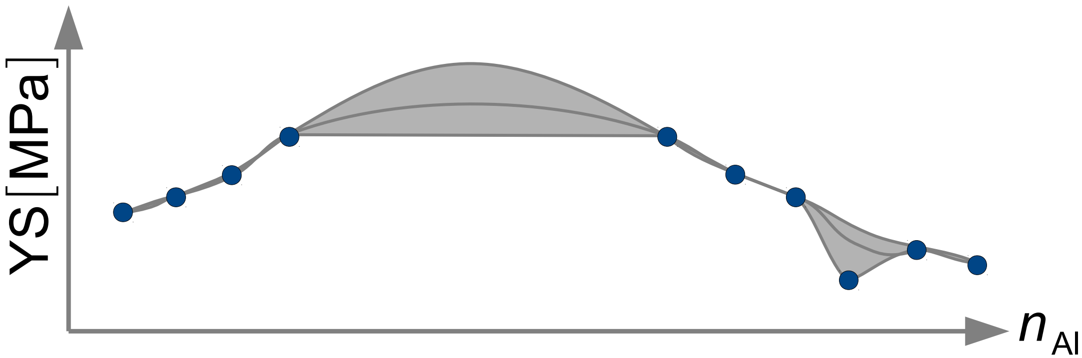

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Resistivity μΩcm
Entropy $Jmol^{-1}K^{-1}$
Low cycle fatigue
High cycle fatigue
Weldability
Creep model

Calculate grid of

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

Properties

Cost $lb^{-1}
γ' fraction
Stability
Density gcm^{-3}
Yield stress MPa
UTS MPa
Oxidation index
Stress rupture MPa
Resistivity μΩcm
Entropy Jmol^{-1}K^{-1}
Low cycle fatigue
High cycle fatigue
Weldability
Creep model

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

↓

Generate neural network models

Properties

- Cost $\$lb^{-1}$
- **γ' fraction**
- Stability
- Density gcm^{-3}
- Yield stress MPa
- UTS MPa
- Oxidation index
- Stress rupture MPa
- Resistivity μΩcm
- Entropy $Jmol^{-1}K^{-1}$
- Low cycle fatigue
- High cycle fatigue
- Weldability
- Creep model

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

↓

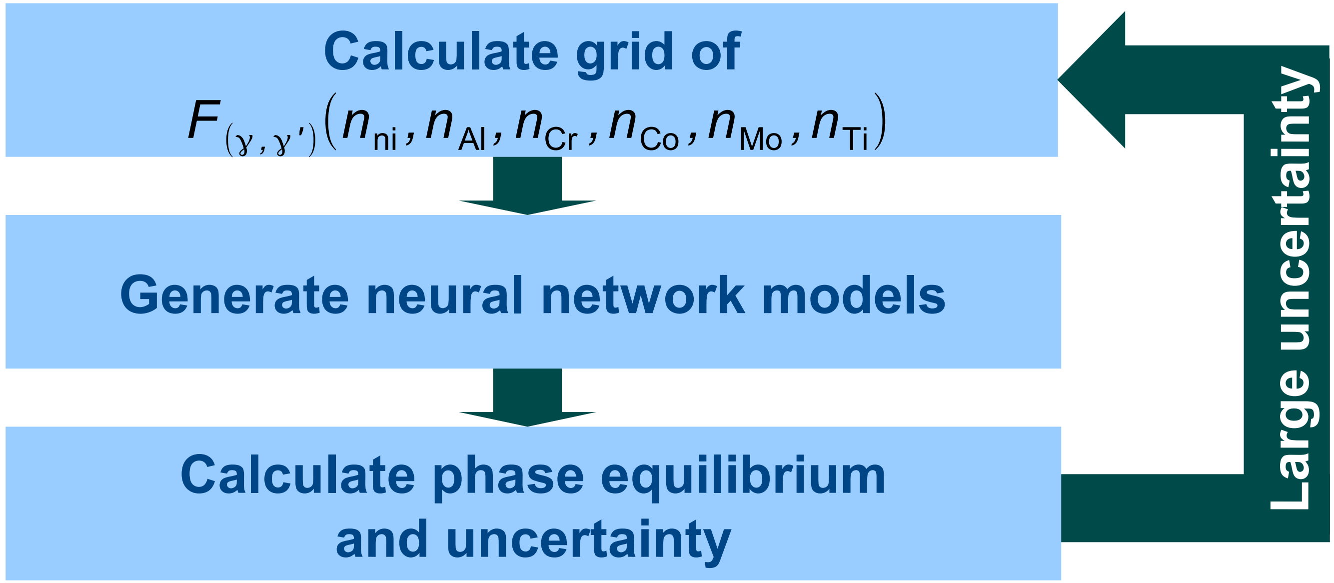
Generate neural network models

↓

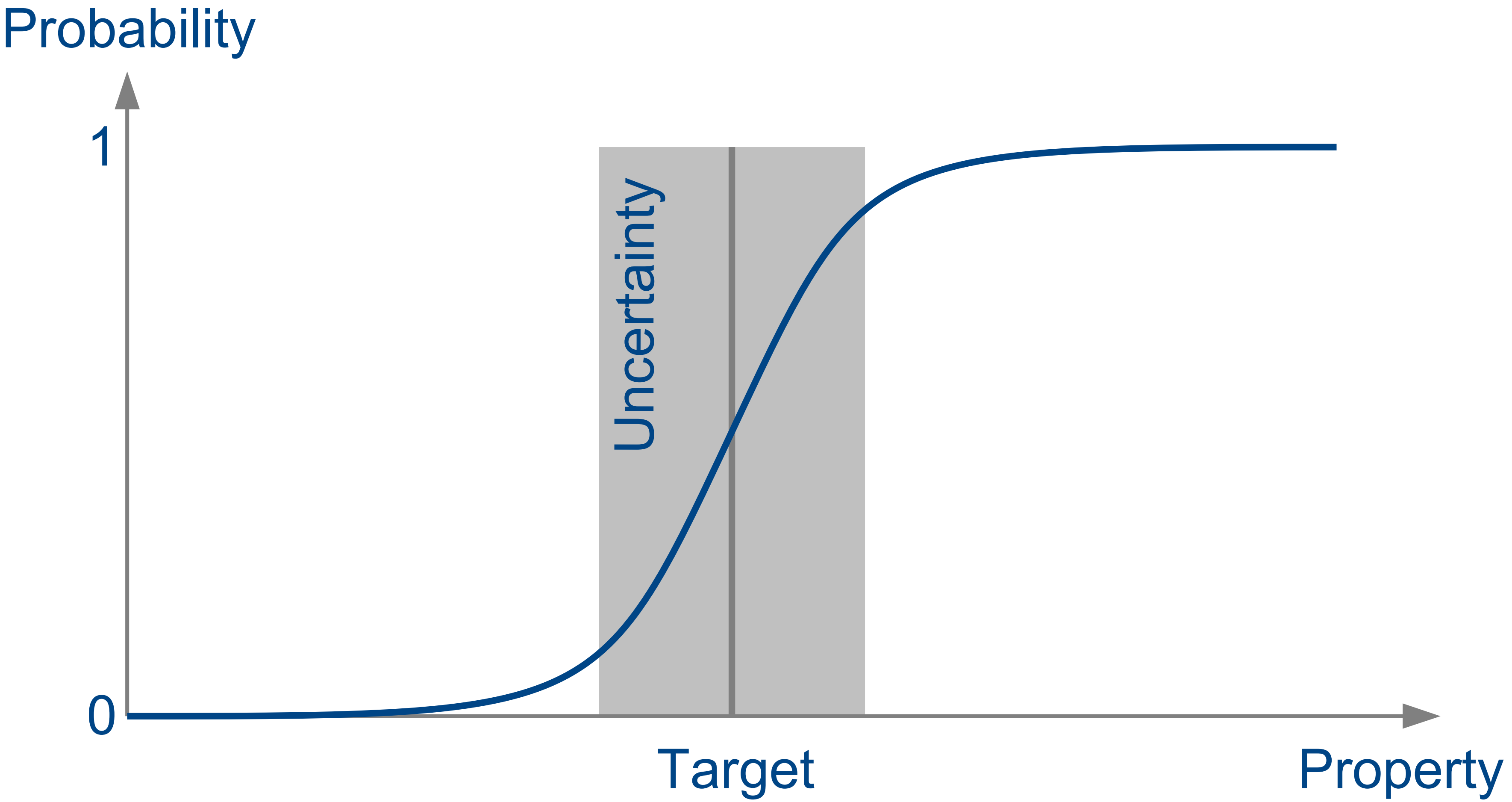
Calculate phase equilibrium and uncertainty

Properties

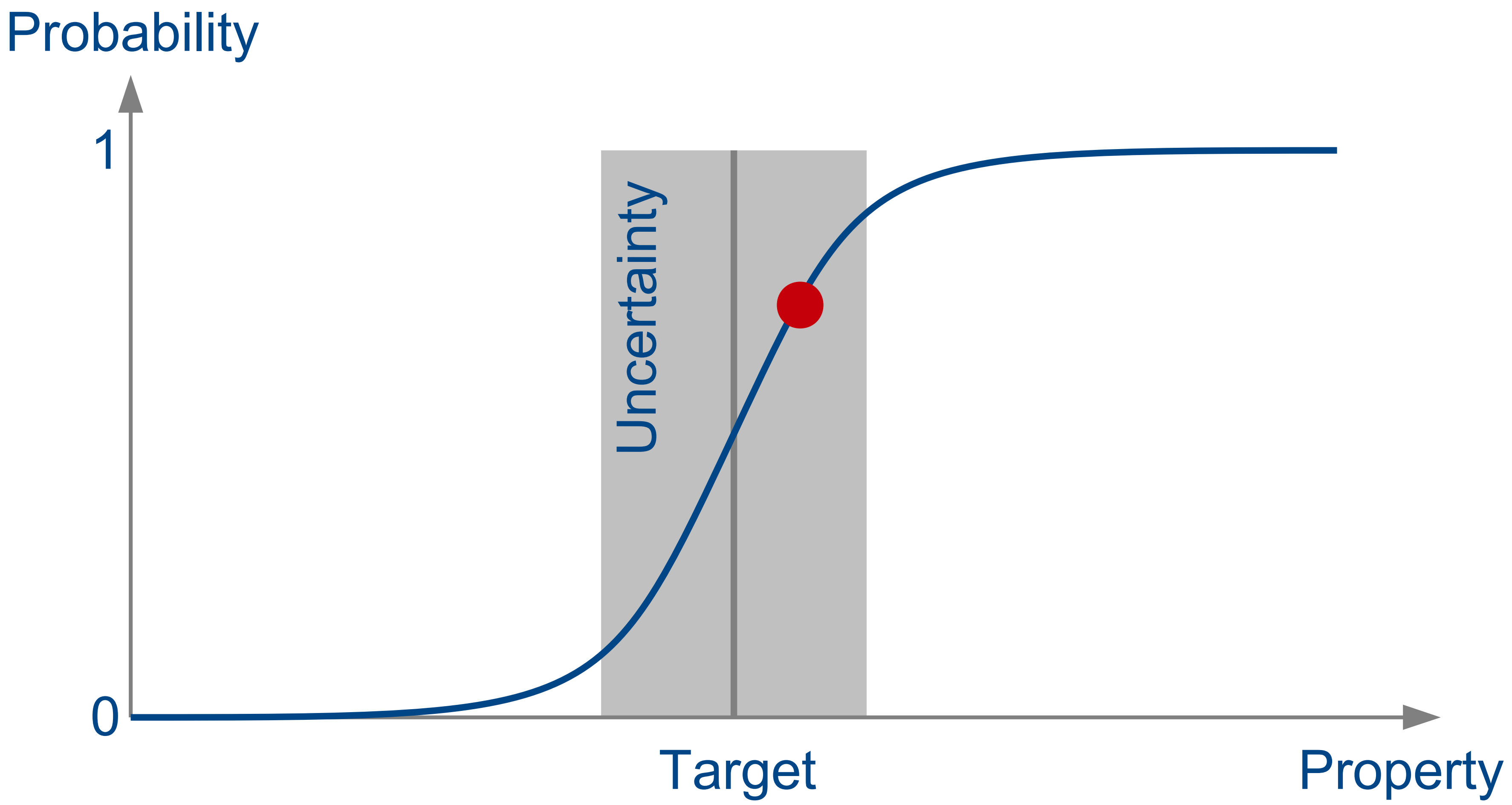
Cost $\$lb^{-1}$
γ' fraction
Stability
Density gcm^{-3}
Yield stress MPa
UTS MPa
Oxidation index
Stress rupture MPa
Resistivity μΩcm
Entropy $Jmol^{-1}K^{-1}$
Low cycle fatigue
High cycle fatigue
Weldability
Creep model



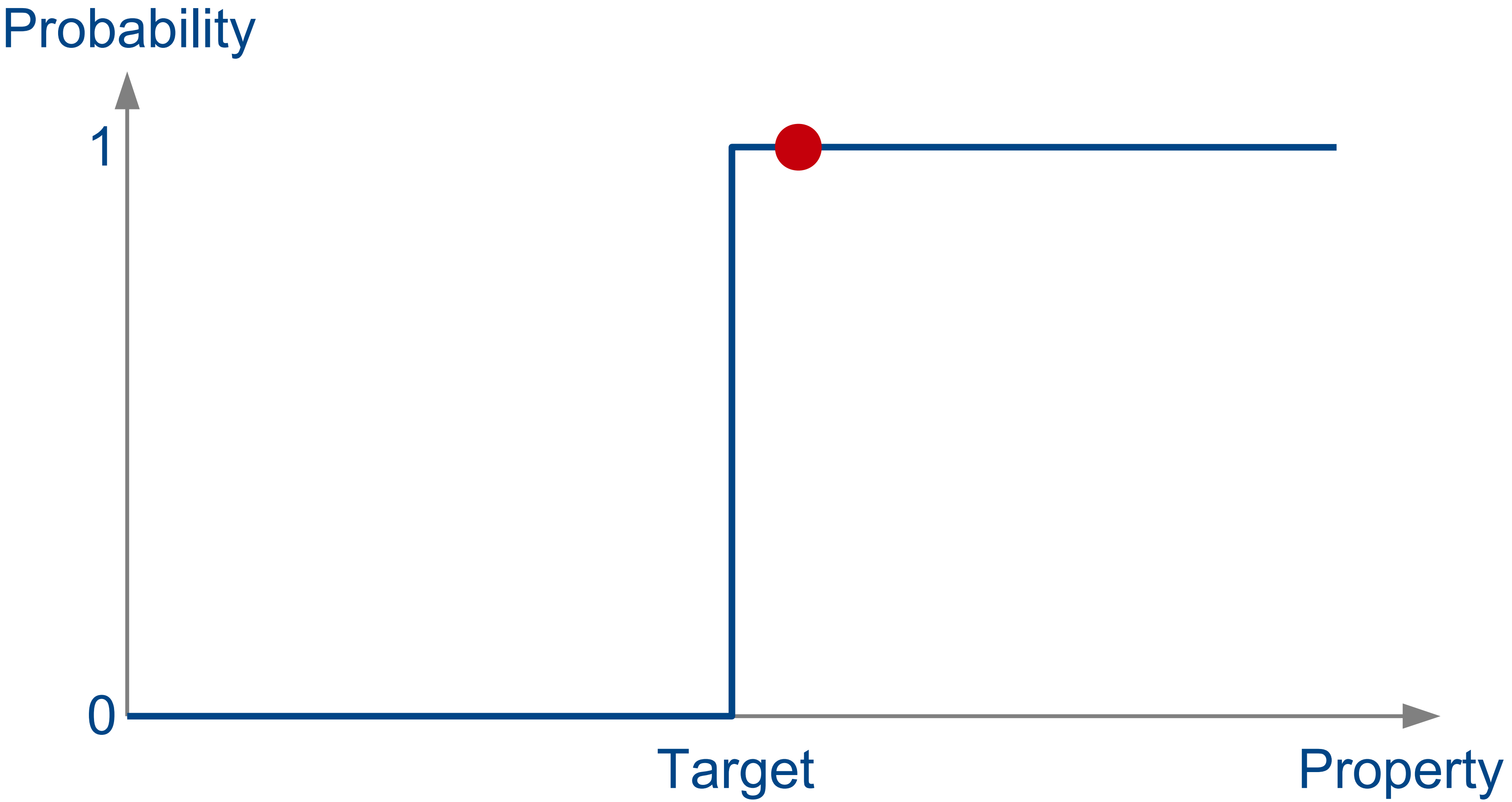
Probability



Probability



Probability

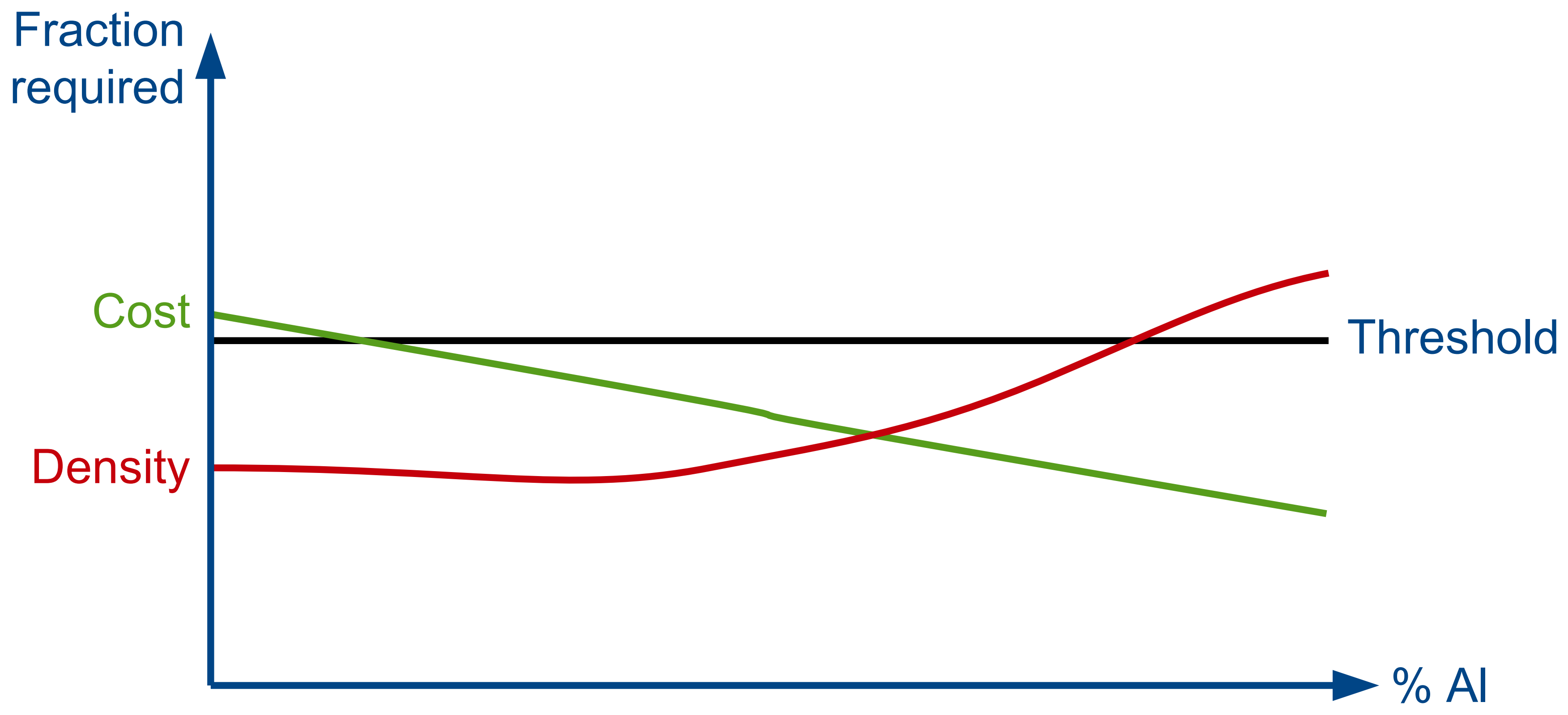


Probability

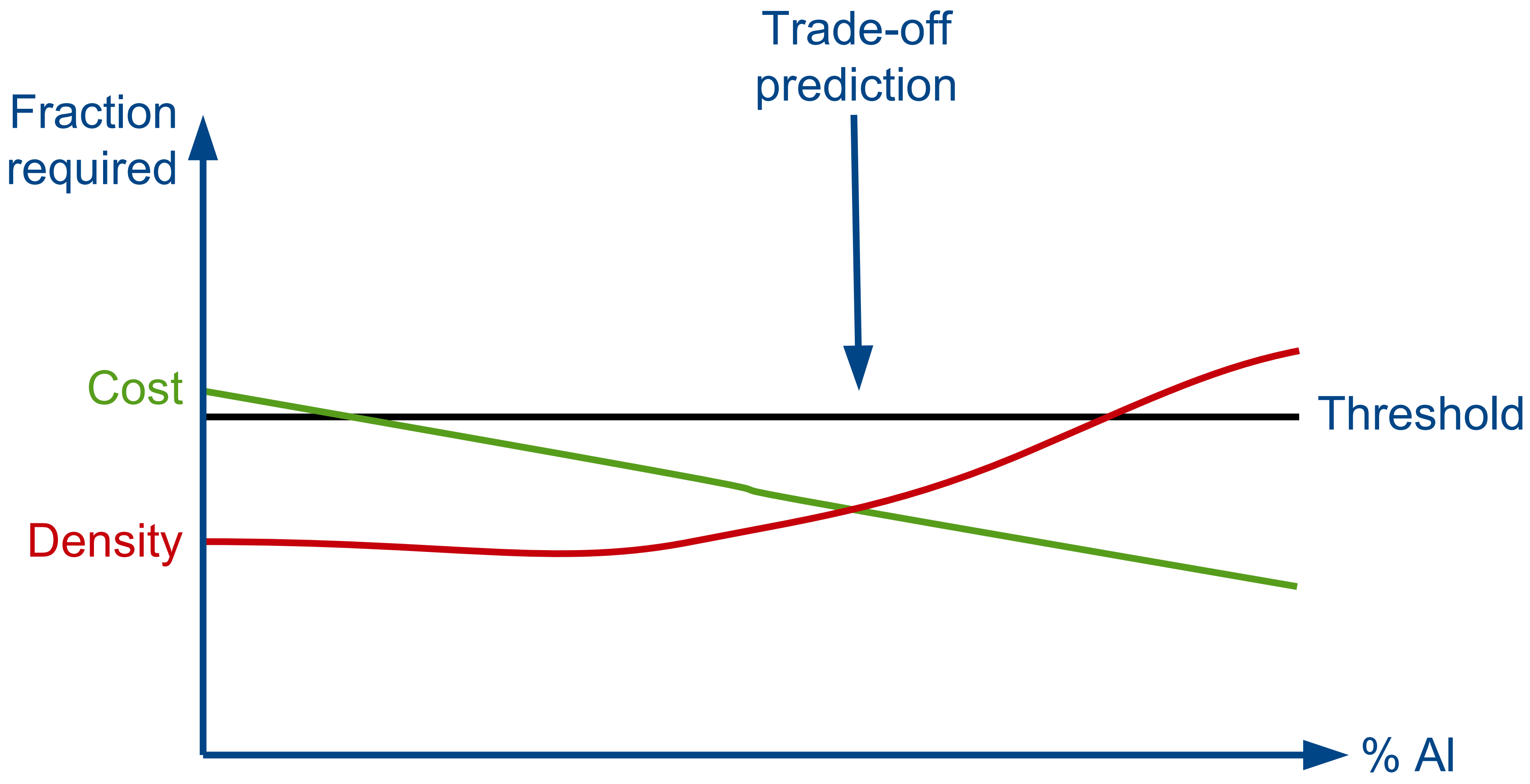
Cost $lb^{-1}	$P_{cost}(\mathbf{C})$
γ' fraction	$P_{\gamma'}(\mathbf{C})$
Stability	$P_{stable}(\mathbf{C})$
Density gcm^{-3}	$P_{density}(\mathbf{C})$
Yield stress MPa	$P_{YS}(\mathbf{C})$
UTS MPa	$P_{UTS}(\mathbf{C})$
Oxidation index	$P_{oxidize}(\mathbf{C})$
Stress rupture MPa	$P_{SR}(\mathbf{C})$
Resistivity μΩcm	$P_{resis}(\mathbf{C})$
Entropy Jmol^{-1}K^{-1}	$P_{entropy}(\mathbf{C})$
Low cycle fatigue	$P_{LCF}(\mathbf{C})$
High cycle fatigue	$P_{HCF}(\mathbf{C})$
Weldability	$P_{weld}(\mathbf{C})$
Creep model	$P_{creep}(\mathbf{C})$

→ $P_{spec}(\mathbf{C})$

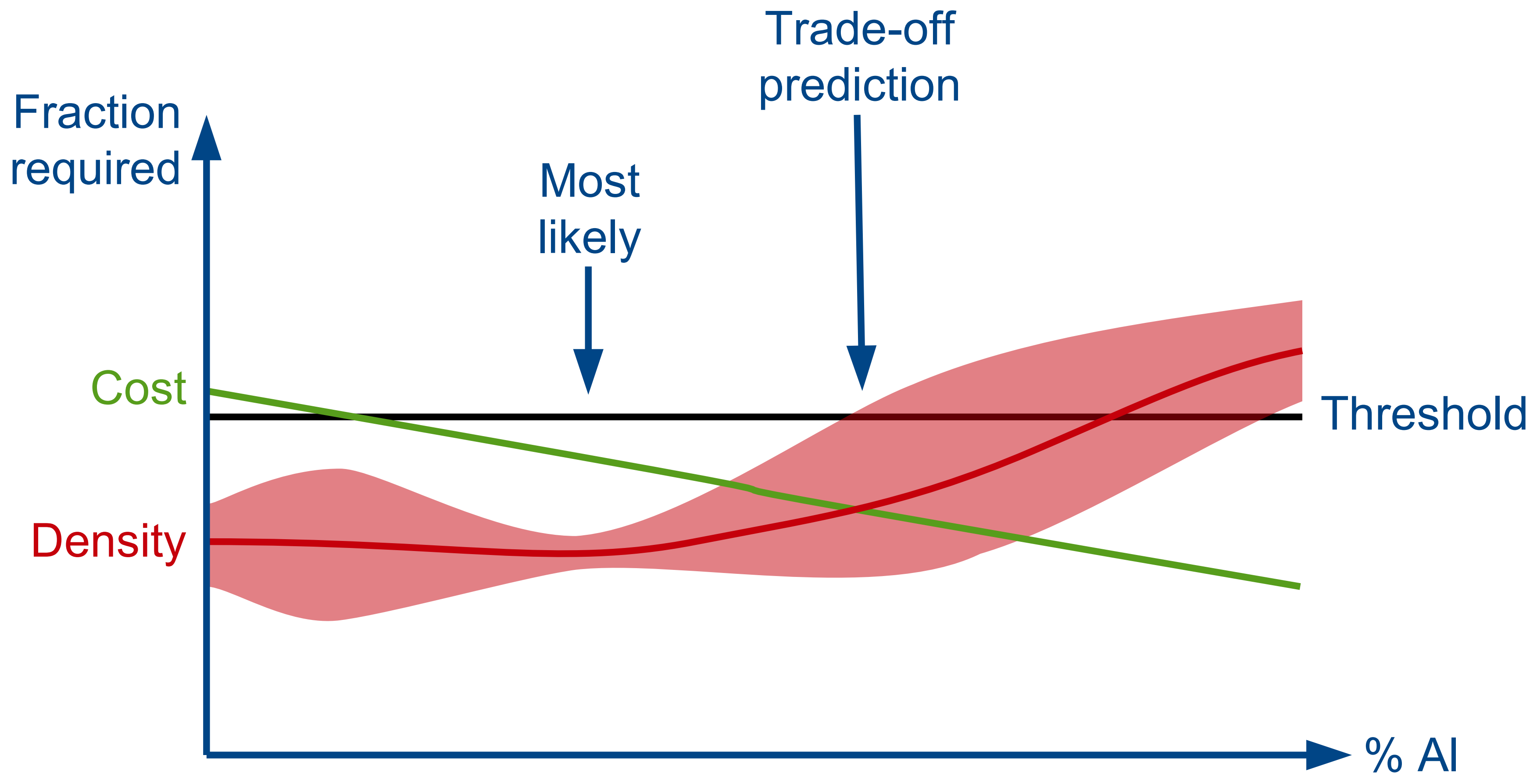
Optimization – probability



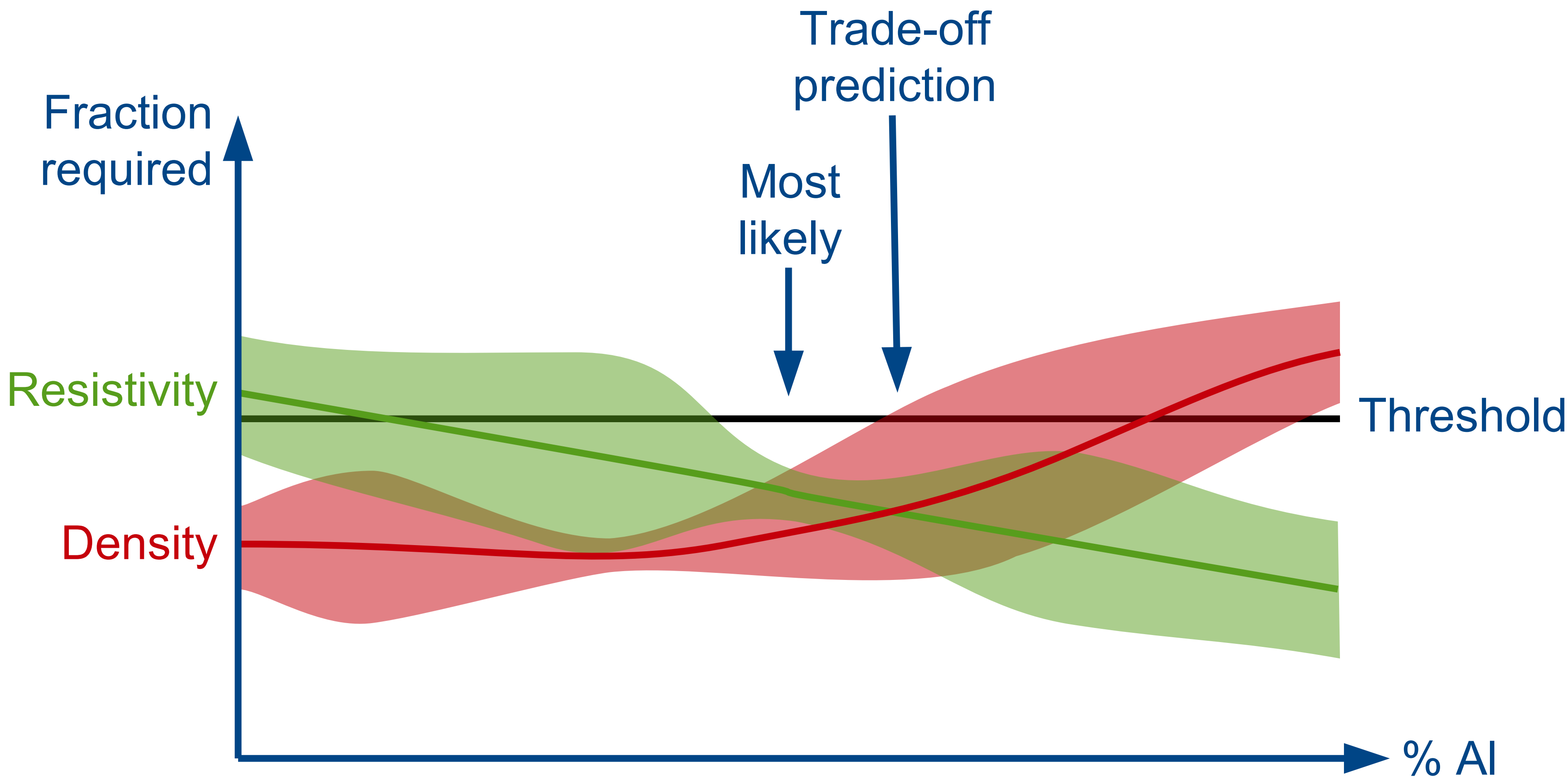
Optimization – probability



Optimization – probability



Optimization – probability



Optimization – probability

10 specified properties,
each with probability of 0.5

$0.5^{10} = 0.001$ chance of success

Multidimensional design space

Cr

Co

Mo

W

Ta

Nb

Al


Ti

Fe

Mn

Si

C

B

Zr


Cu

N

P

V

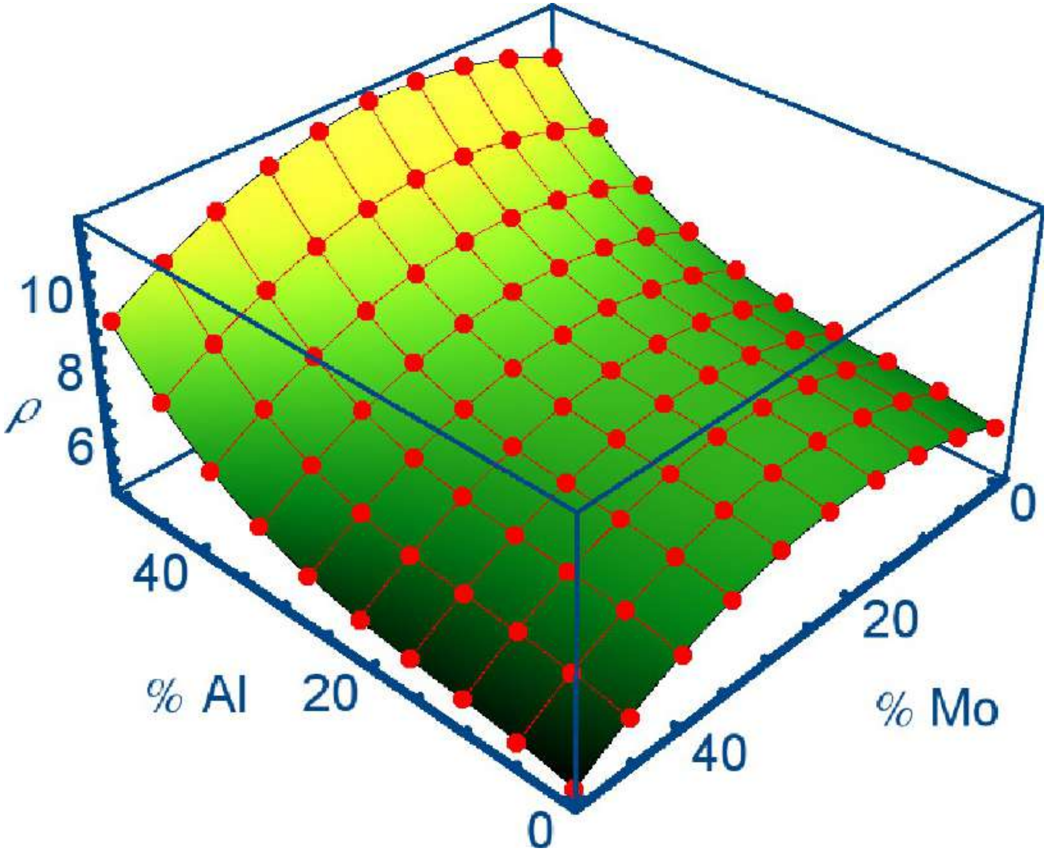
Hf

Mg

Ni

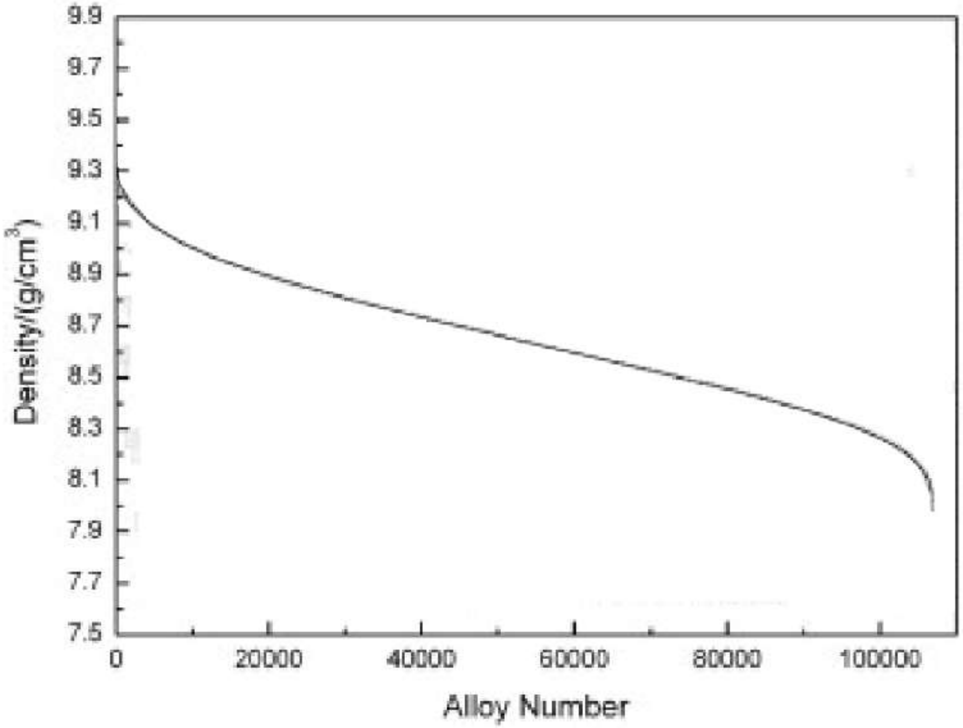

Heat treatment


Optimization – tradeoff diagrams



R.C. Reed, T. Tao & N. Warnken, Acta Materialia **57**, 5898 (2009)

Optimization – tradeoff diagrams



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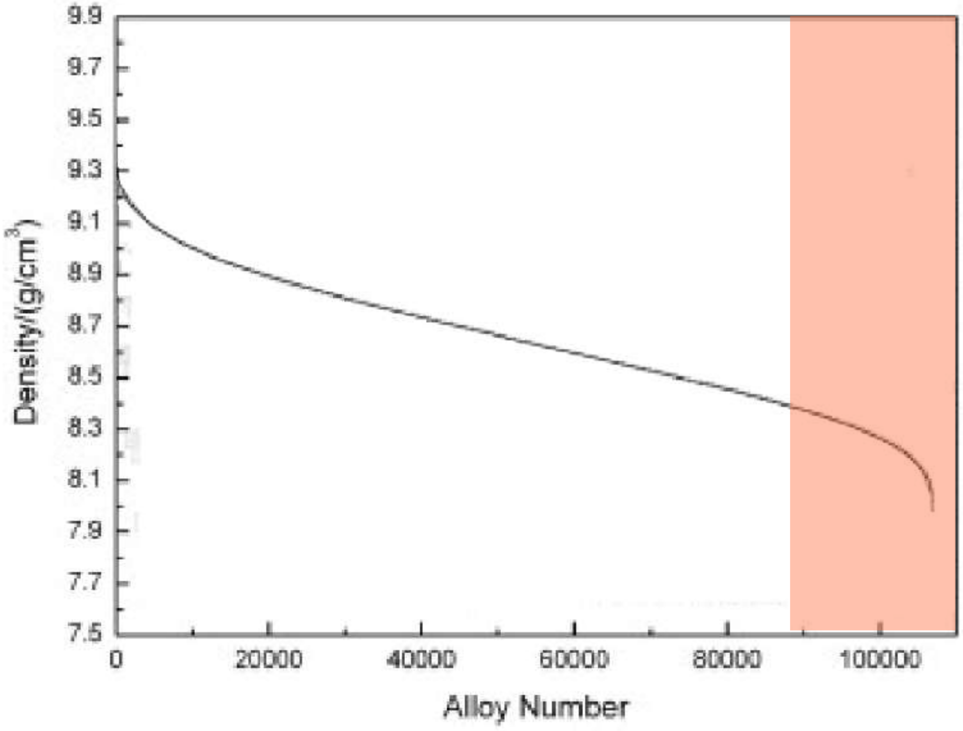

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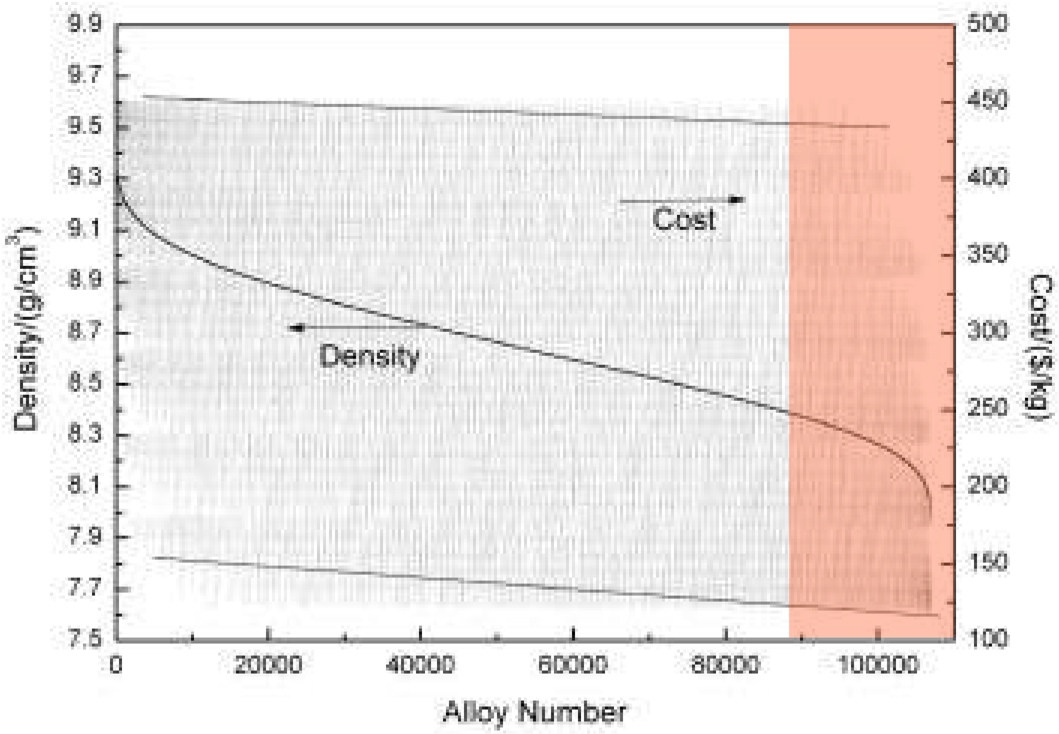

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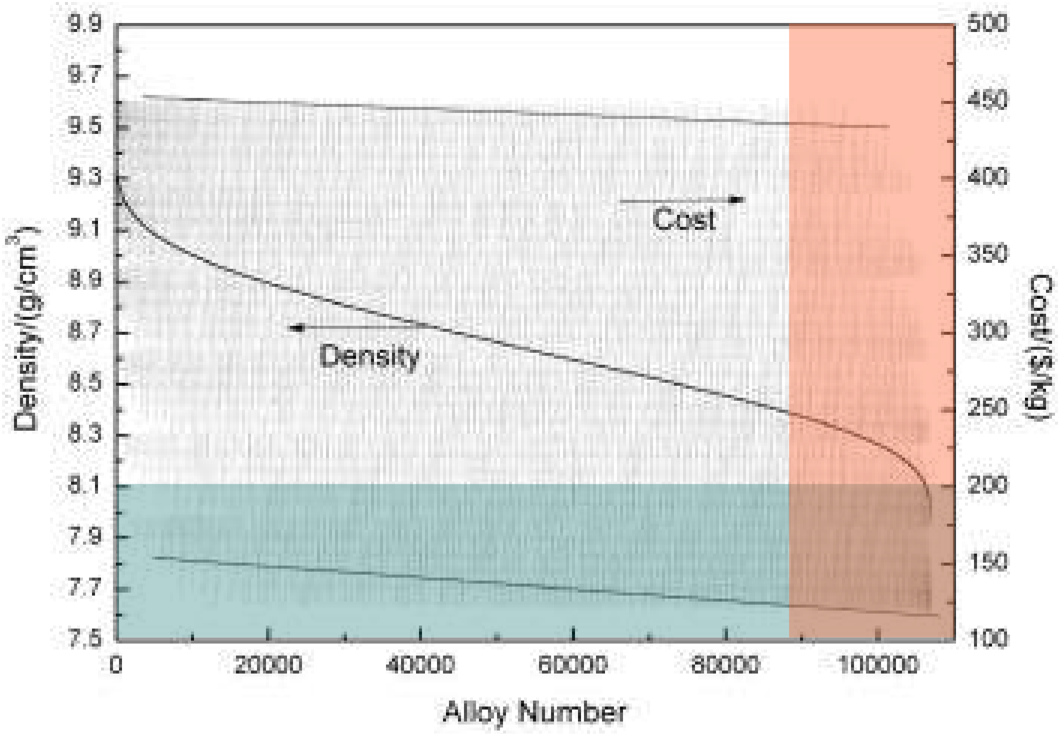

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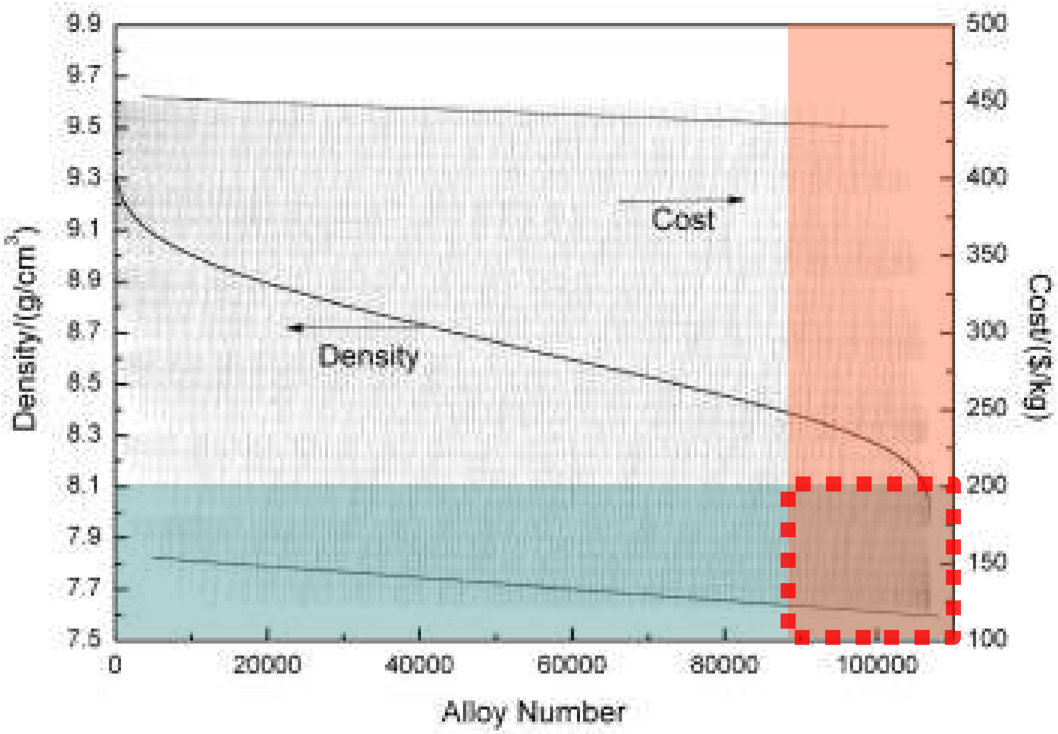

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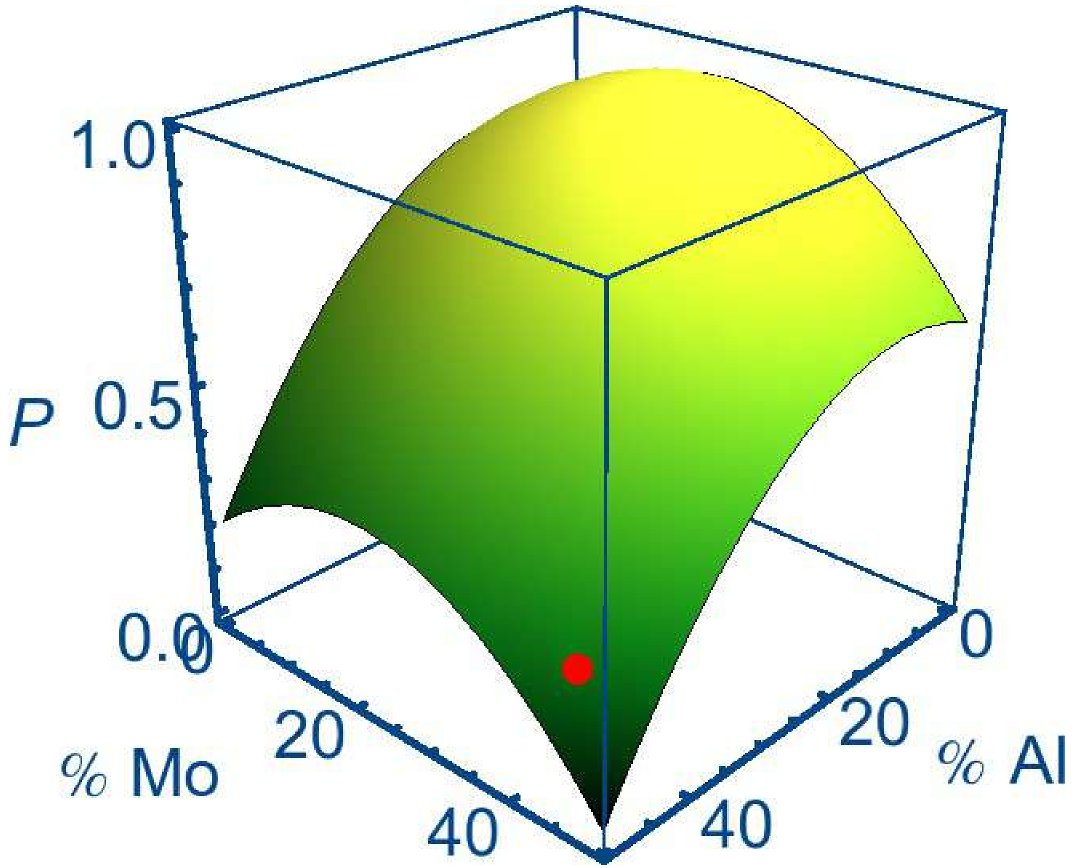
Optimization – tradeoff diagrams

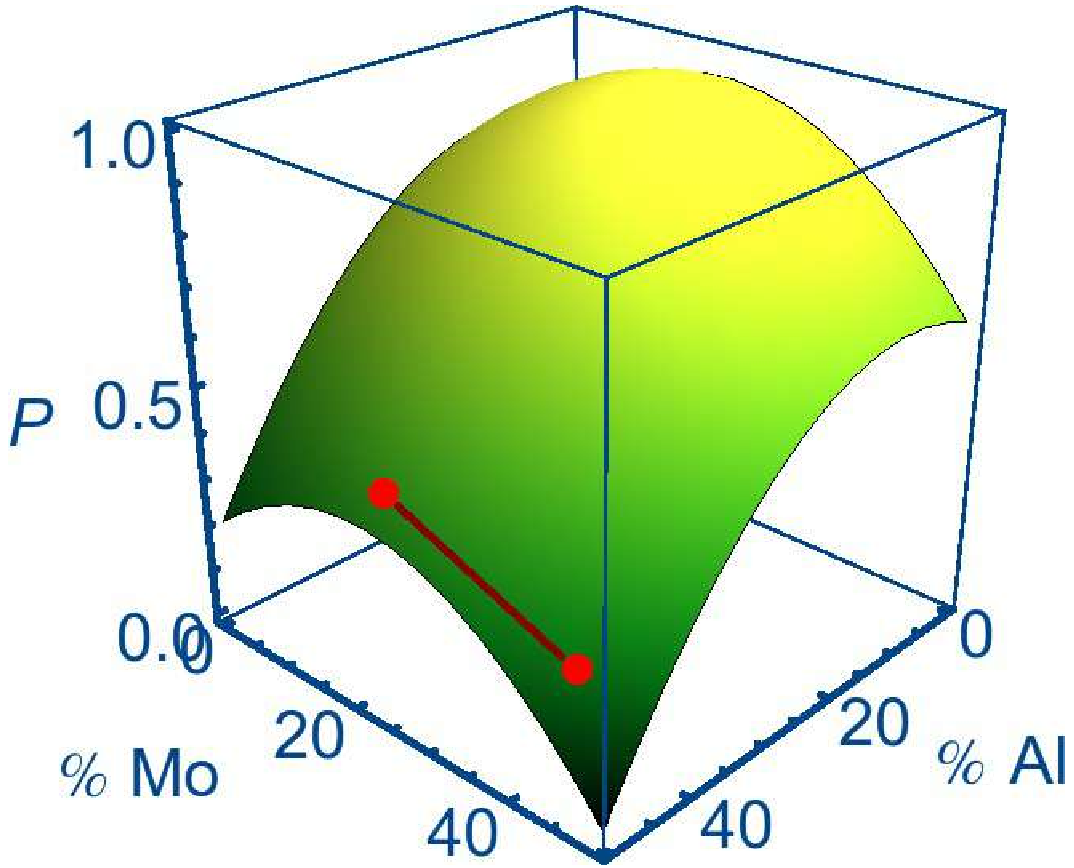
30 design variables, at 0.1% accuracy, and evaluation time of 1ms

$1000^{30} = 3\times10^{79}$ years

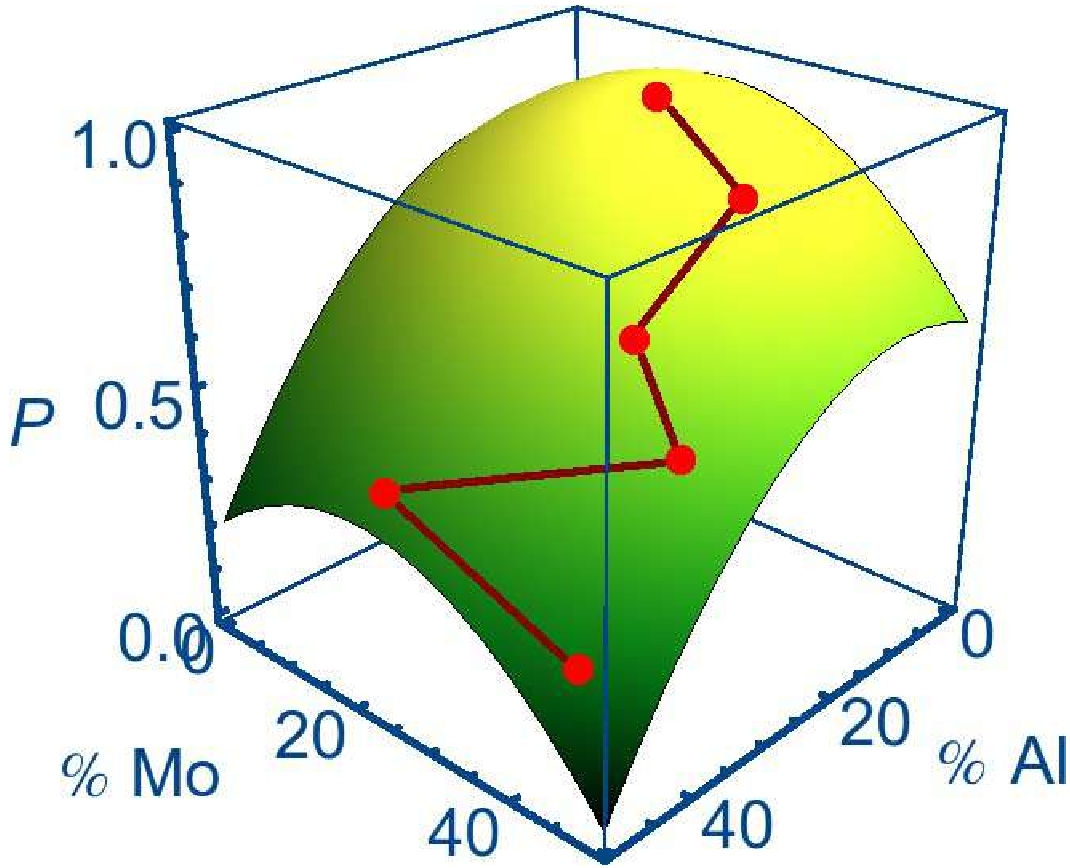
Optimization – replica exchange sampling



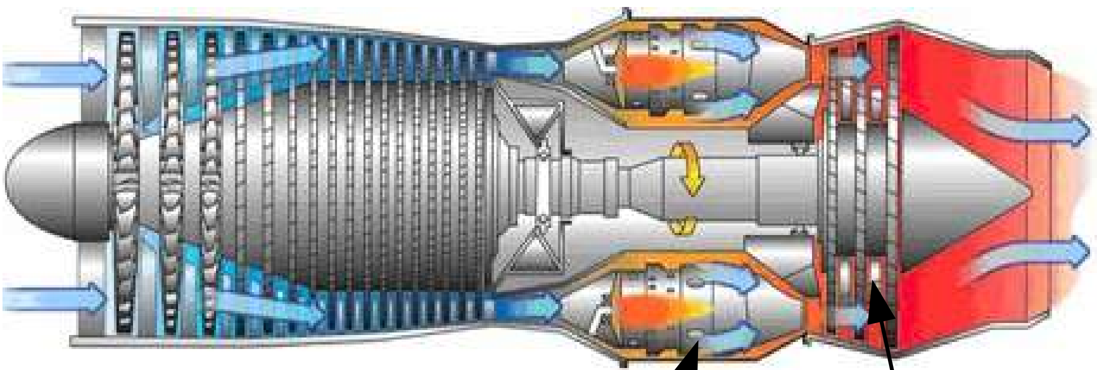
Optimization – replica exchange sampling



Optimization – replica exchange sampling



Predicted alloys

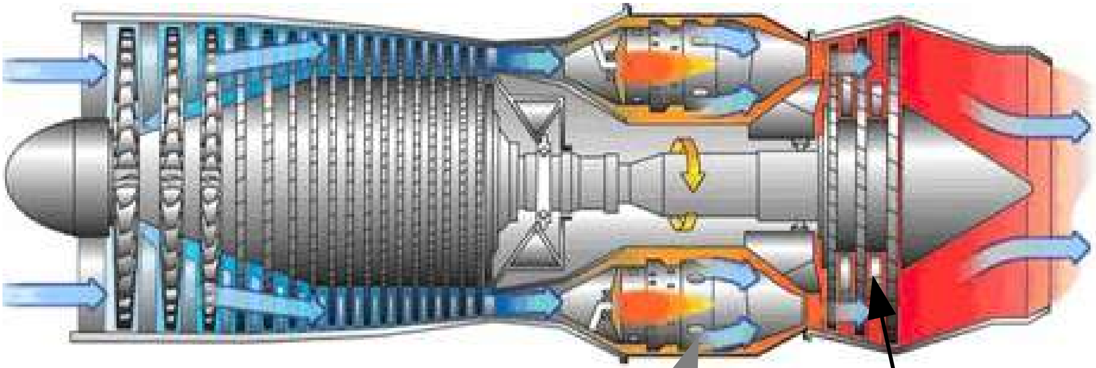


Combustor liner

2x disc alloy

2x forging hammer

Predicted alloys



Combustor liner

2x disc alloy

2x forging hammer

Case study: improved disc alloy











Ni	Cr	Co	Mo	Ti	Al	Ta	Hf	C	T	t
52	15	19	5	3.6	3	2	0.5	0.1	800	8

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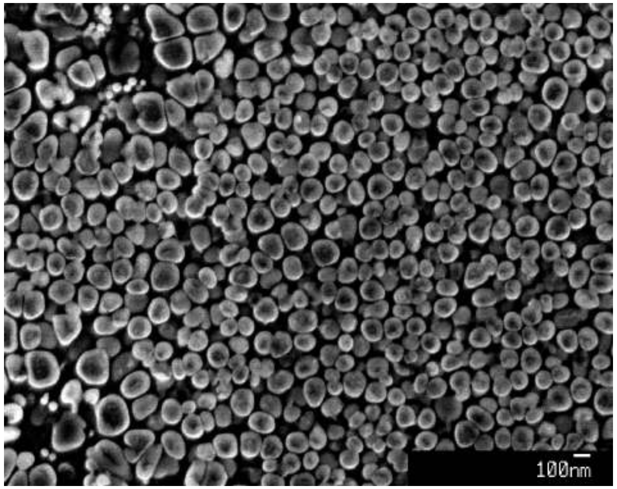
Case study: improved disc alloy

										
Ni	**Cr**	**Co**	**Mo**	**Ti**	**Al**	**Ta**	**Hf**	**C**	**T**	**t**
56	17	1.0	4.0	1.5	4.3	0.2	0.1	0.2	980	61

							
W	**Mn**	**B**	**V**	**Si**	**Zr**	**Nb**	**Fe**
6.0	0.1	0.1	0.1	0.1	0.2	5.6	3.4

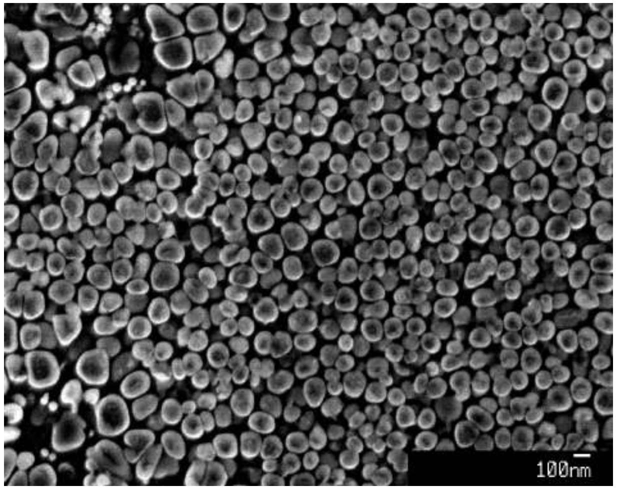
Electron micrograph – Ni disc alloy

Ni disc alloy

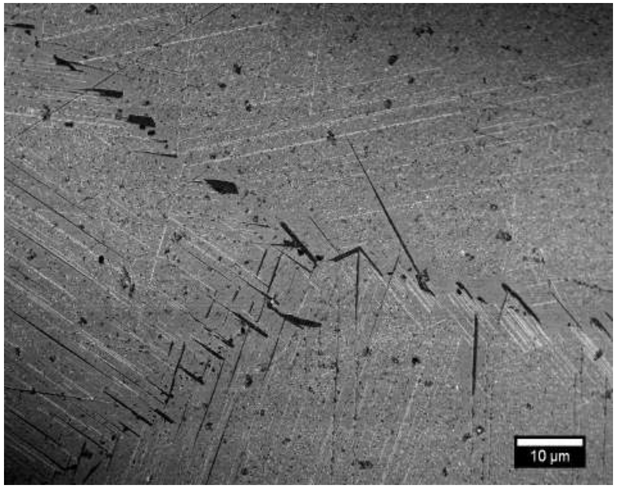


Electron micrograph – Ni disc alloy

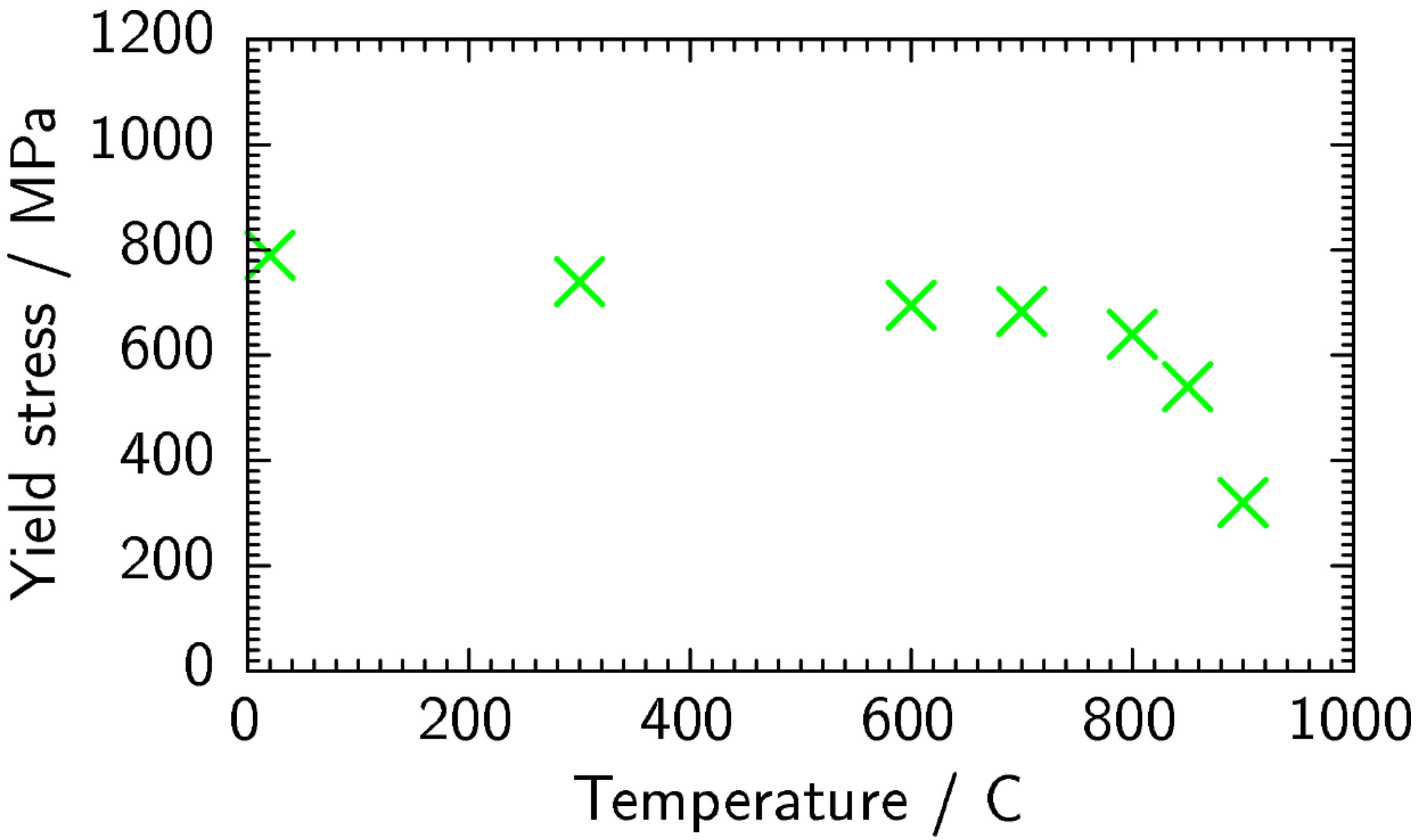
Ni disc alloy



η contaminated alloy



Yield stress



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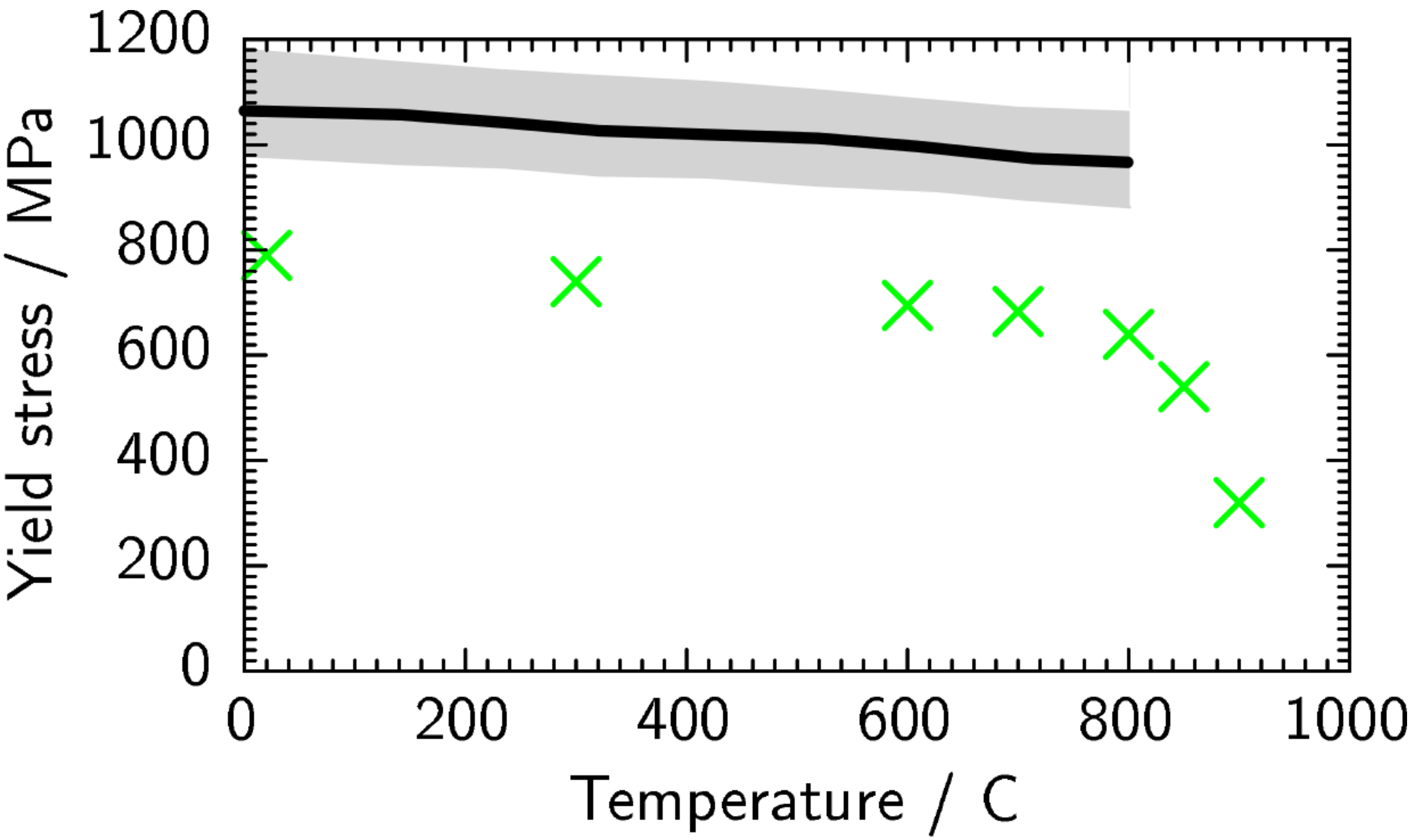

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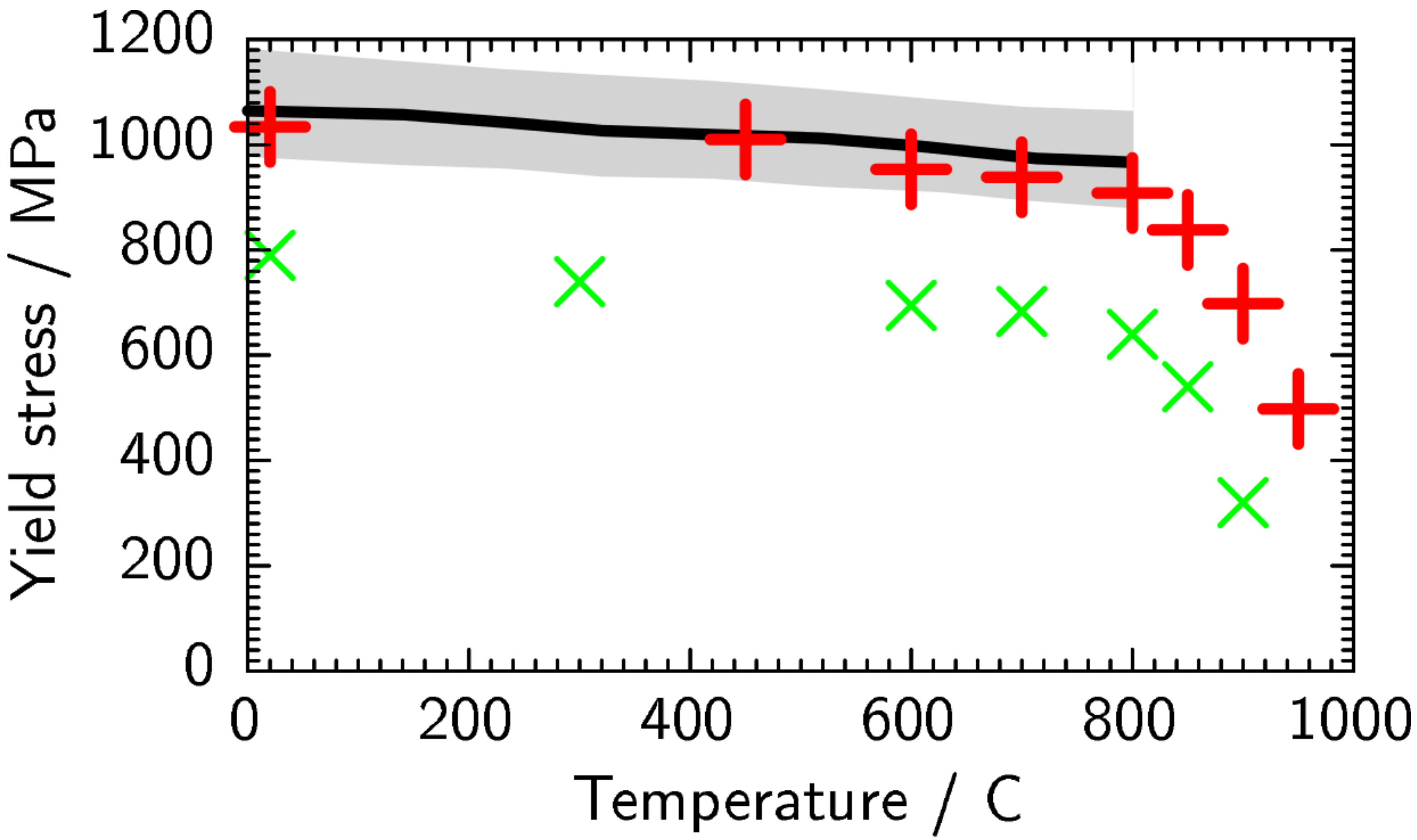
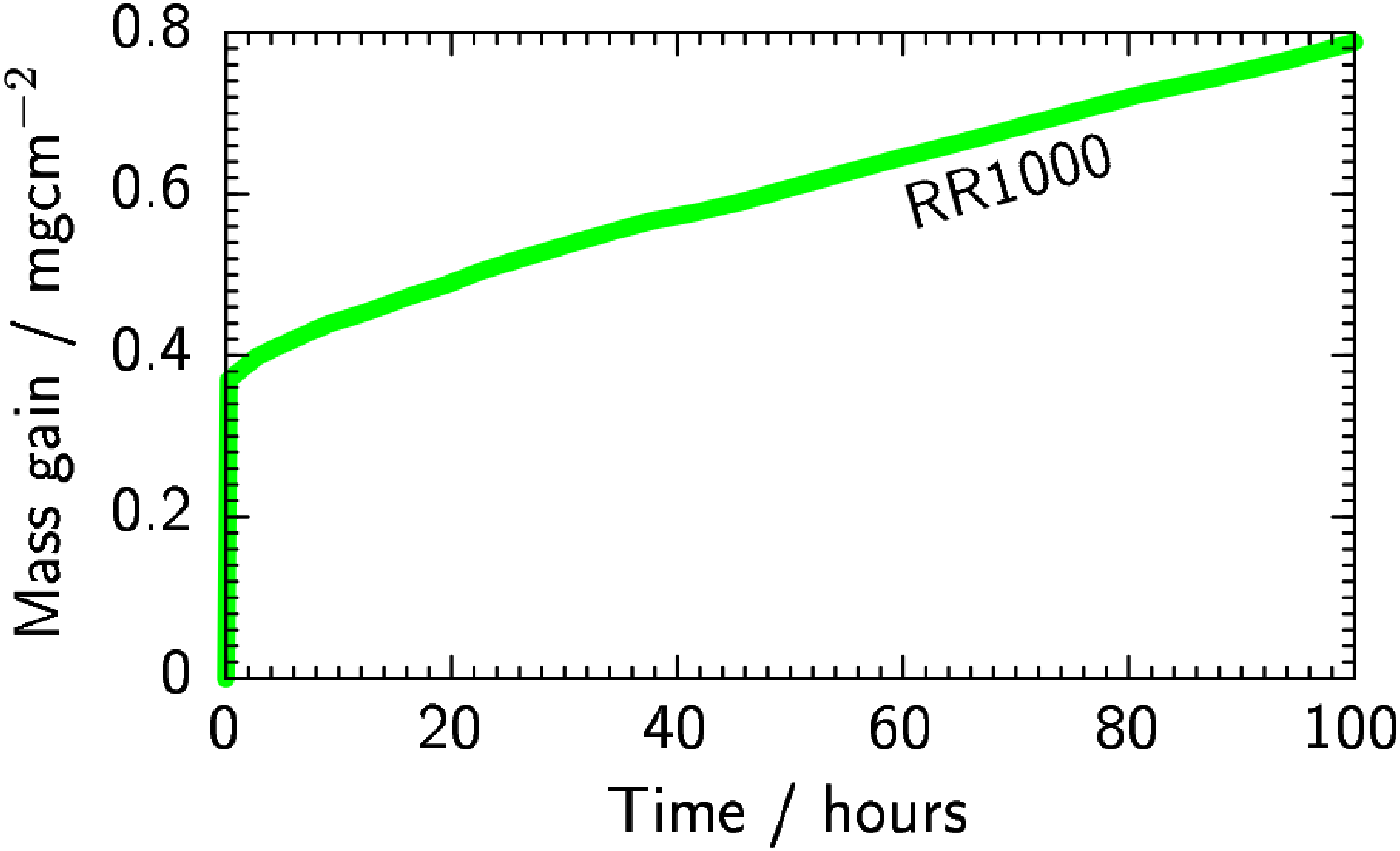
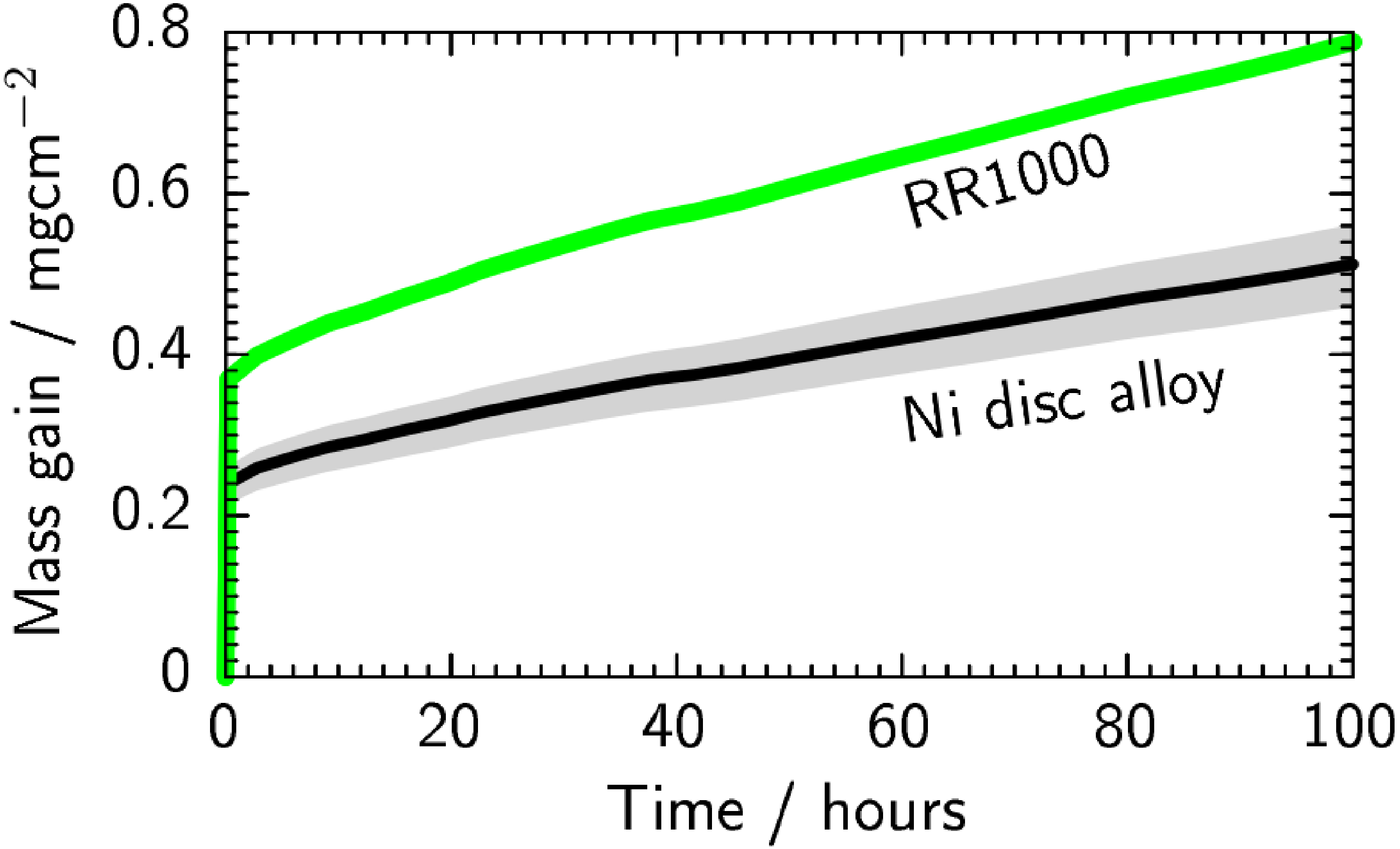


Oxidation

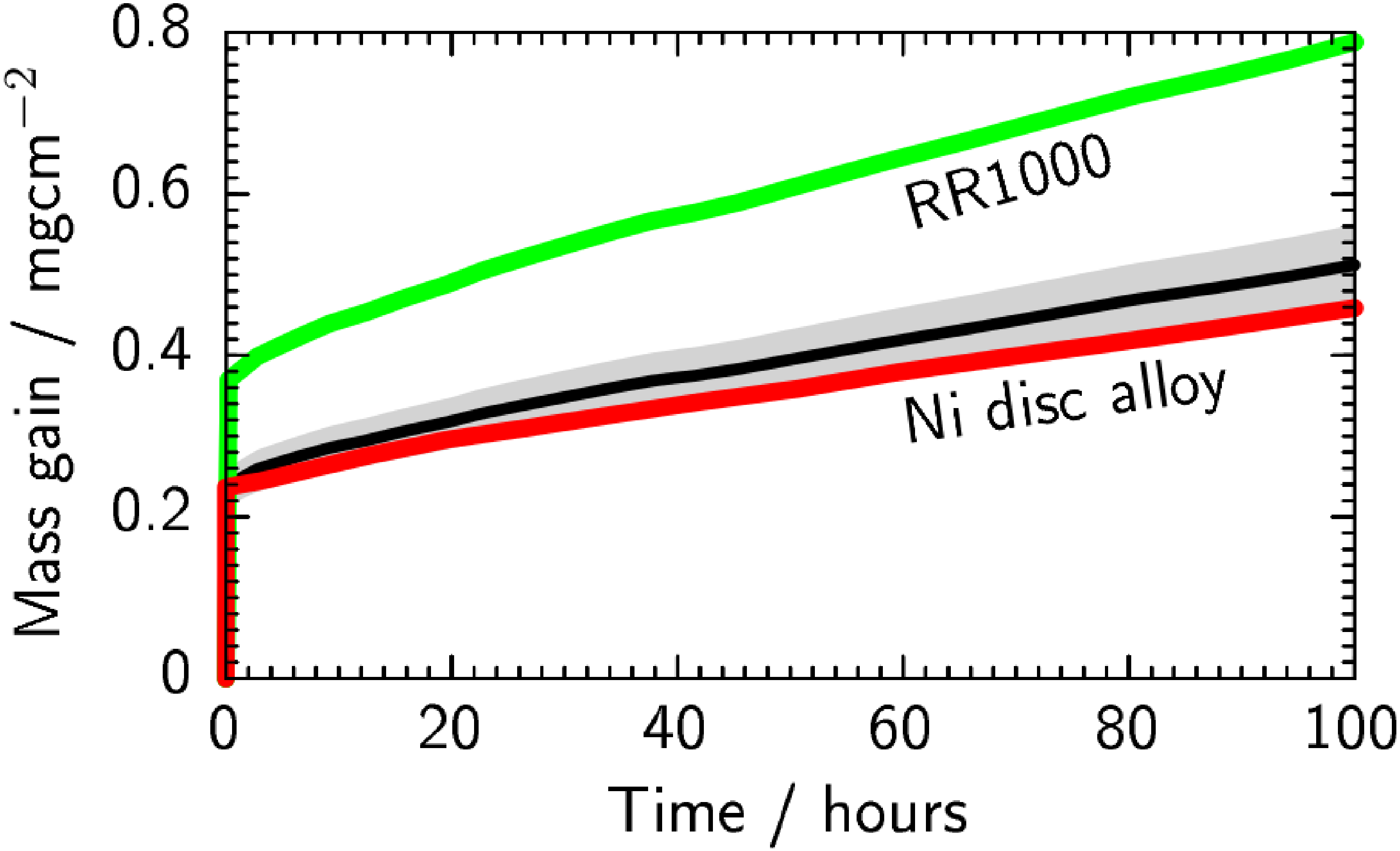


Oxidation



0.8
0.6
0.4
0.2
0
Mass gain / mgcm^{-2}
0
20
40
60
80
100
Time / hours
RR1000
Ni disc alloy

Oxidation



0.8
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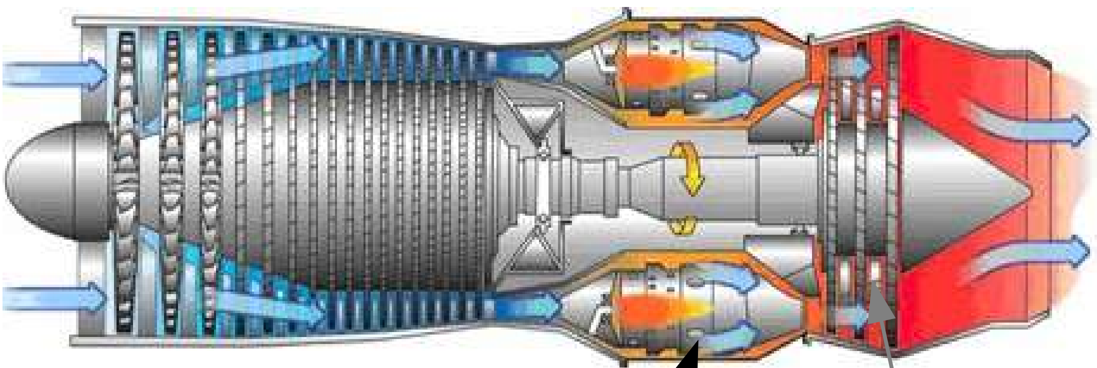
Ni disc alloy

Predicted alloys

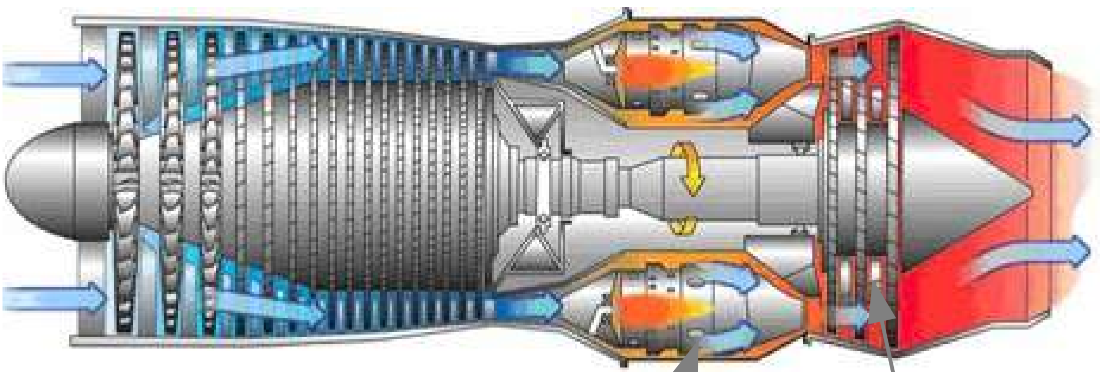


Combustor liner

2x disc alloy

2x forging hammer

Predicted alloys



Combustor liner

2x disc alloy

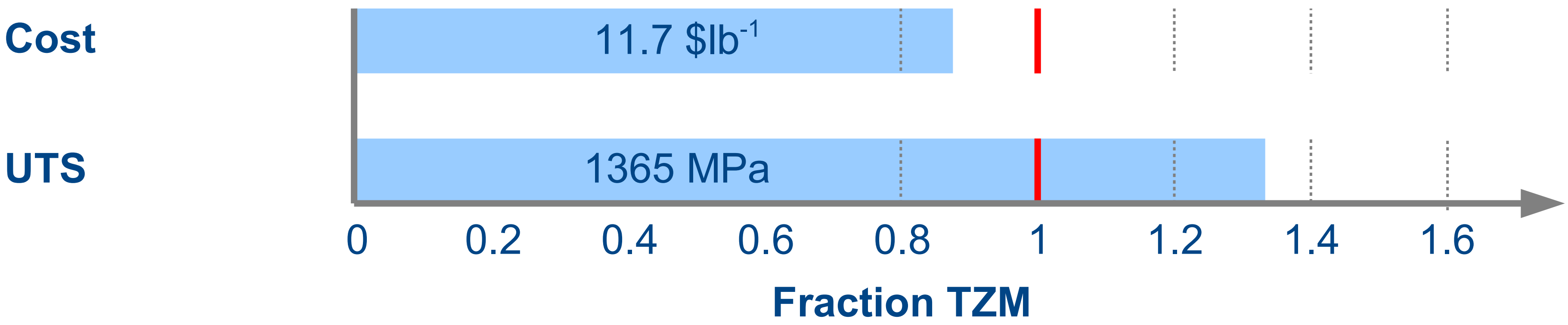
2x forging hammer

Case study: improved forging alloy




	Mo	Ti	C	Zr
TZM	99.4	0.5	0.02	0.08

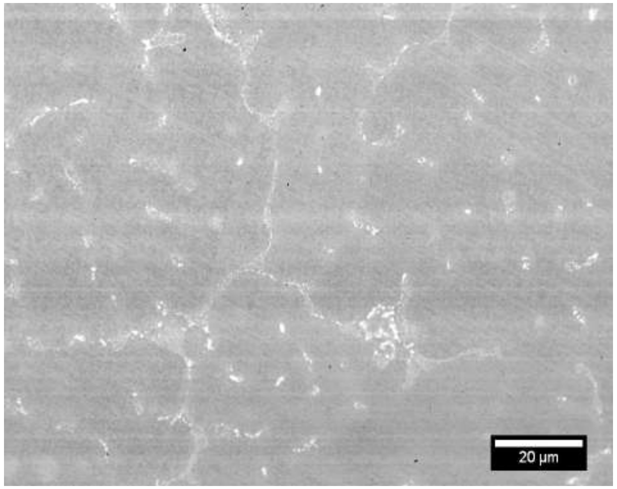
Case study: improved forging alloy



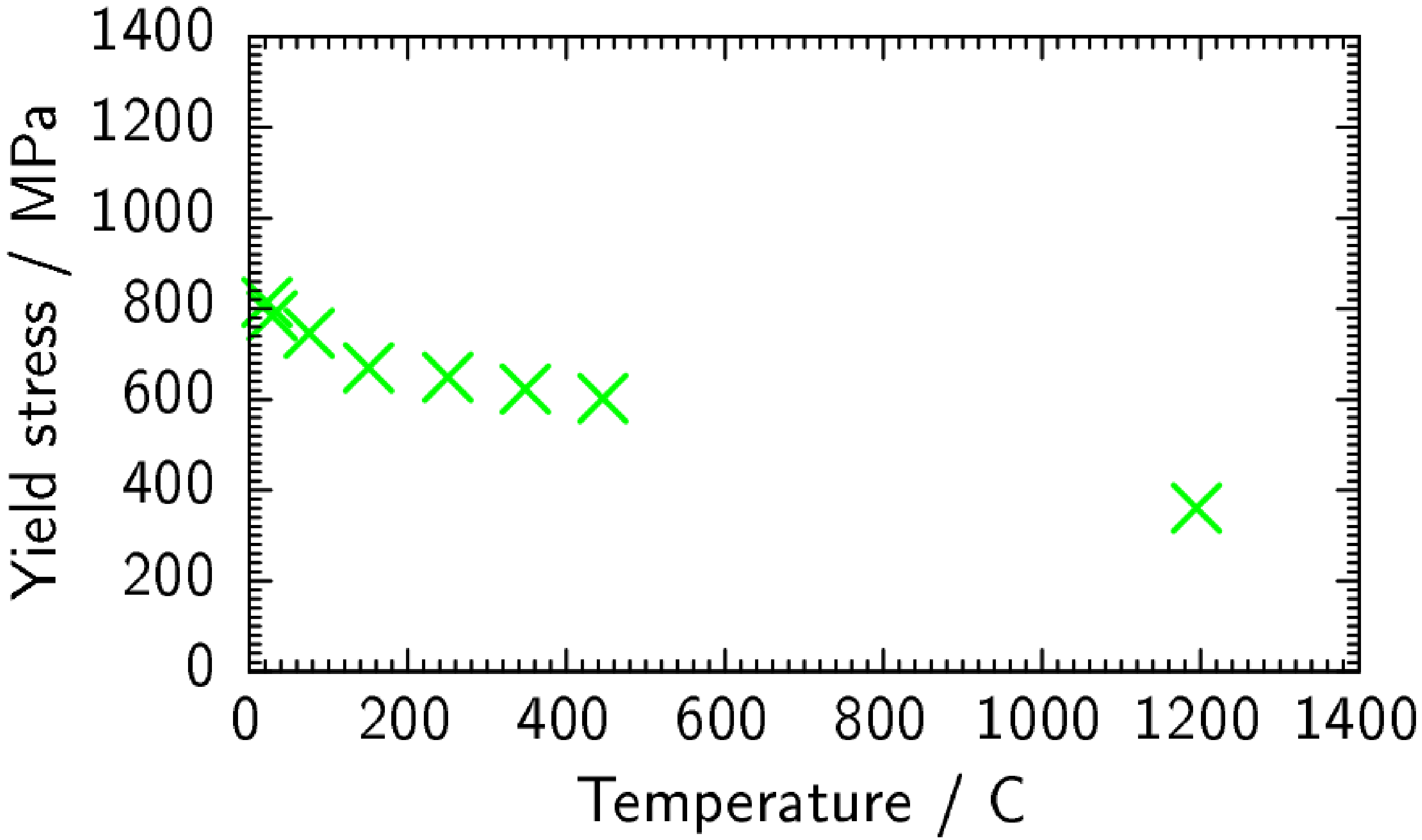
	Mo	Ti	C	Zr	Hf	W	Nb
TZM	99.4	0.5	0.02	0.08			
Optimal	82.7	1.0	0.2	0.9	9.0	0.5	5.7

Electron micrograph – Mo forging alloy

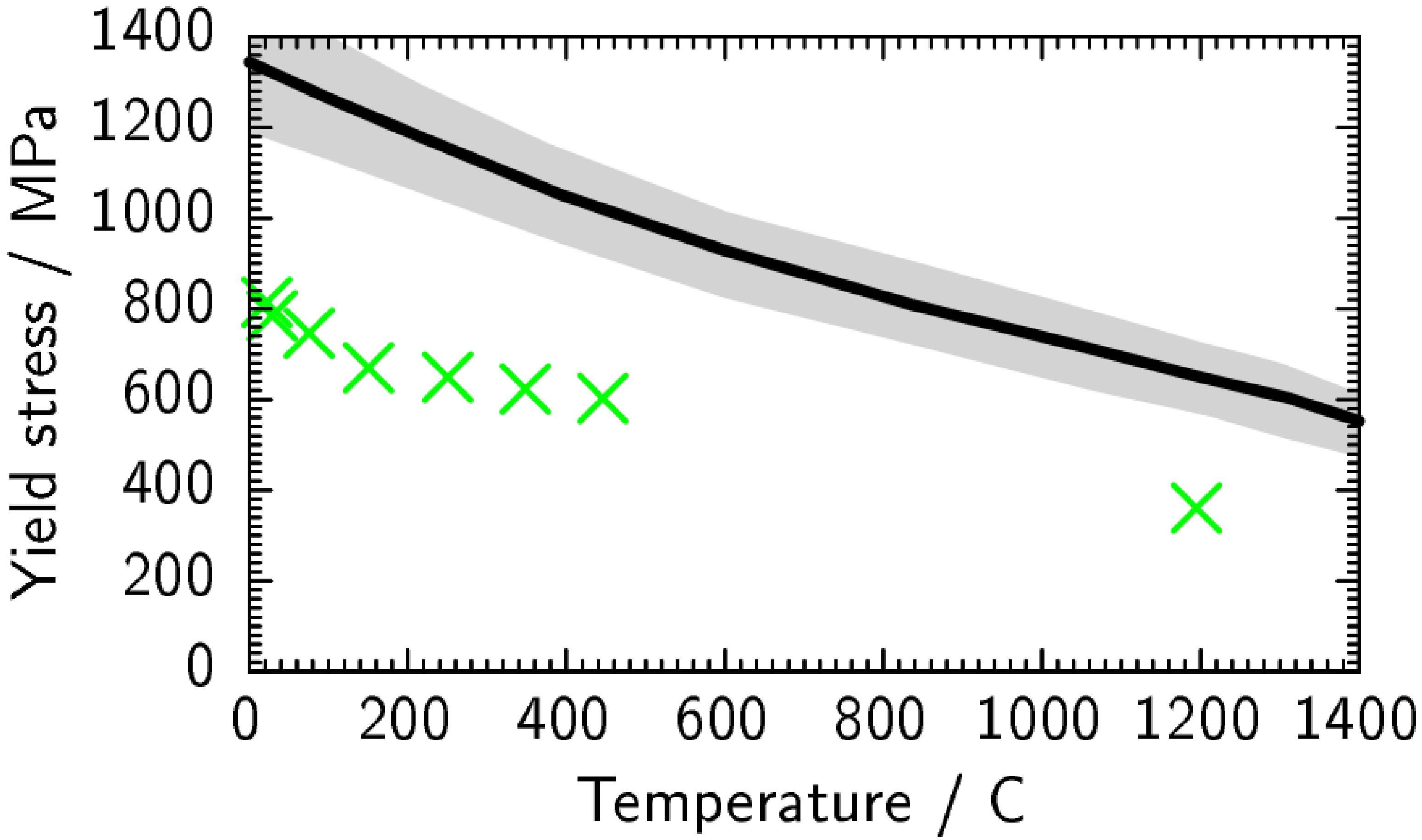
Mo forging alloy



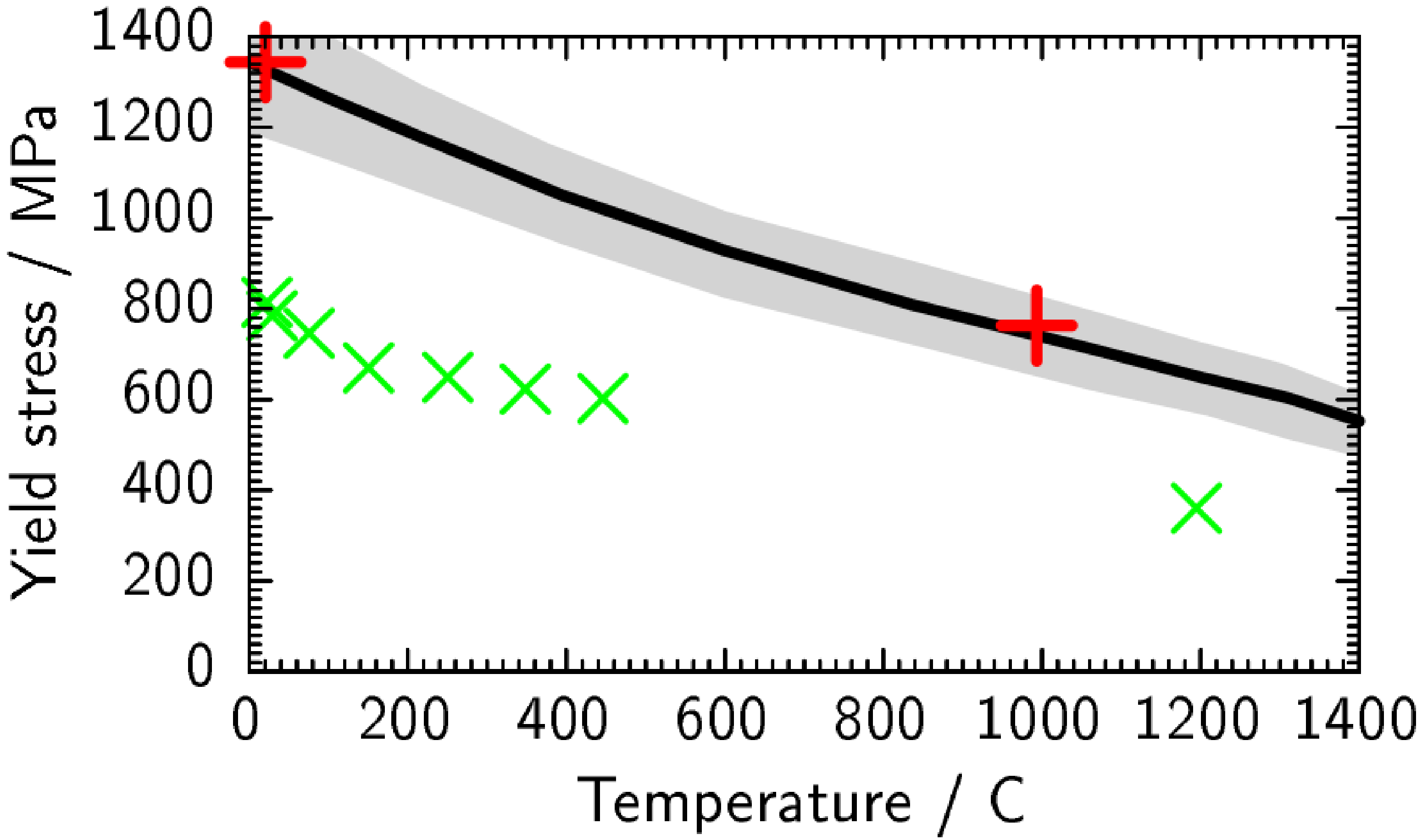
Yield stress



Yield stress

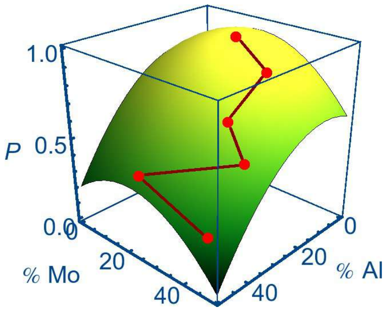


Yield stress

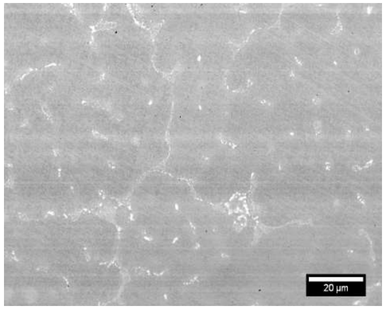


Concurrent materials design

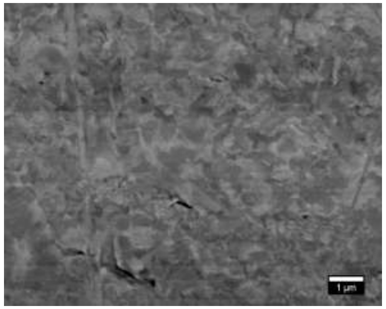
Discovery algorithm
Patent GB1302743.8 (2013)



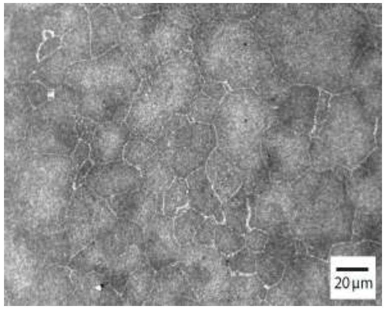
Mo-Hf forging alloy
Patent GB1307533.8 (2013)



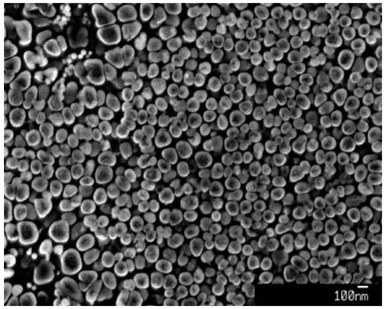
Mo-Nb forging alloy
Patent GB1307535.3 (2013)



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



Ni disc alloy
Rolls-Royce invention NC12261 (2012)



Ni combustor liner
Rolls-Royce invention NC13006 (2013)