UNIVERSITY OF CAMBRIDGE

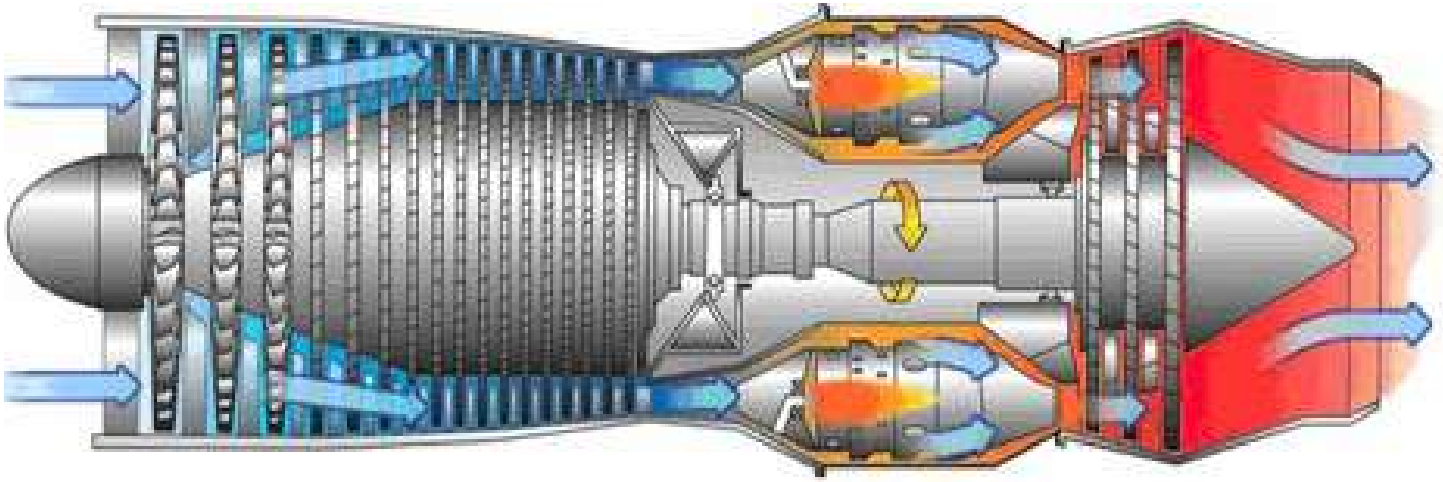
Concurrent materials design

Gareth Conduit

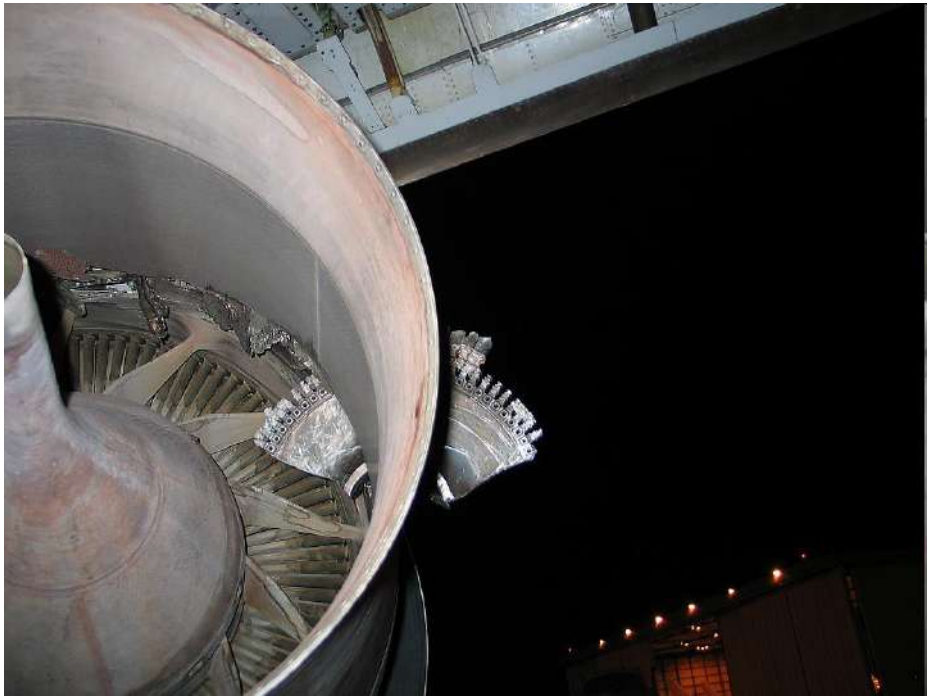
Patent GB1302743.8 (2013)
Patent GB1307533.8 (2013)
Patent GB1307535.3 (2013)
Acta Materialia, **61**, 3378 (2013)
Rolls-Royce Group plc invention submission NC12261 (2012)
Rolls-Royce Group plc invention submission NC13006 (2013)

TCM Group, Department of Physics

Jet engine



Jet engine: disc failure



Jet engine: bird strike

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24 May 2013 Last updated at 16:41

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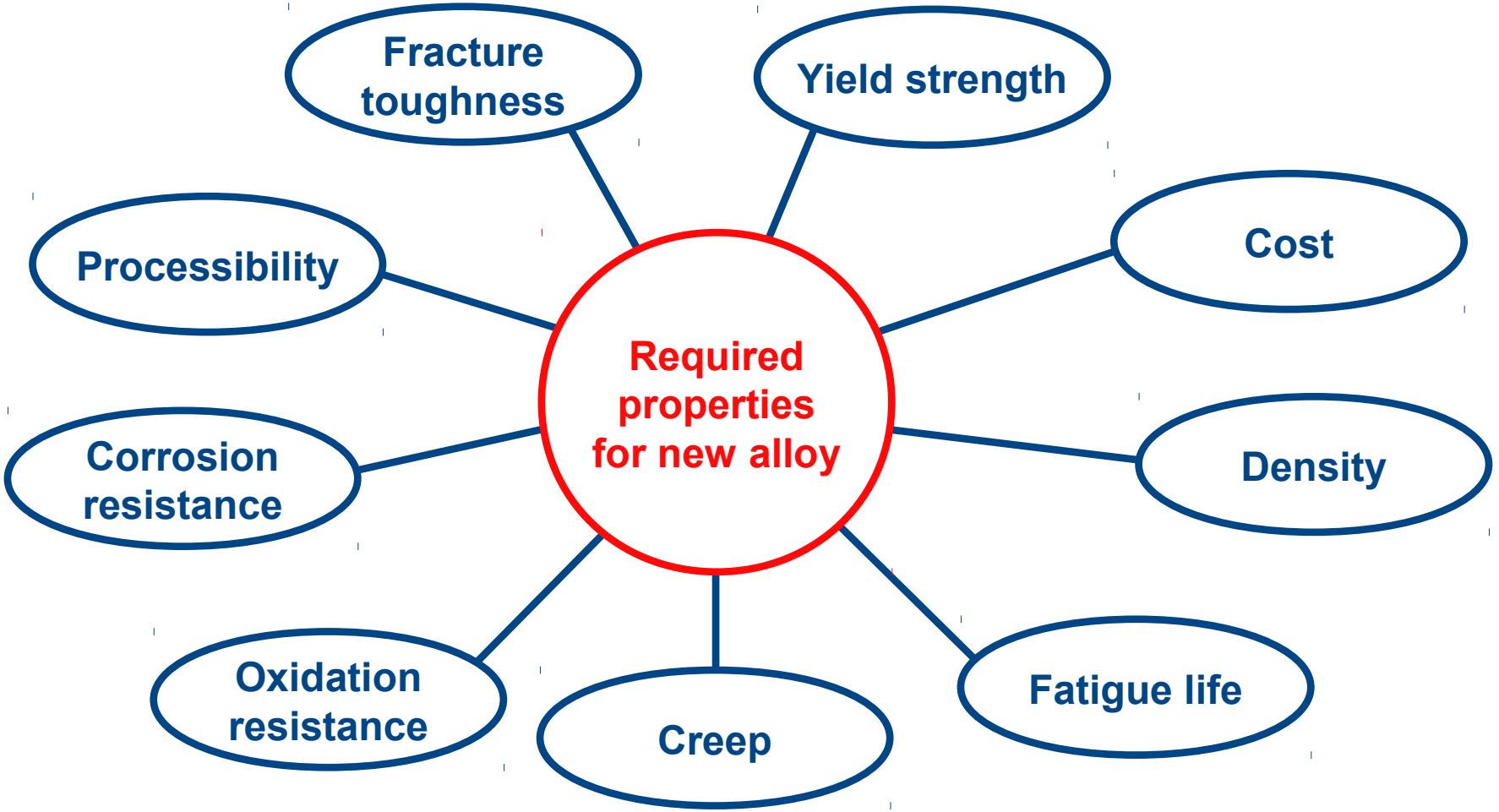
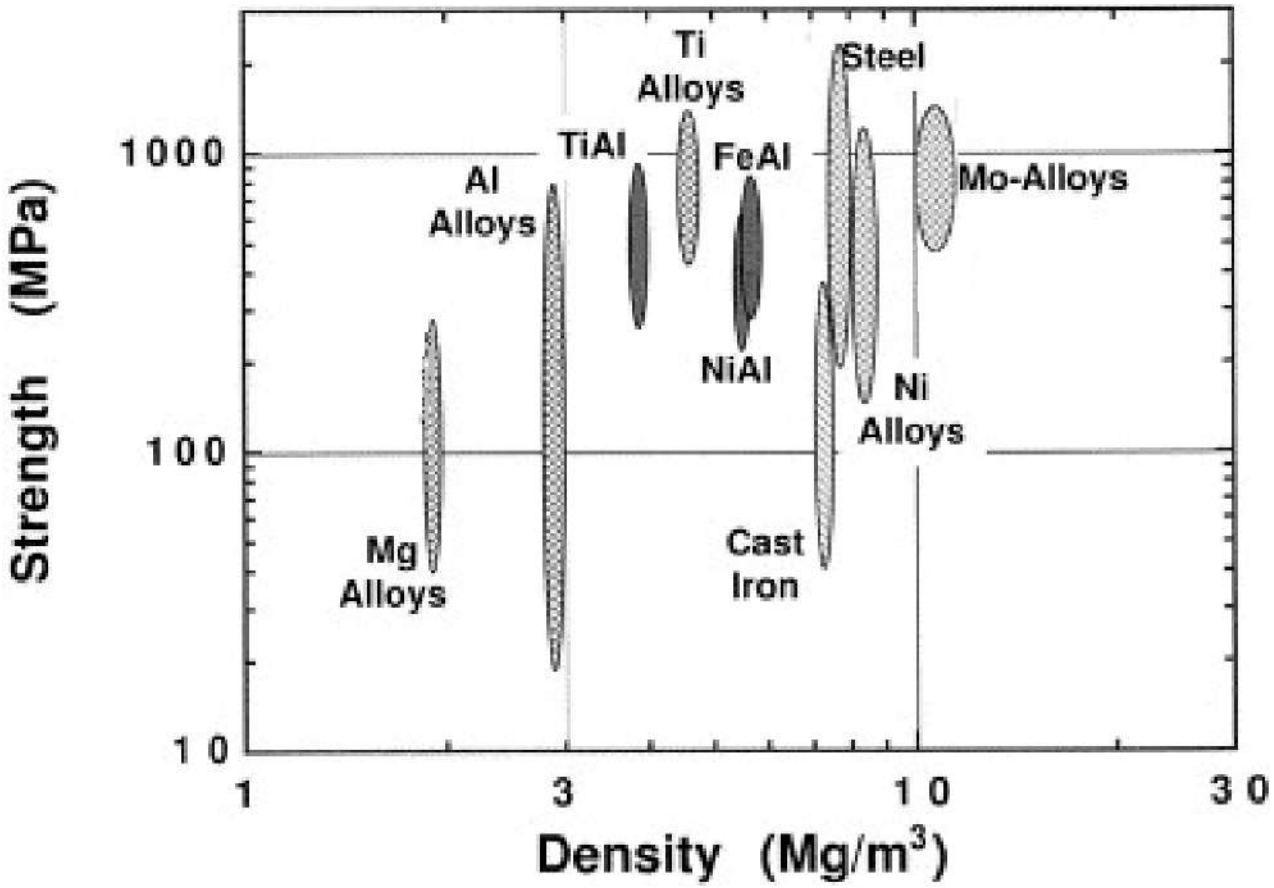
Plane 'fire' closes Heathrow runways

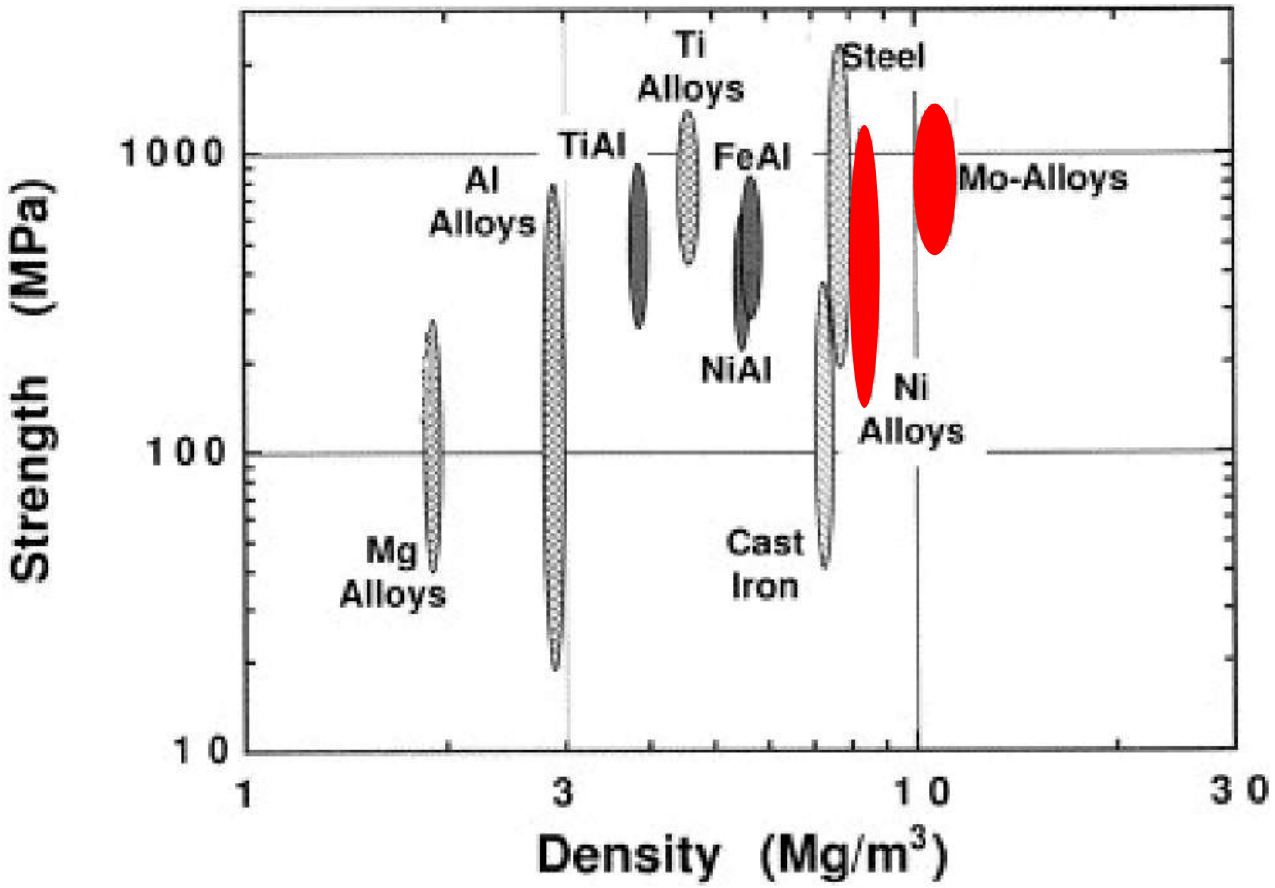
Designing a new alloy – what is required ?



Materials selection



Materials selection



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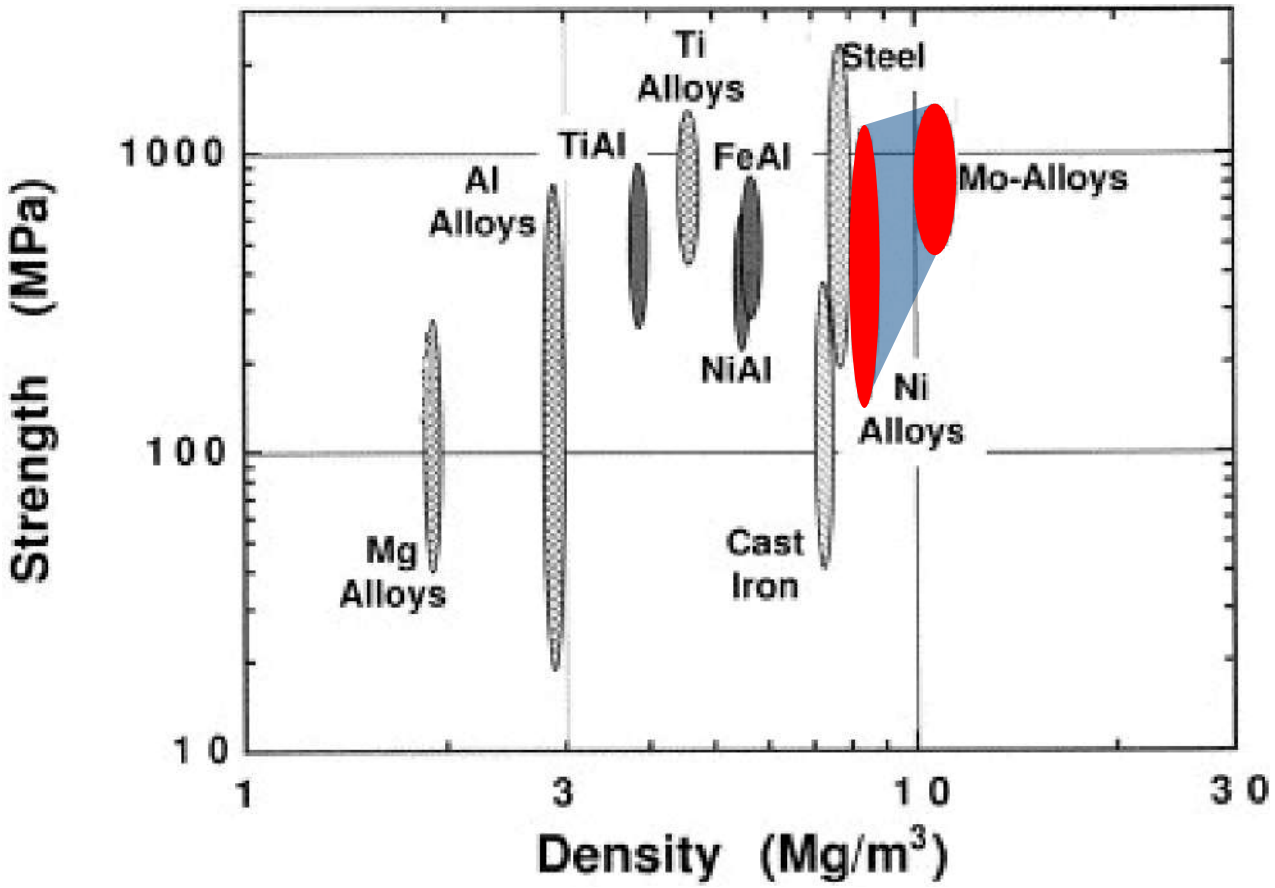

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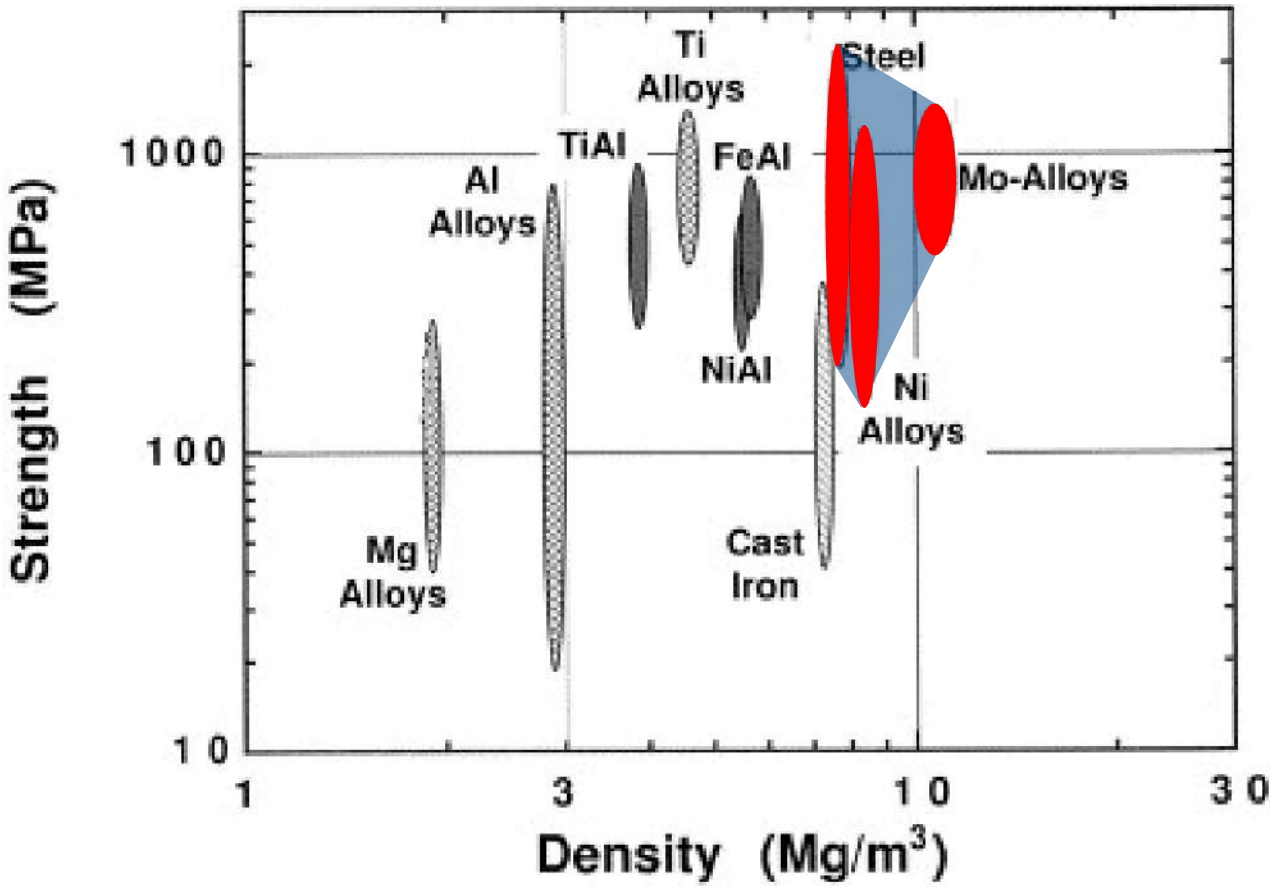
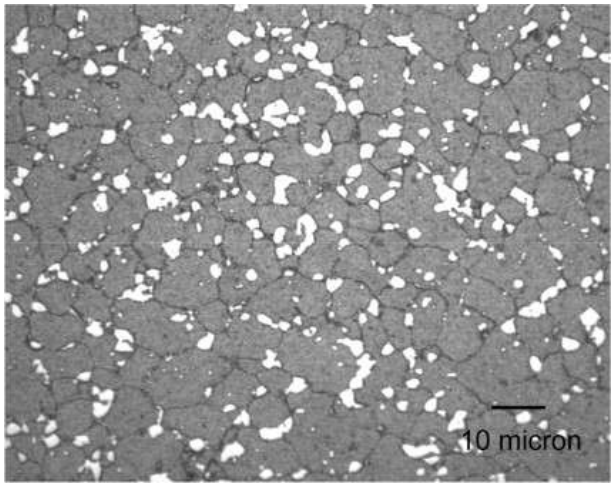
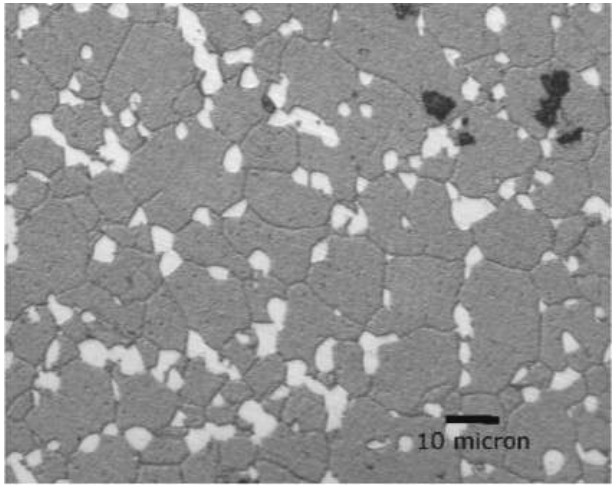


Contemporary alloys

RR1000

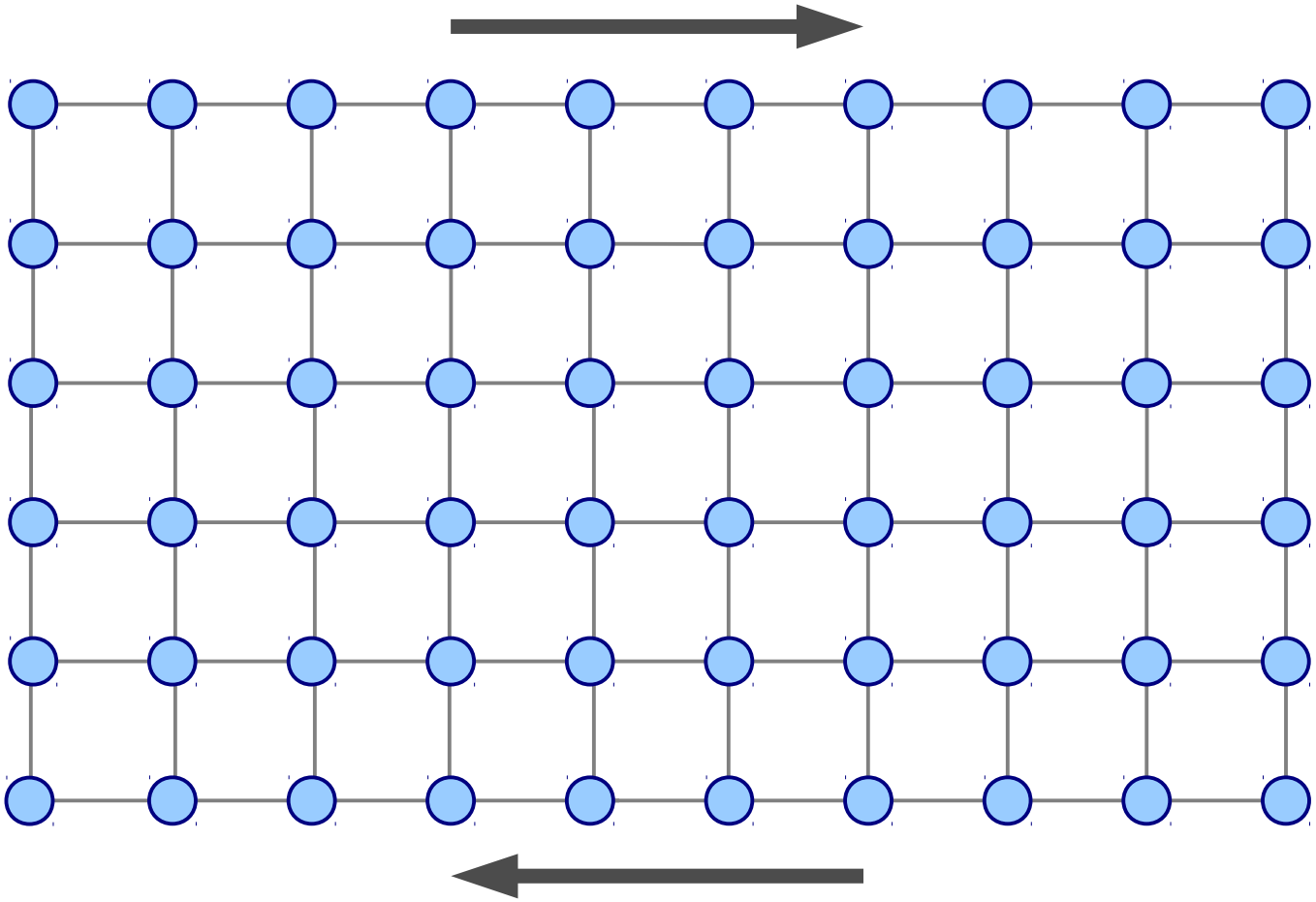


N18



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		

Creep



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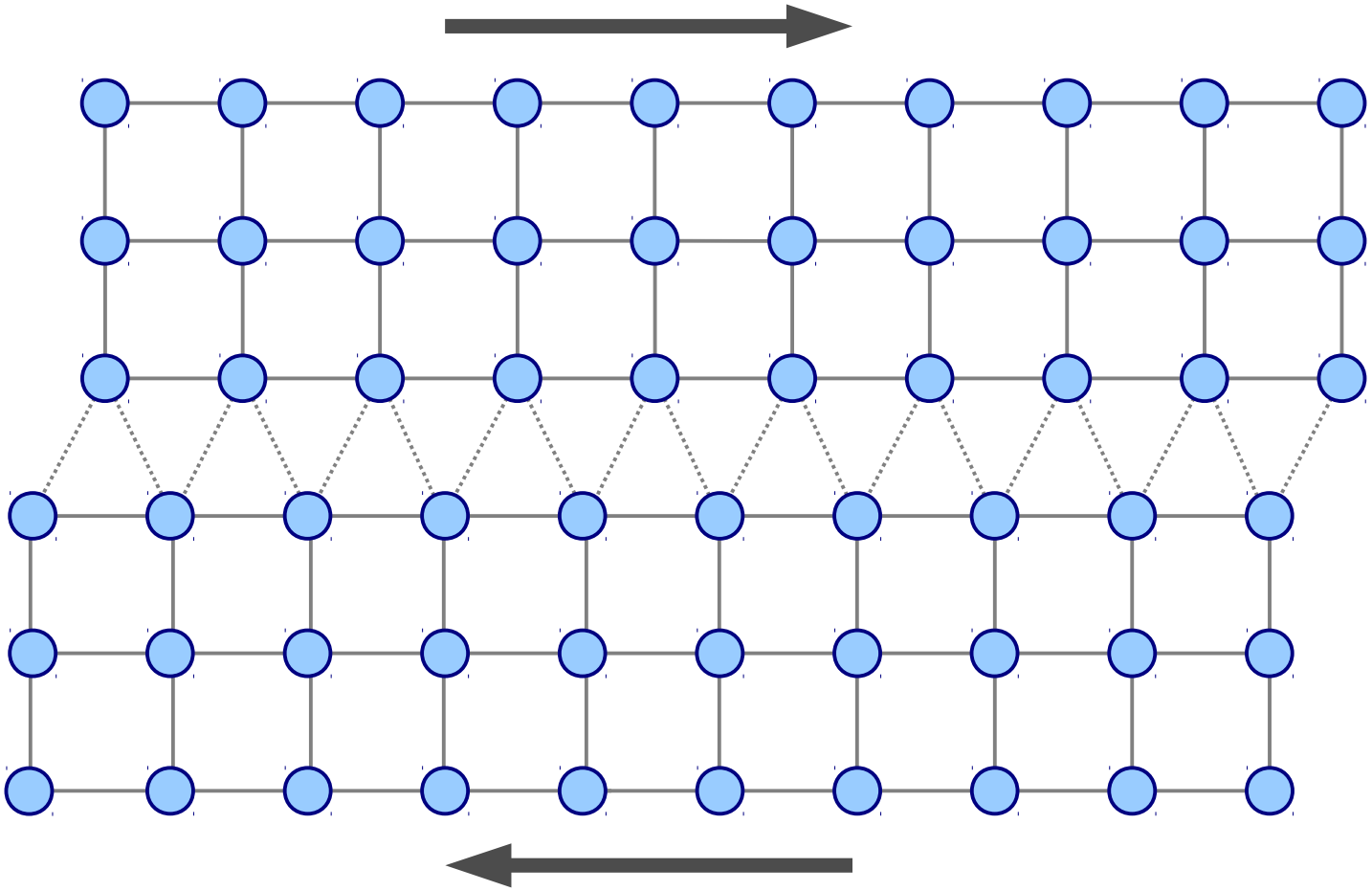

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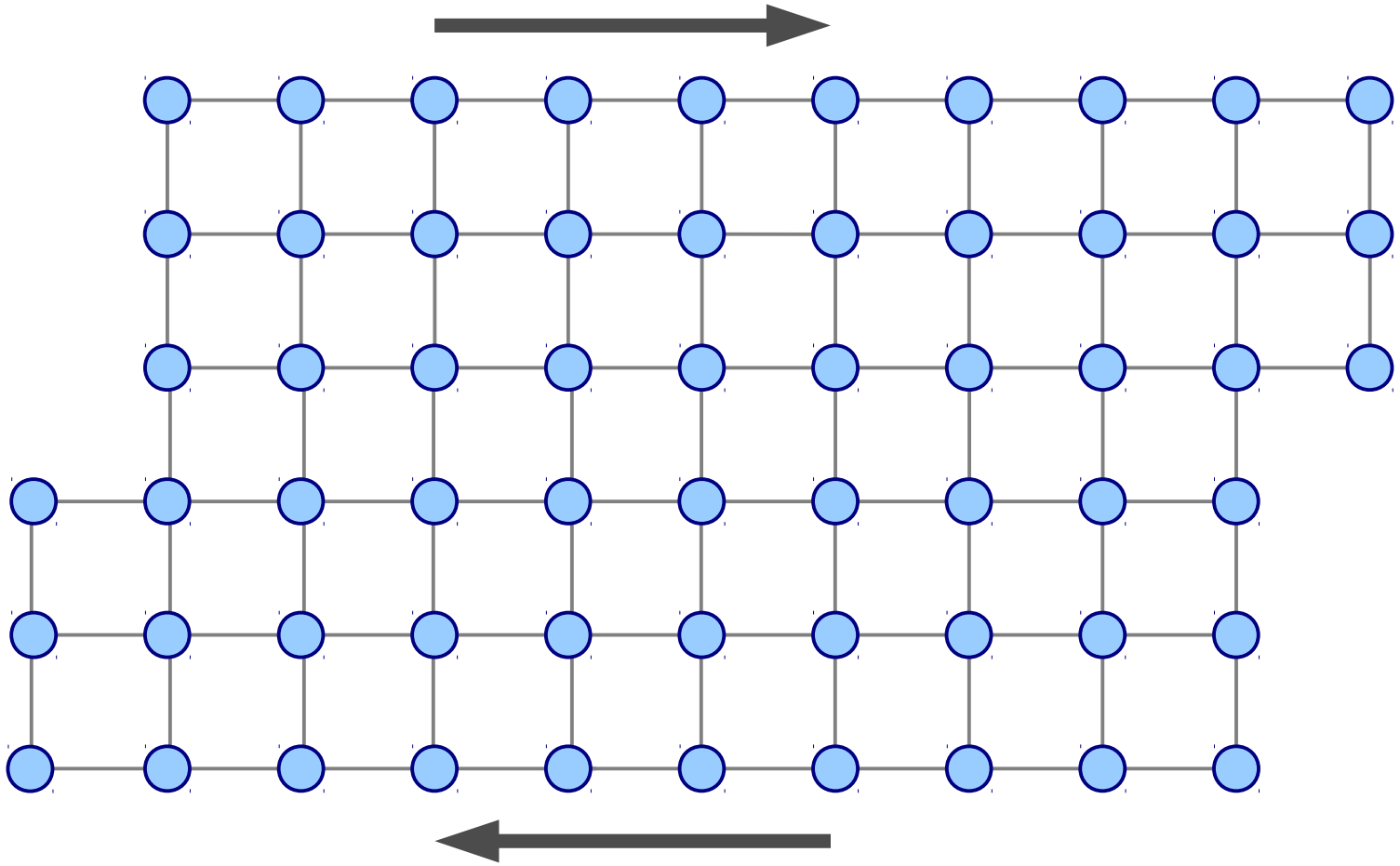

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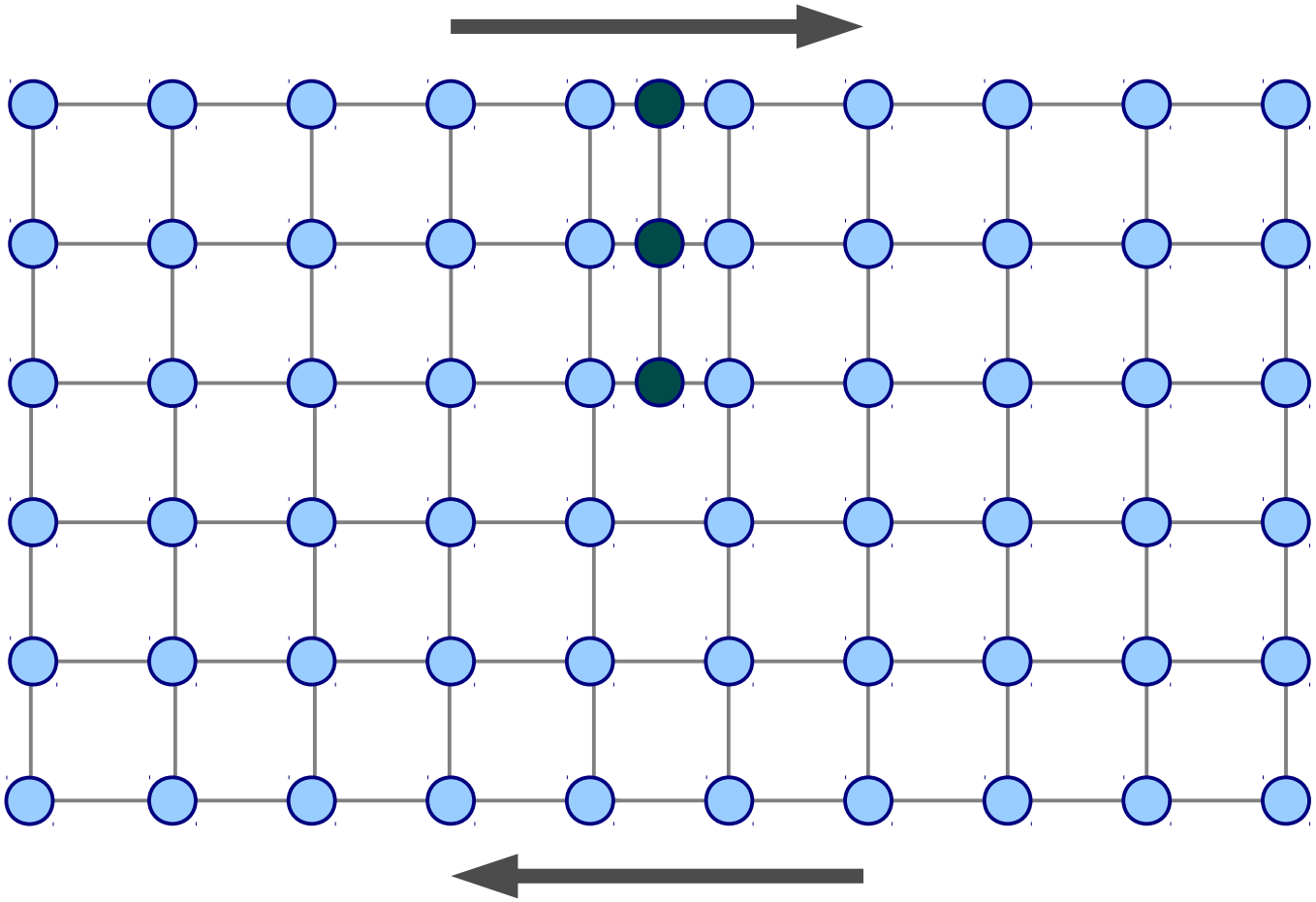

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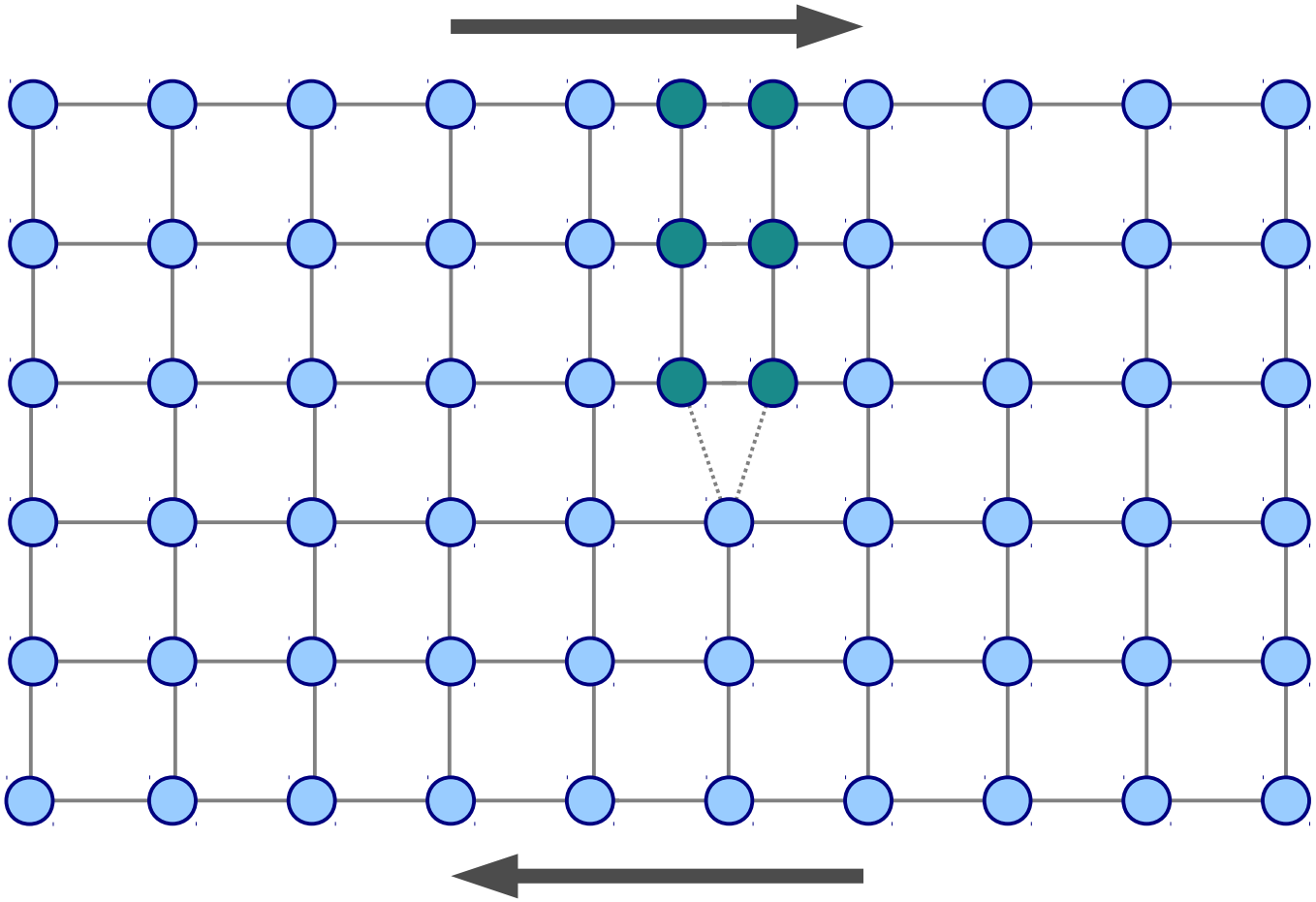

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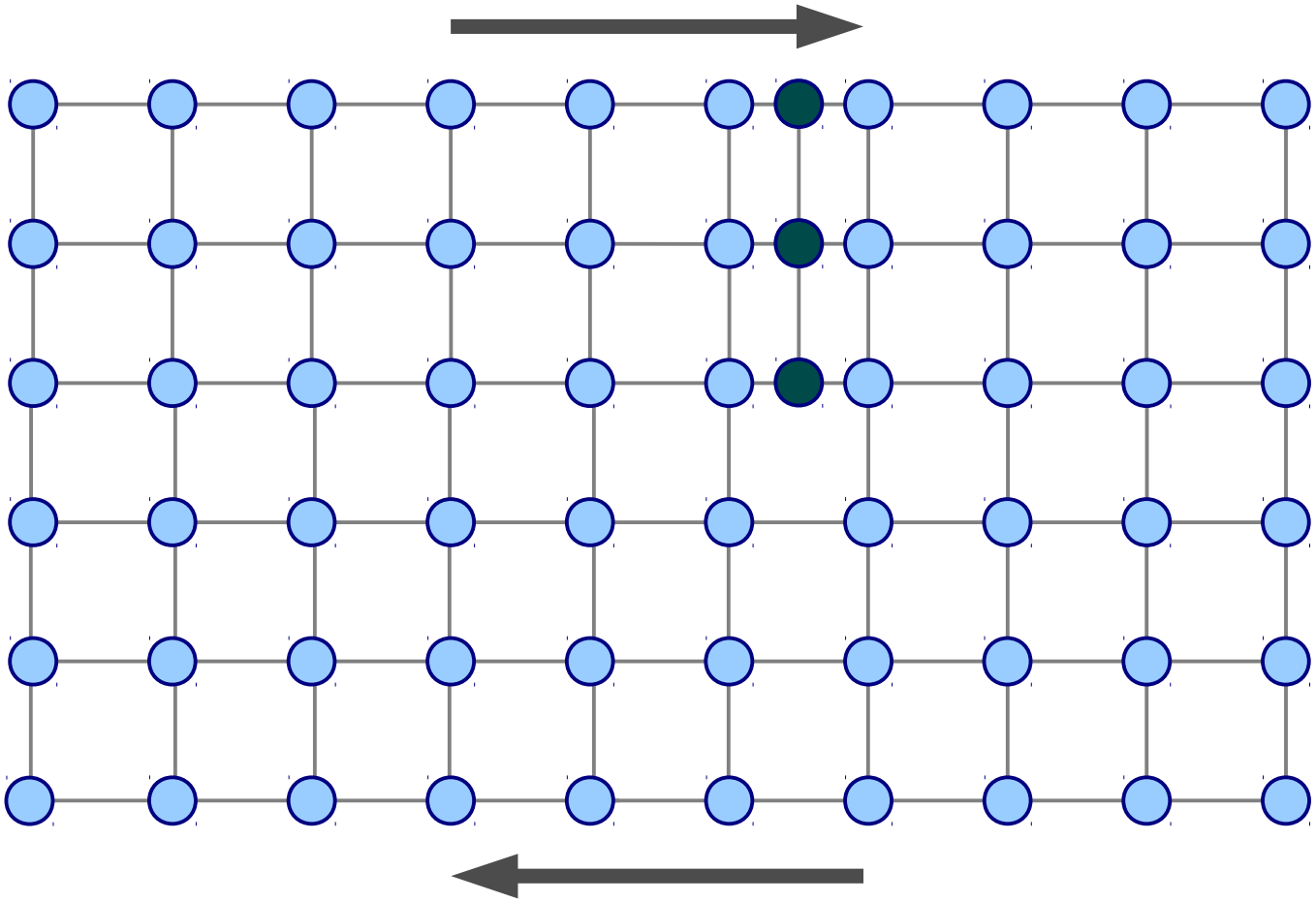

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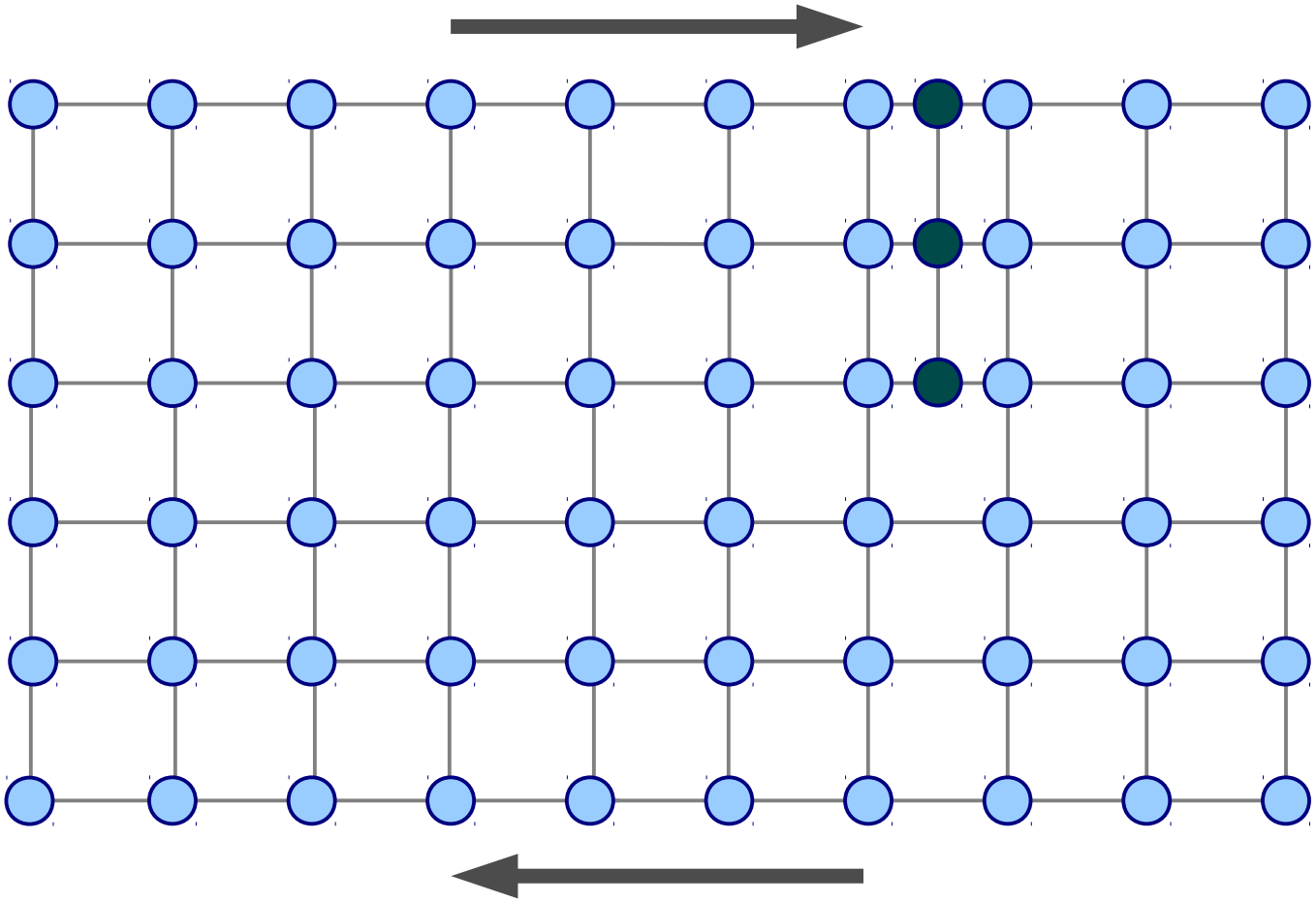
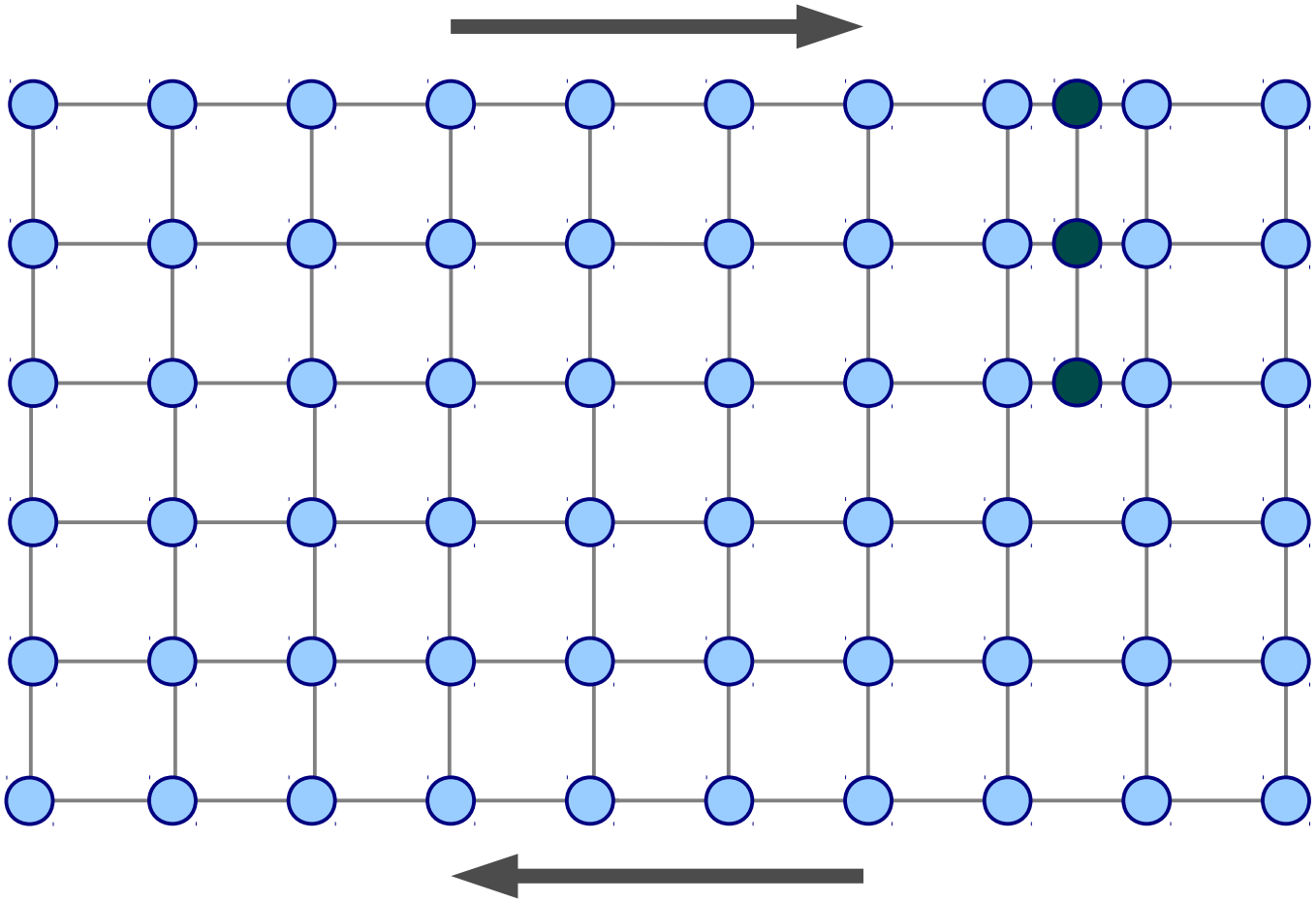
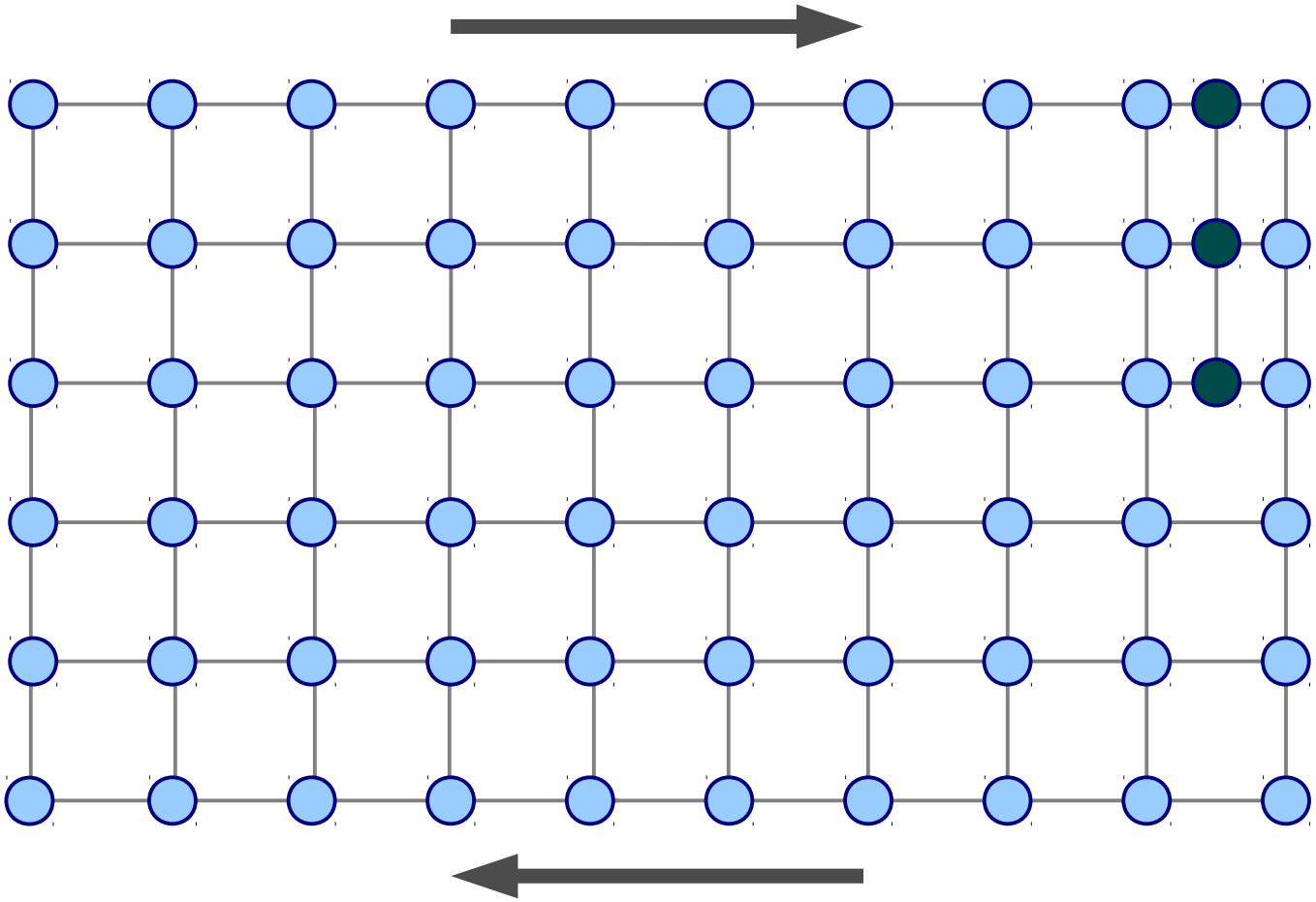


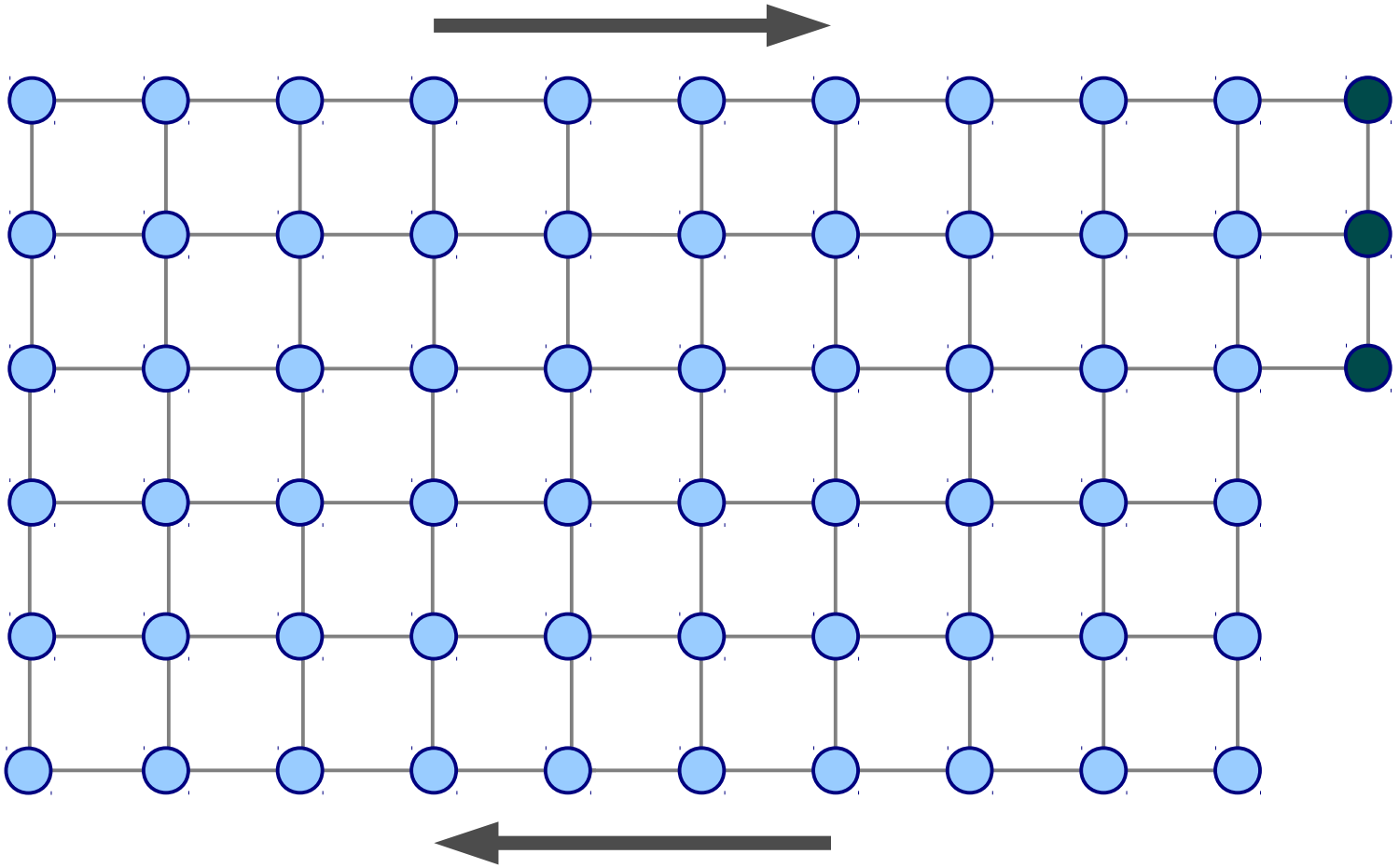
Creep



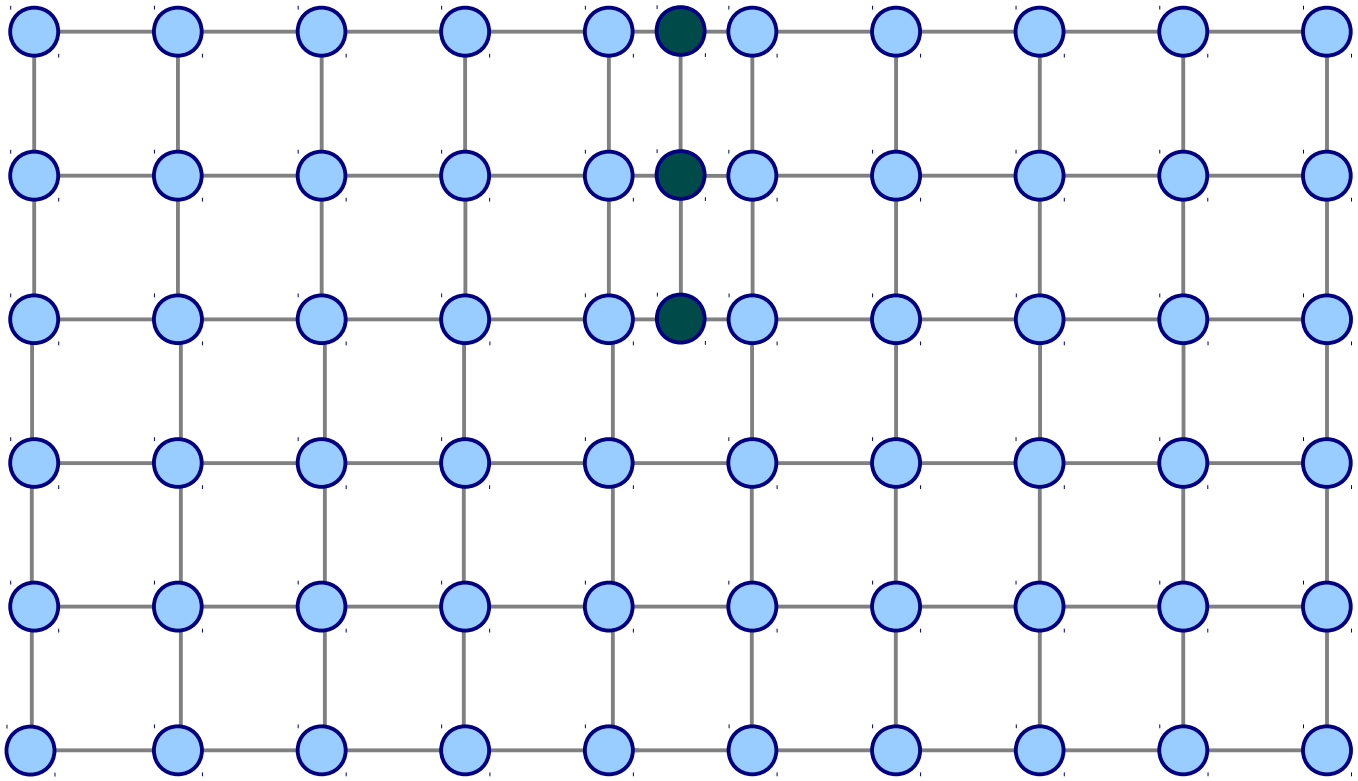
Creep



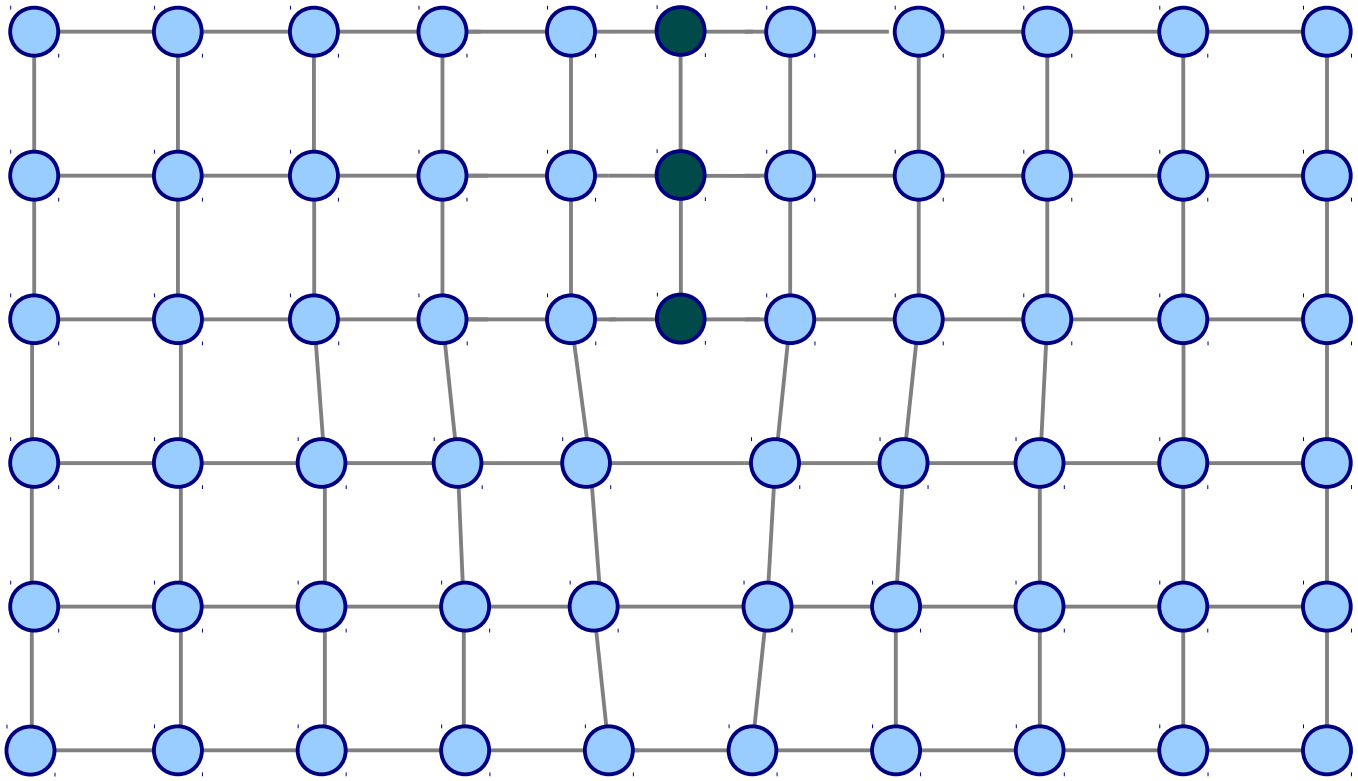
Creep



Solution hardening



Solution hardening



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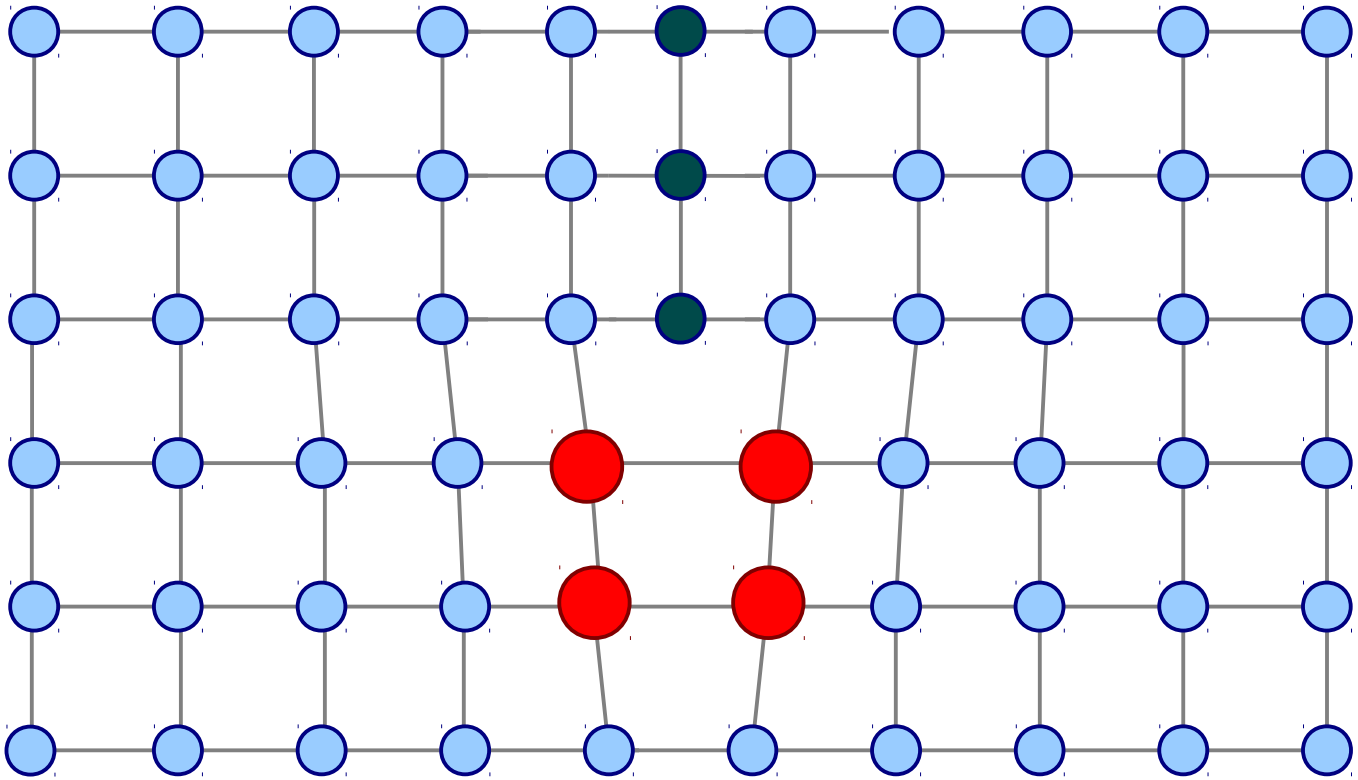

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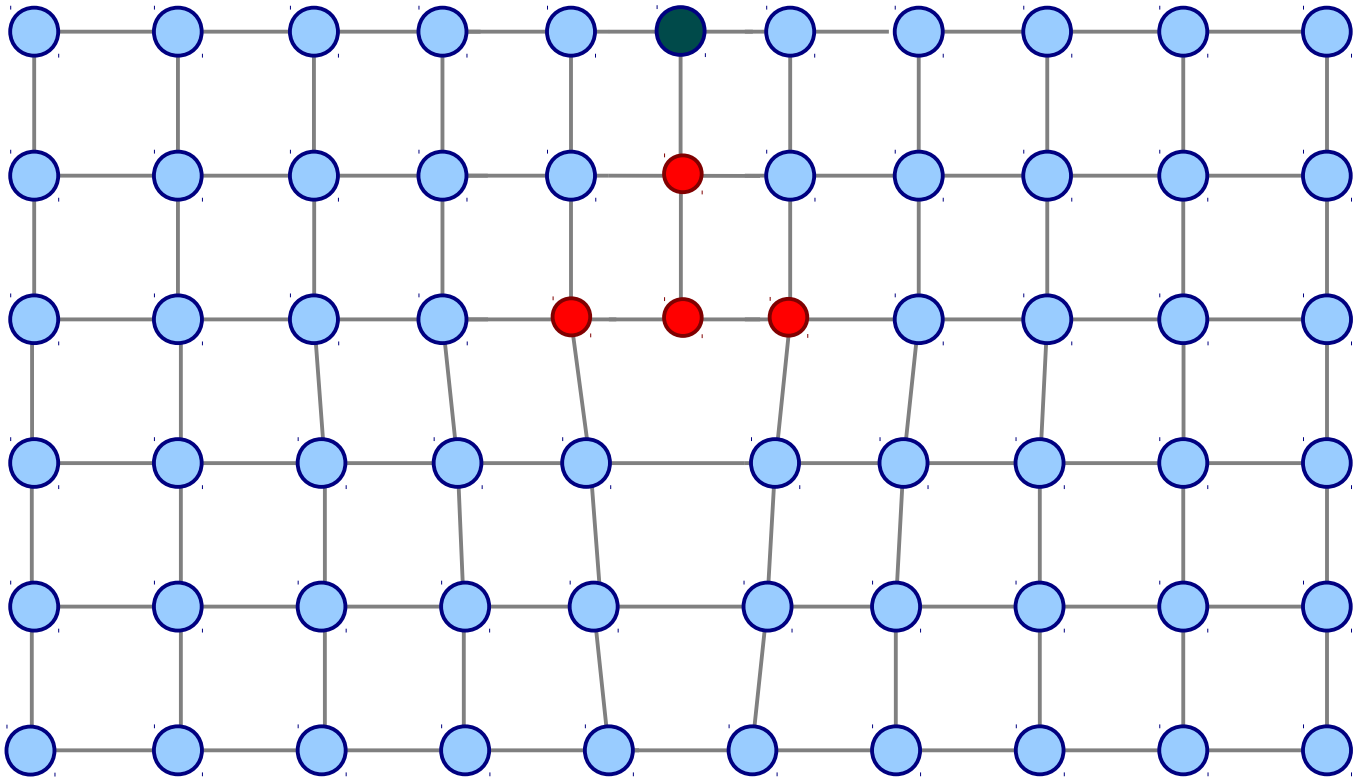
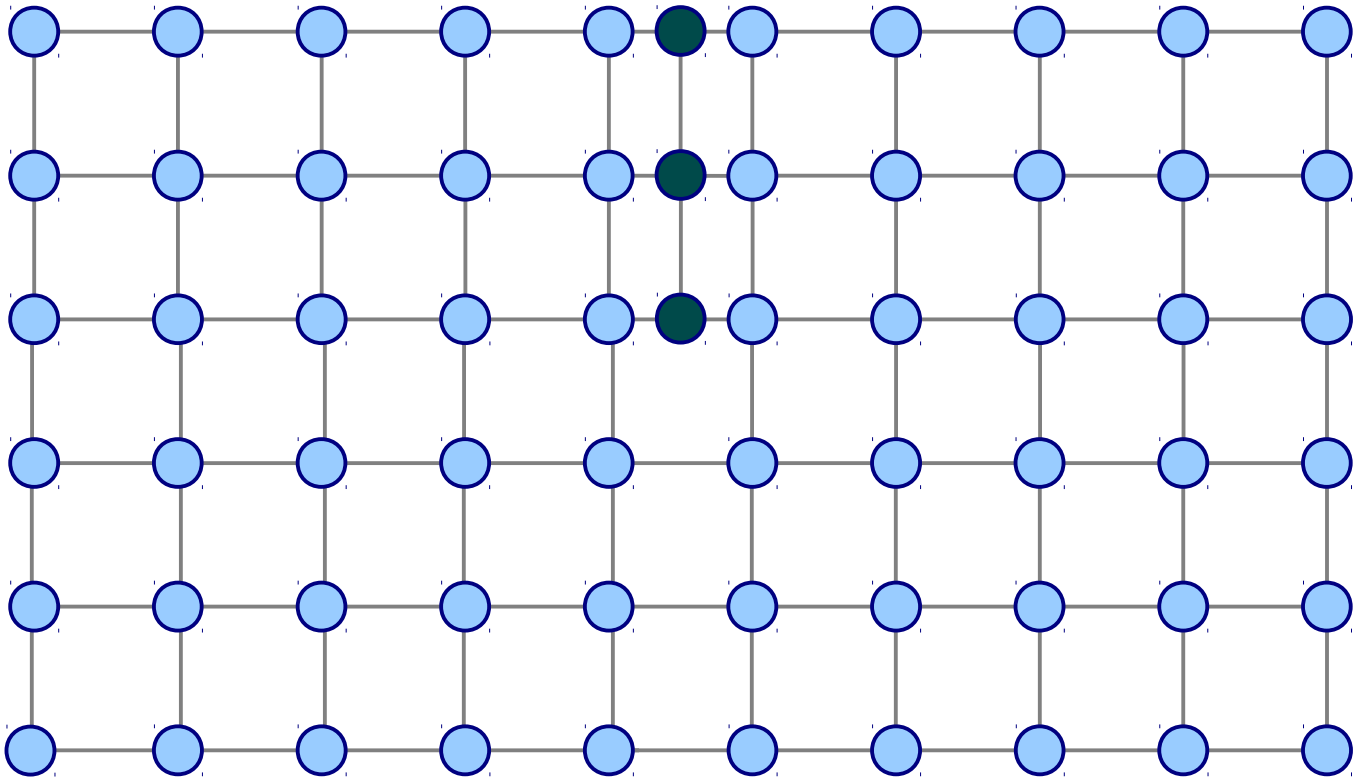


Precipitate hardening



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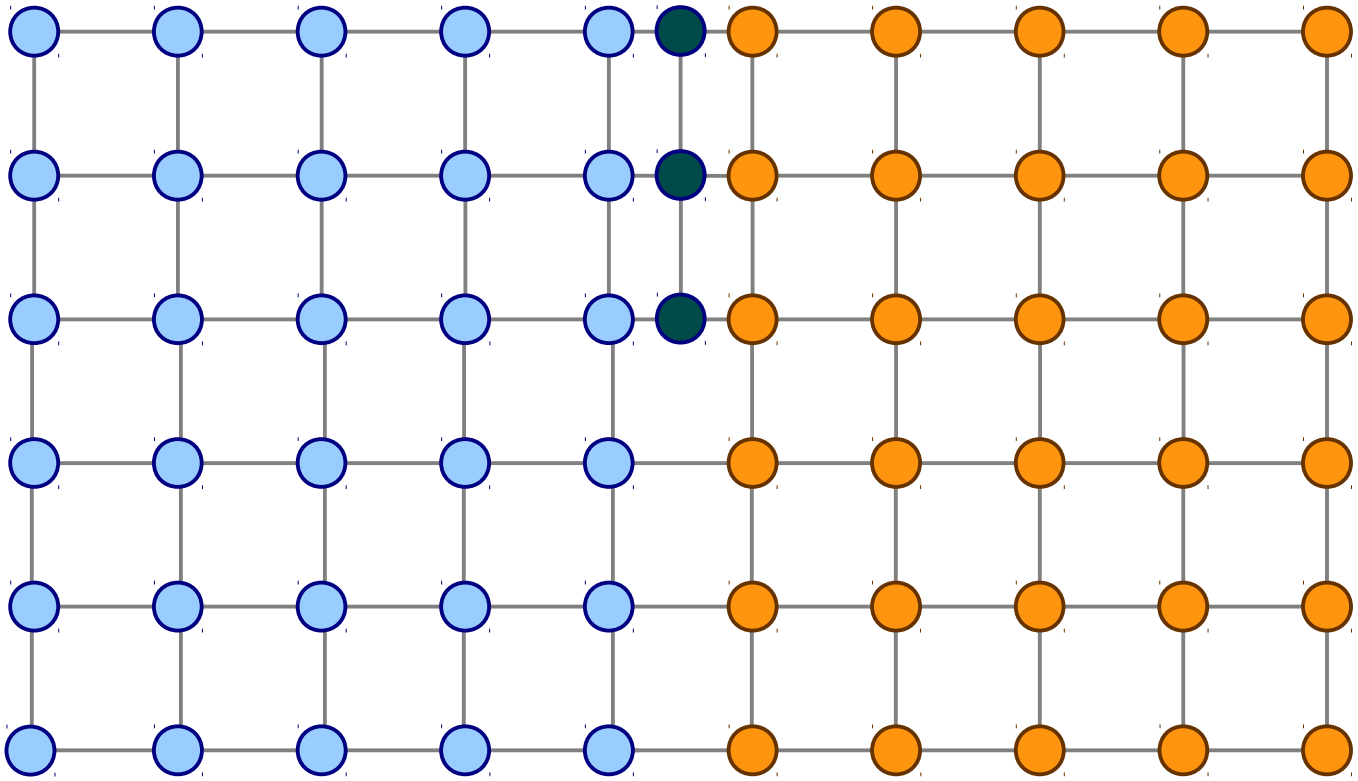
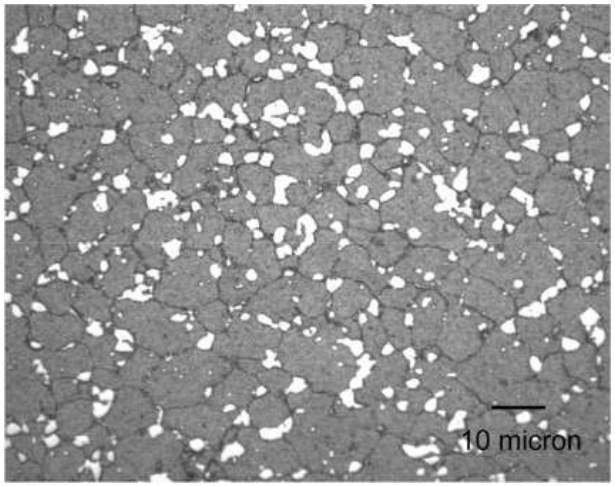


Contemporary alloys

RR1000



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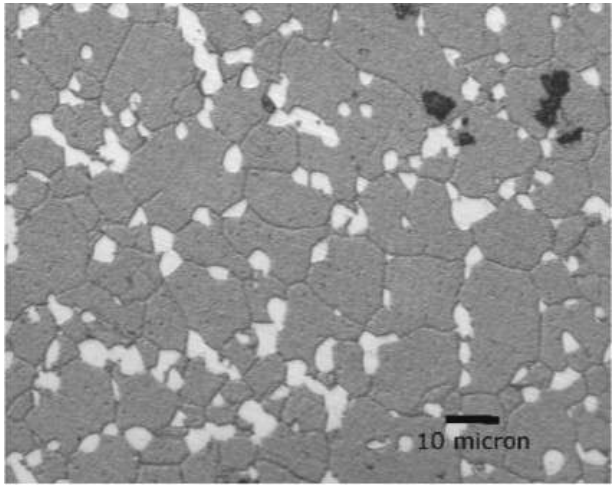

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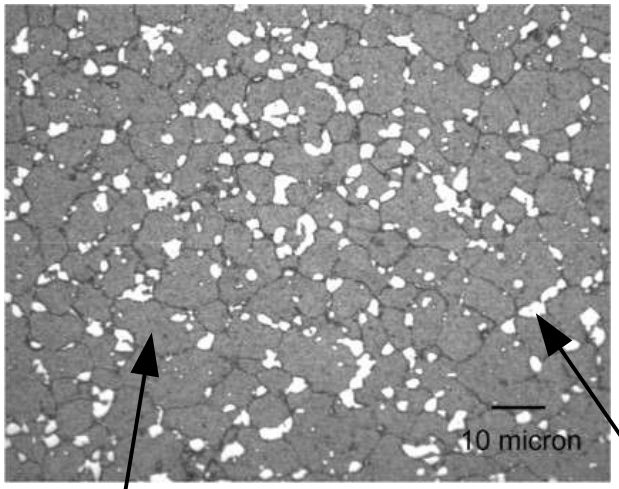
Contemporary alloys

RR1000



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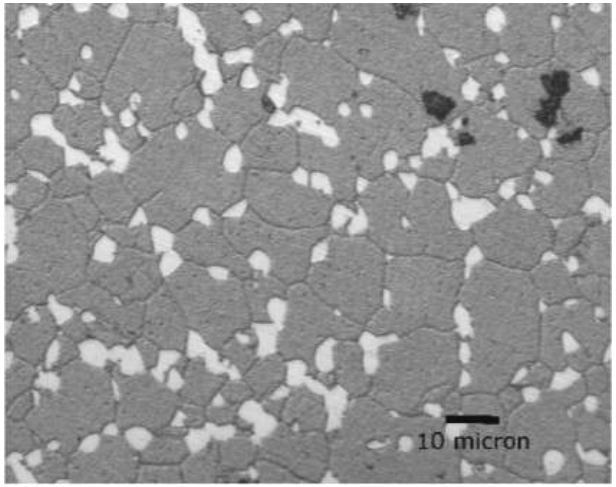
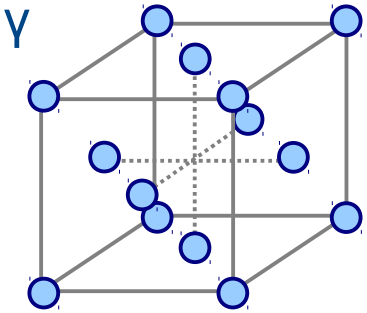
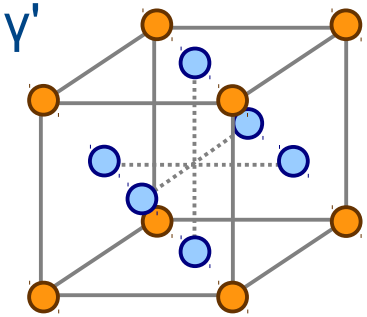


γ



γ'

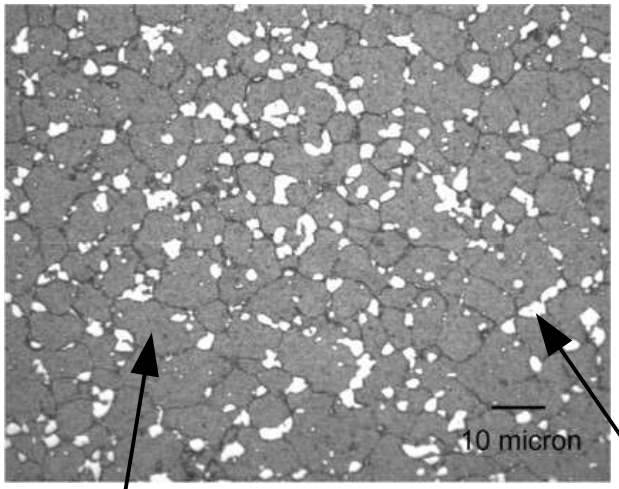


Ni

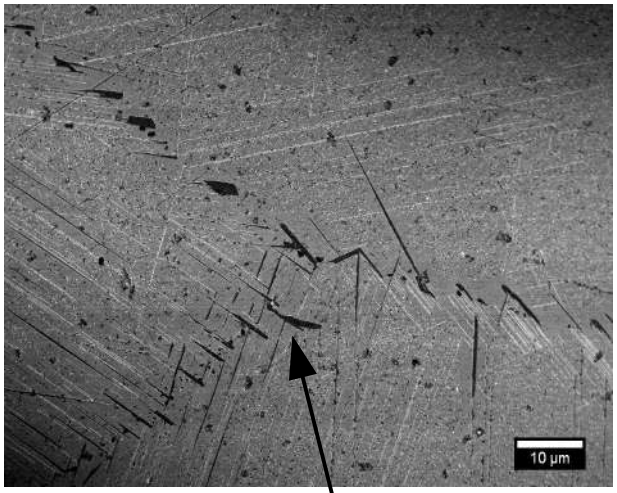
Al

Solution strengthened alloy

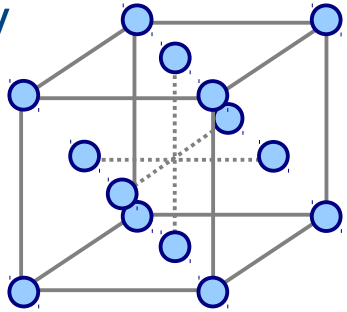
RR1000



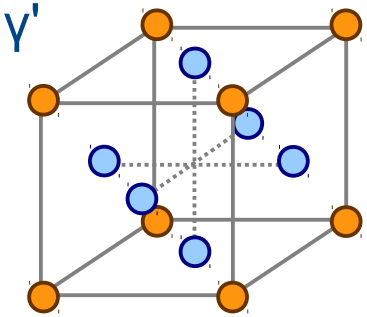
Attempted alloy



γ



γ'



η (HCP $D0_{24}$)

Ni_3Al structure

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



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
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High cycle fatigue
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Creep model

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

Properties

Cost $lb^{-1}

γ' fraction

Stability

Density gcm^{-3}

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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

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

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

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

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

Calculate uncertainty in neural network model

Properties

Cost $lb^{-1}
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Stability
Density gcm^{-3}
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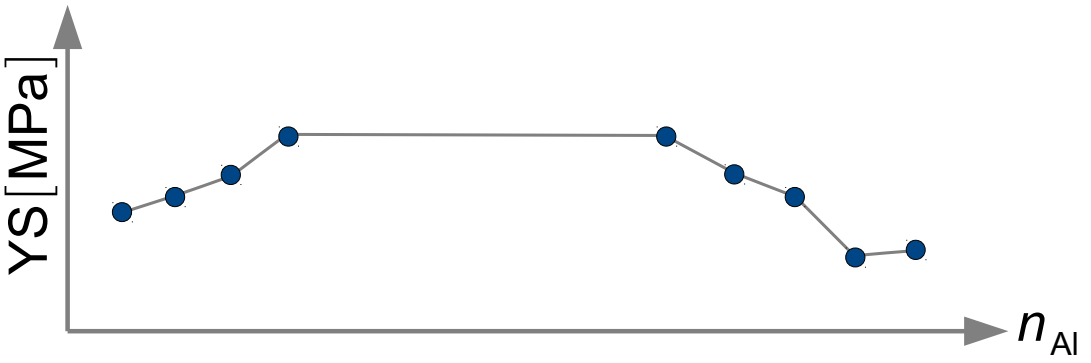

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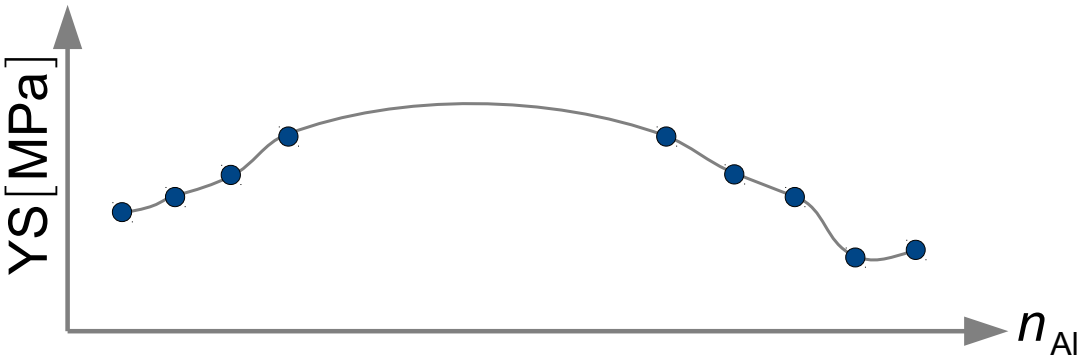
Calculate uncertainty in neural network model



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Collect data for yield stress from 2248 alloys

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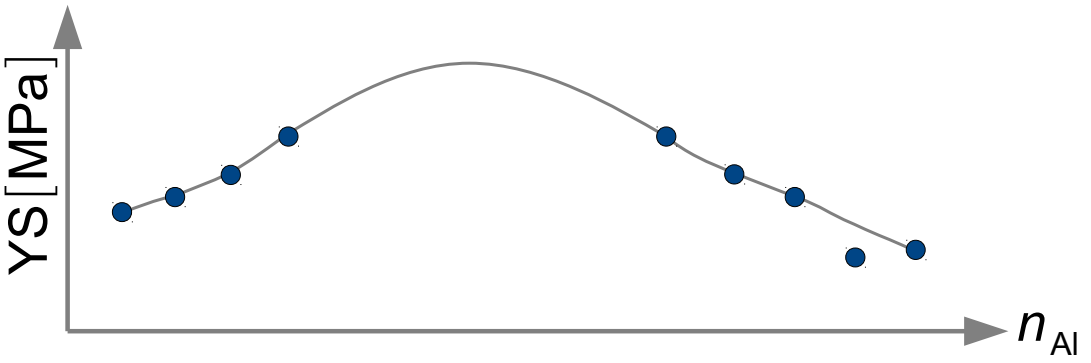
Calculate uncertainty in neural network model



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Generate neural network model

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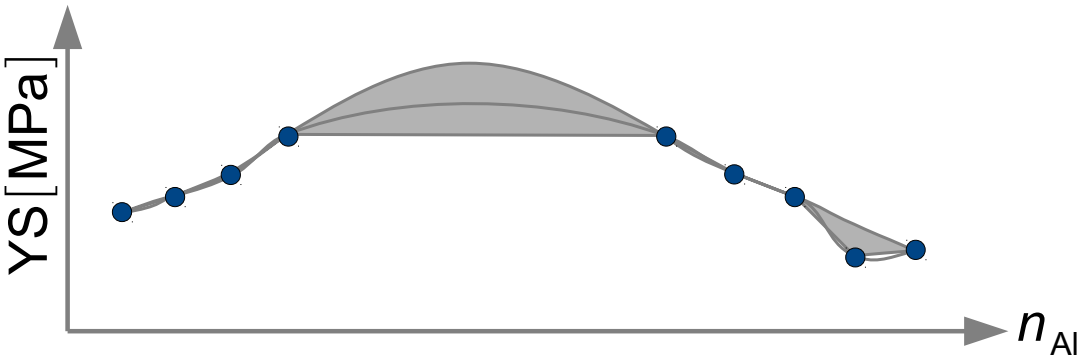
Calculate uncertainty in neural network model



Properties

Cost $lb^{-1}

γ' fraction

Stability

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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

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

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

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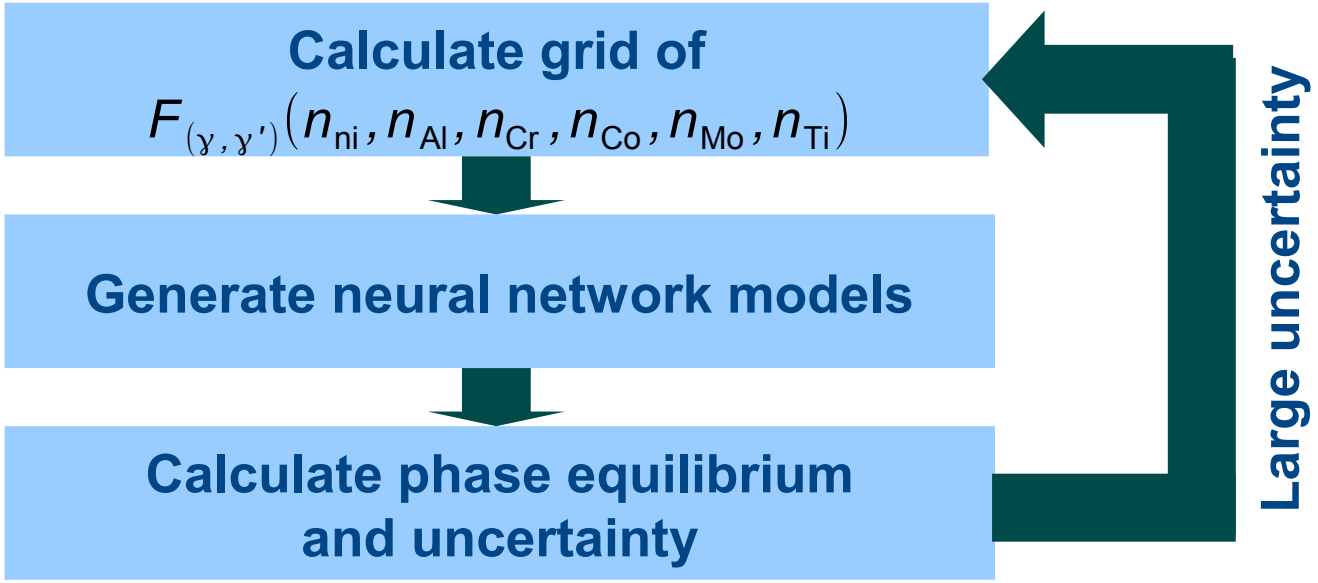
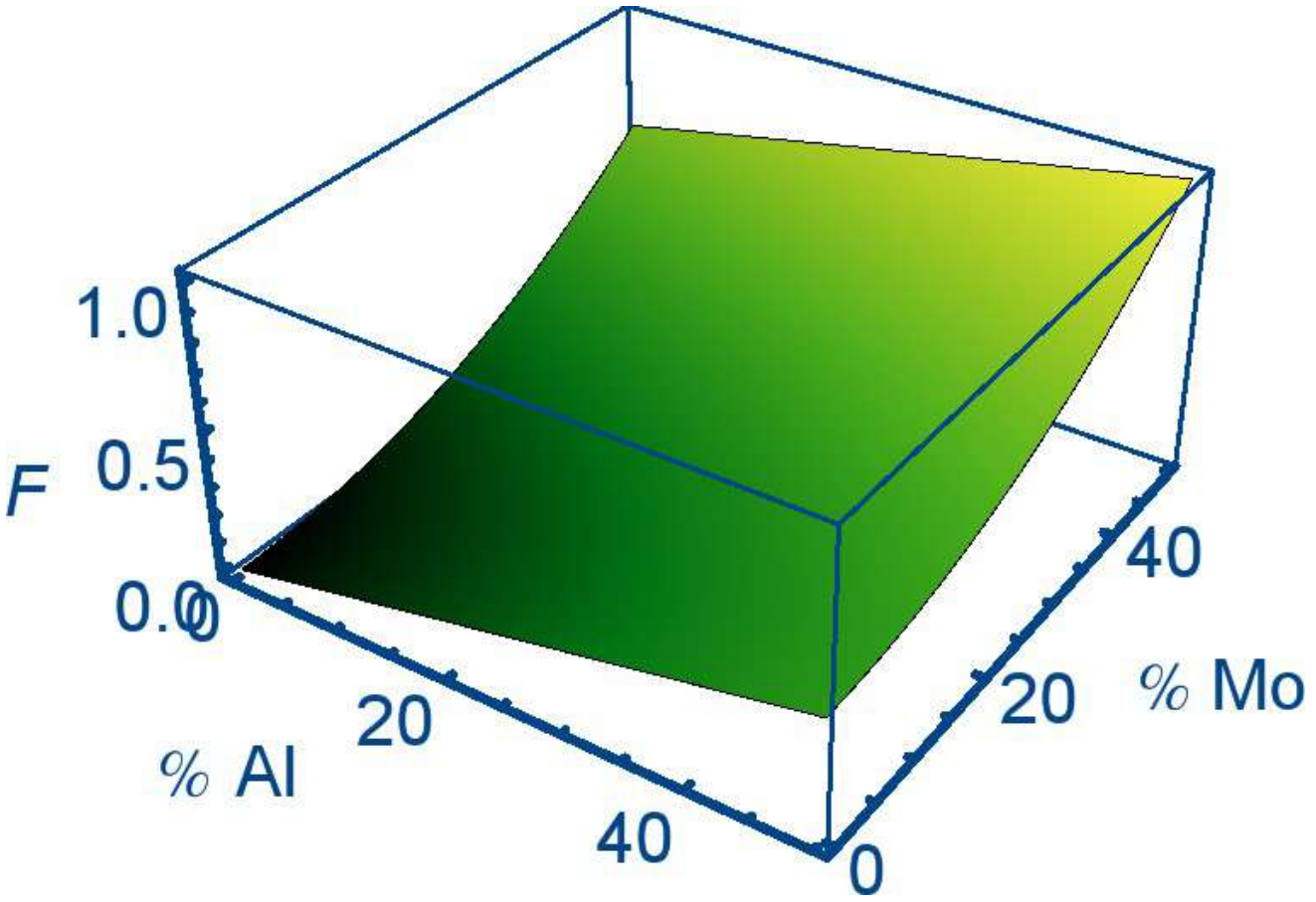
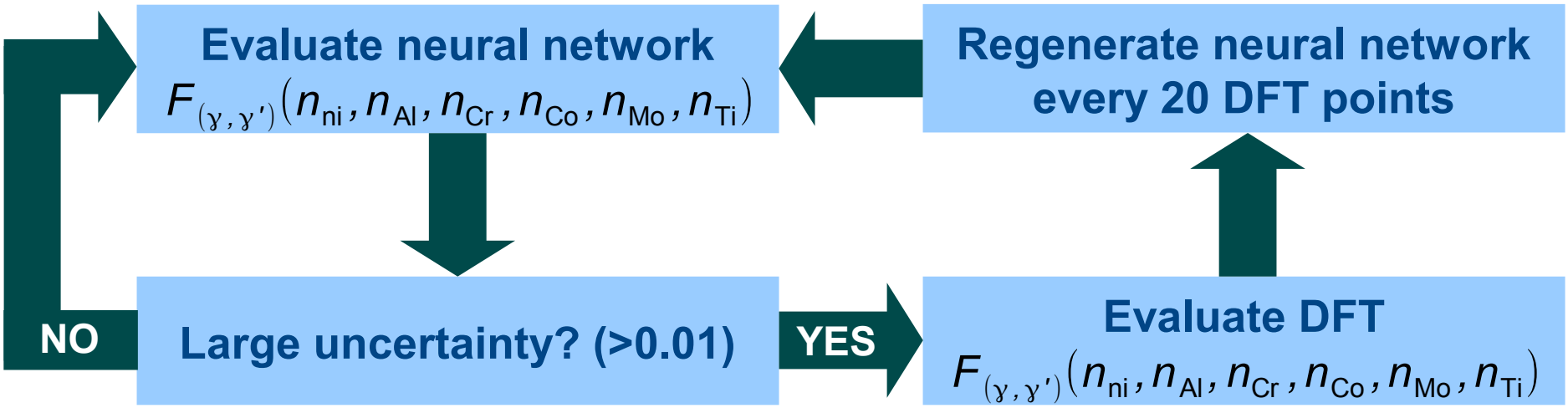


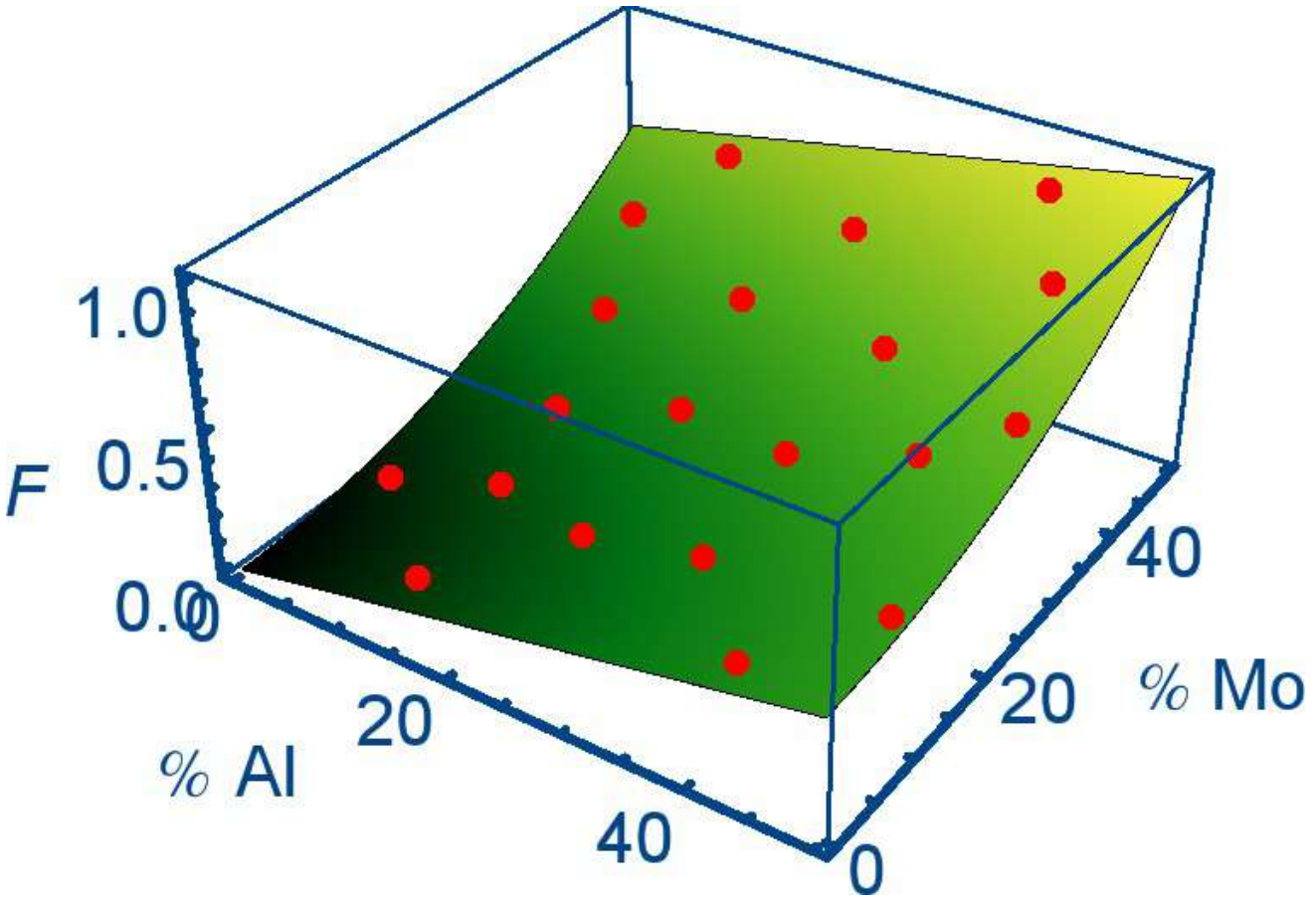
Reinforcement learning



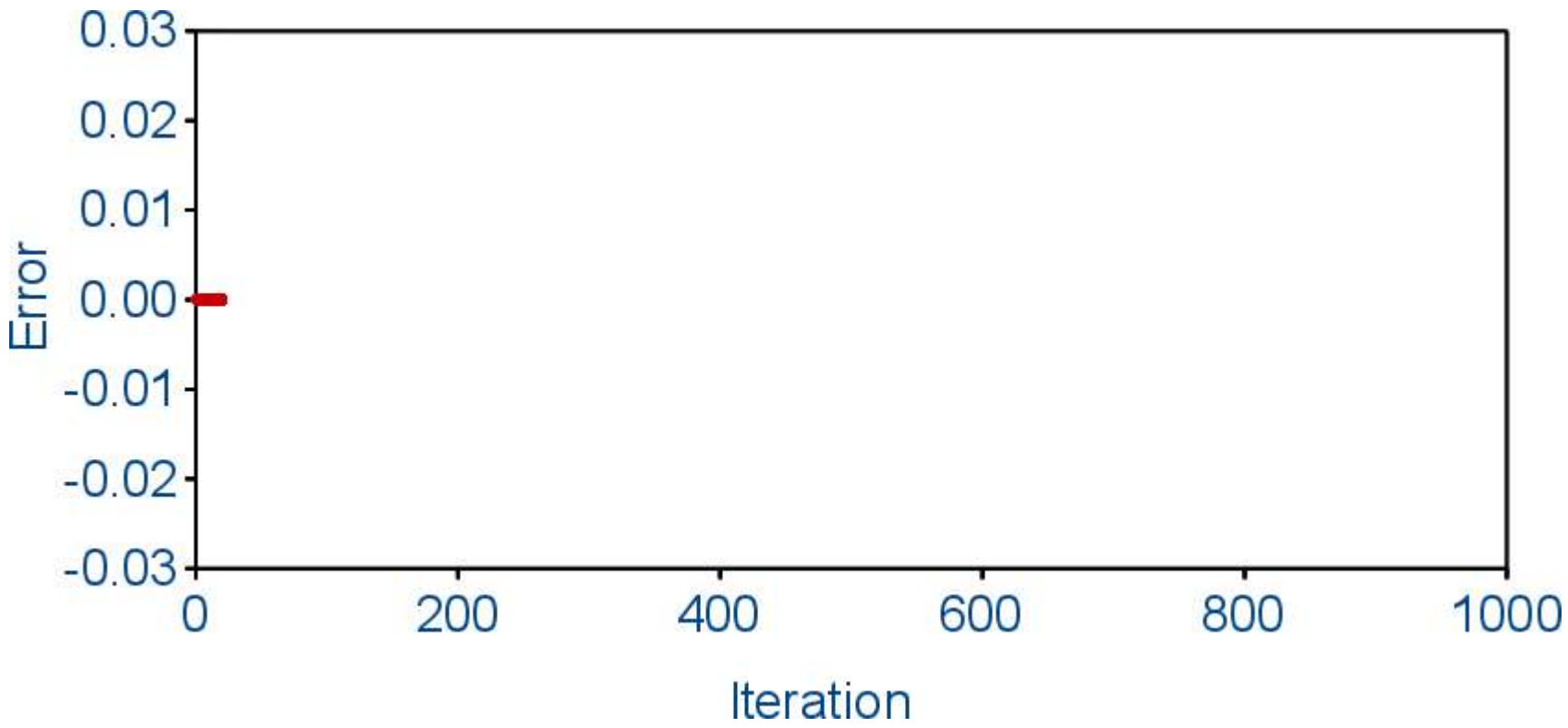
Reinforcement learning



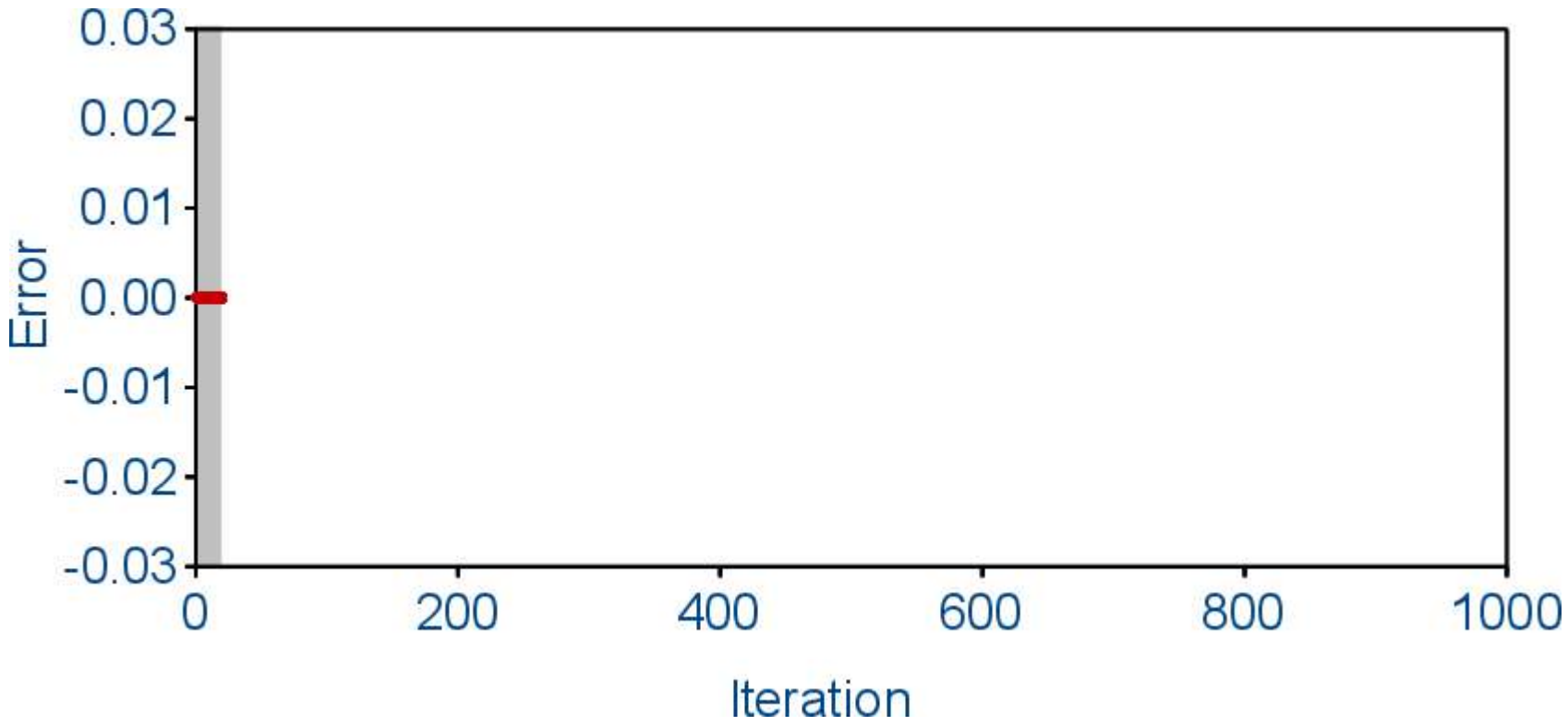
Reinforcement learning



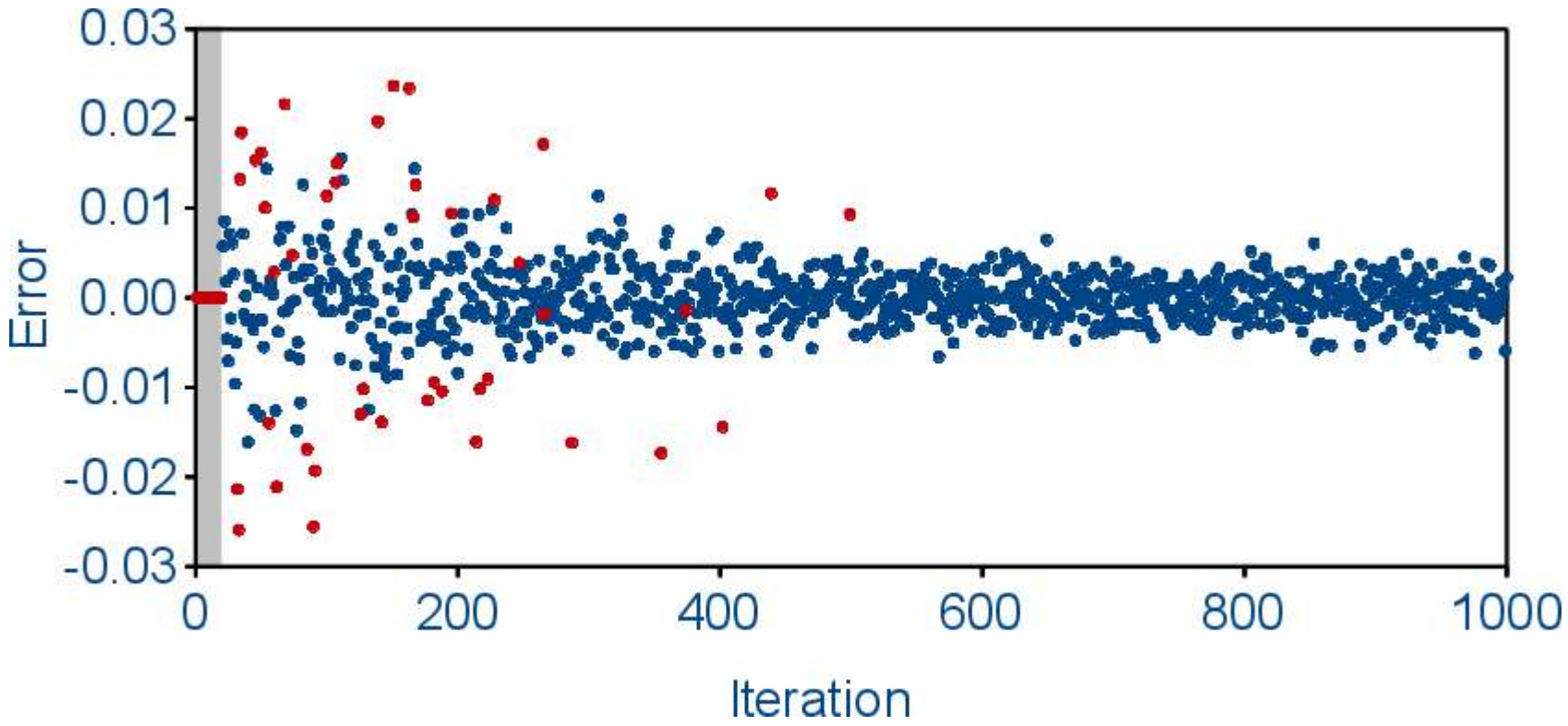
Reinforcement learning



Reinforcement learning

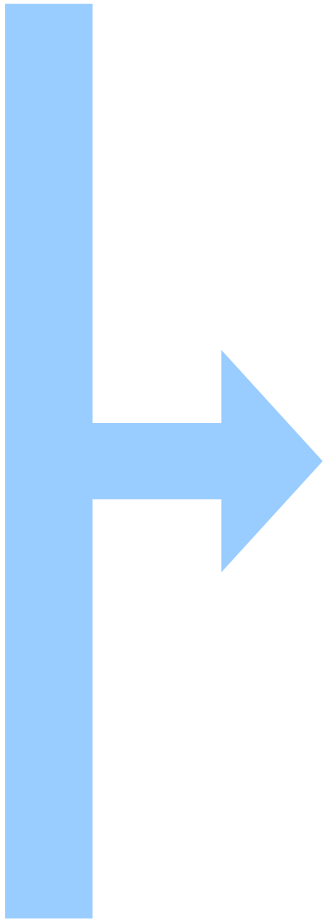


Reinforcement learning



Probability

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



$P_{spec}(C)$

Multidimensional design space

Cr Co Mo W Ta Nb Al







Ti Fe Mn Si C B Zr







Cu N P V Hf Mg Ni



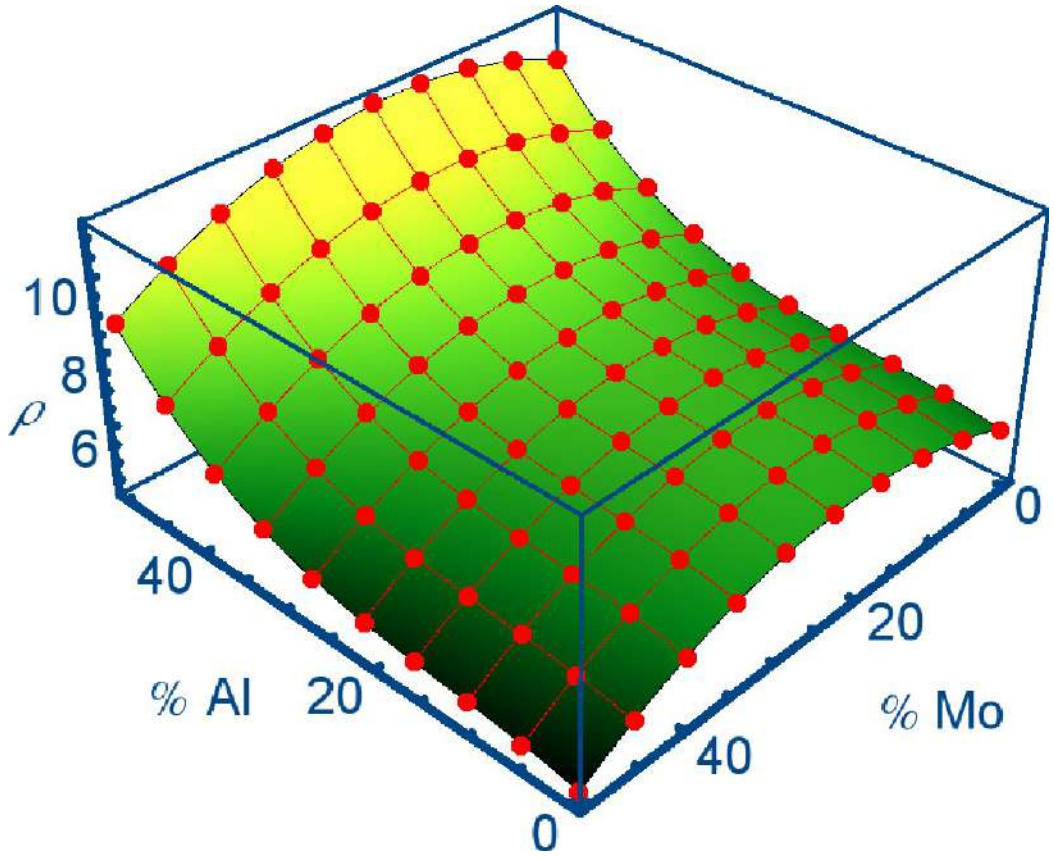




Heat treatment

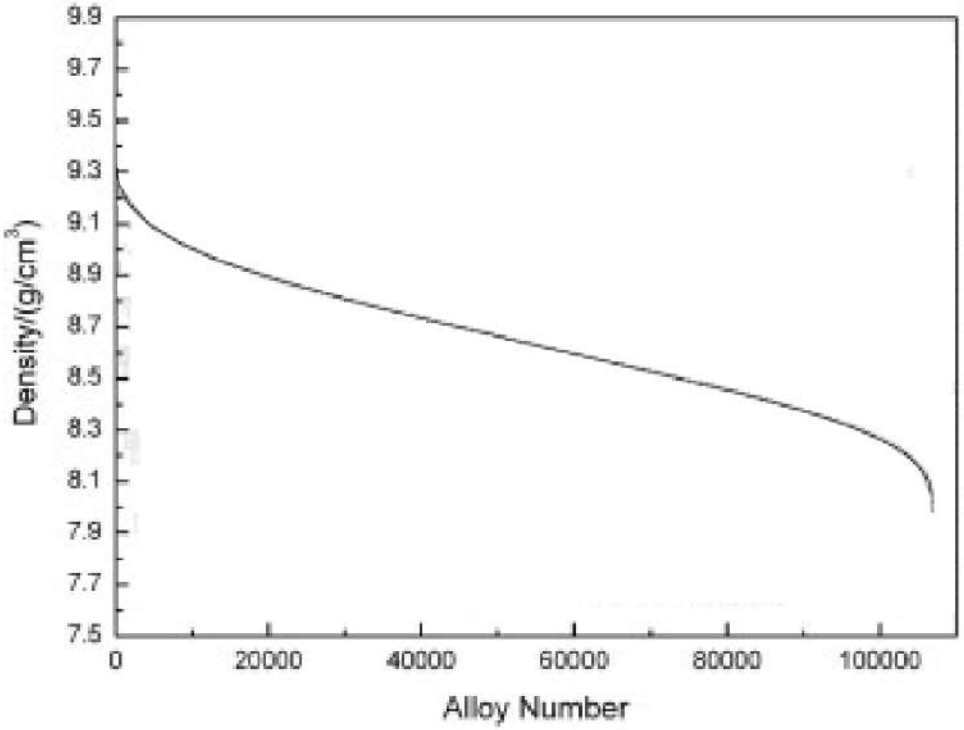


Optimization – tradeoff diagrams



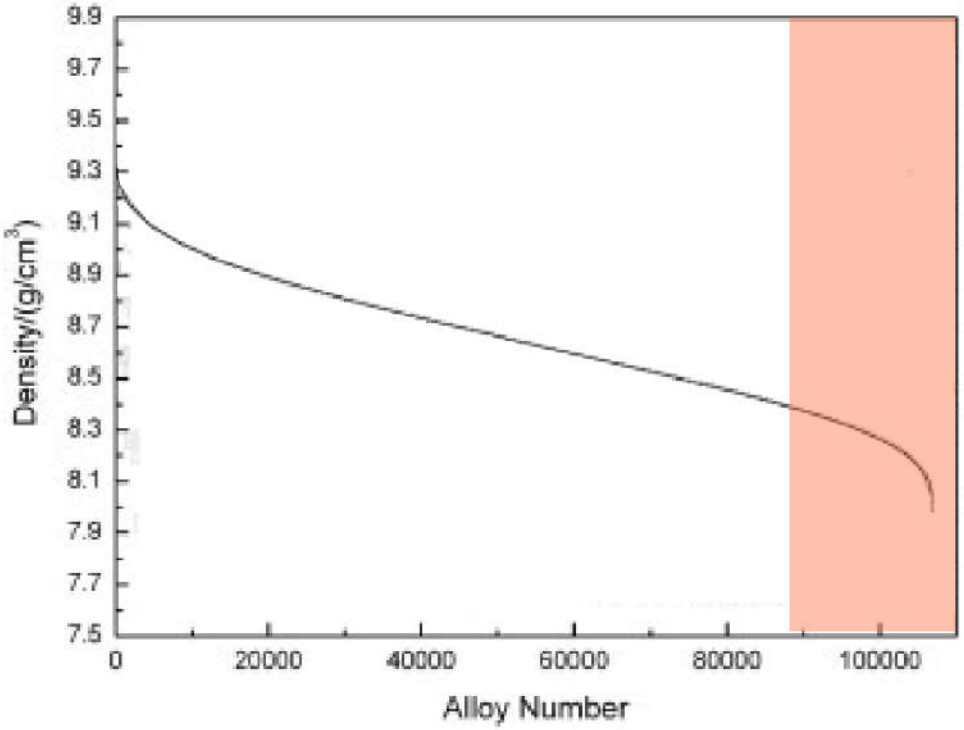
R.C. Reed, T. Tao & N. Warnken, Acta Materialia **57**, 5898 (2009)

Optimization – tradeoff diagrams



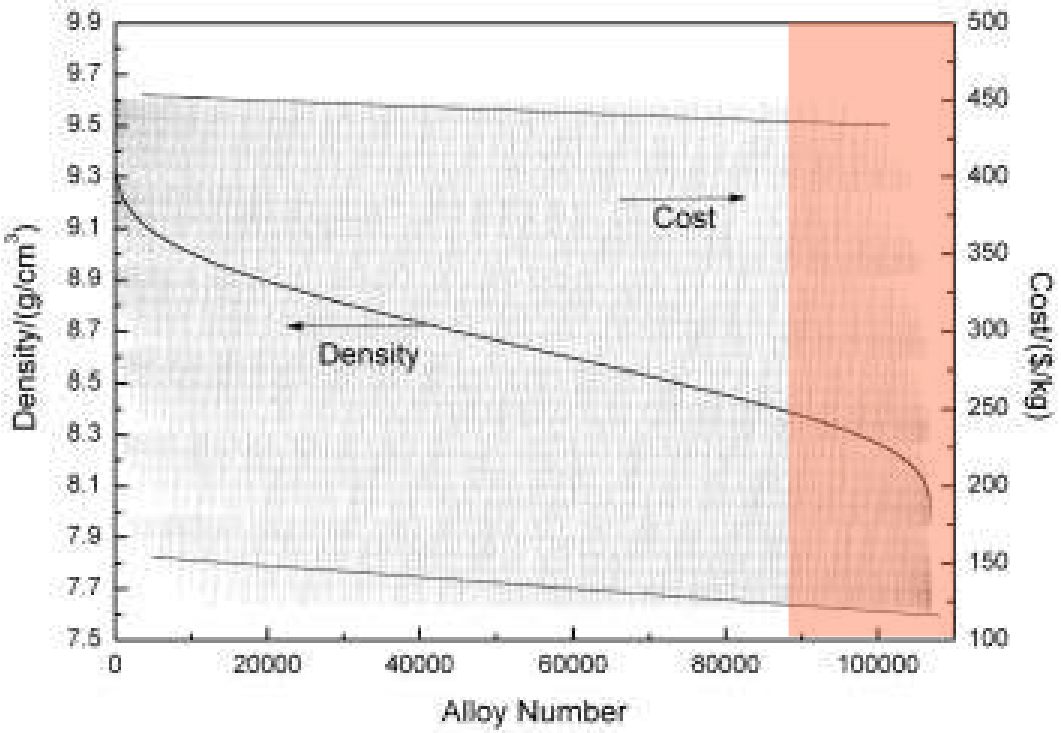
R.C. Reed, T. Tao & N. Warnken, Acta Materialia **57**, 5898 (2009)

Optimization – tradeoff diagrams



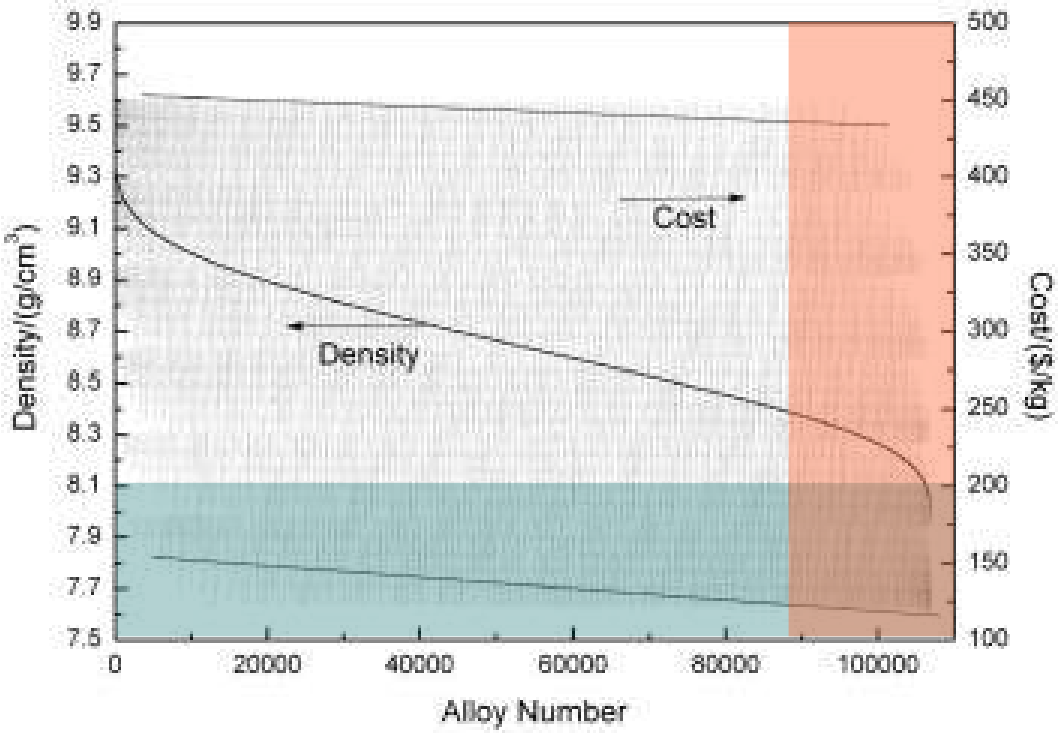
R.C. Reed, T. Tao & N. Warnken, Acta Materialia **57**, 5898 (2009)

Optimization – tradeoff diagrams



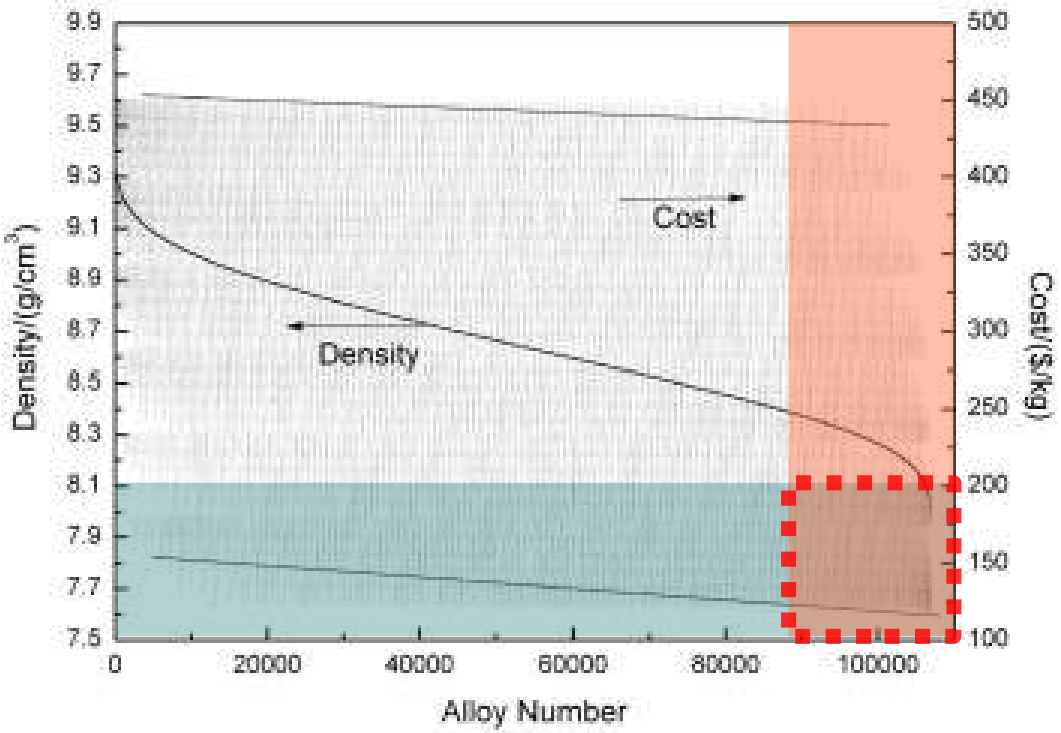
R.C. Reed, T. Tao & N. Warnken, Acta Materialia **57**, 5898 (2009)

Optimization – tradeoff diagrams



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

Optimization – tradeoff diagrams



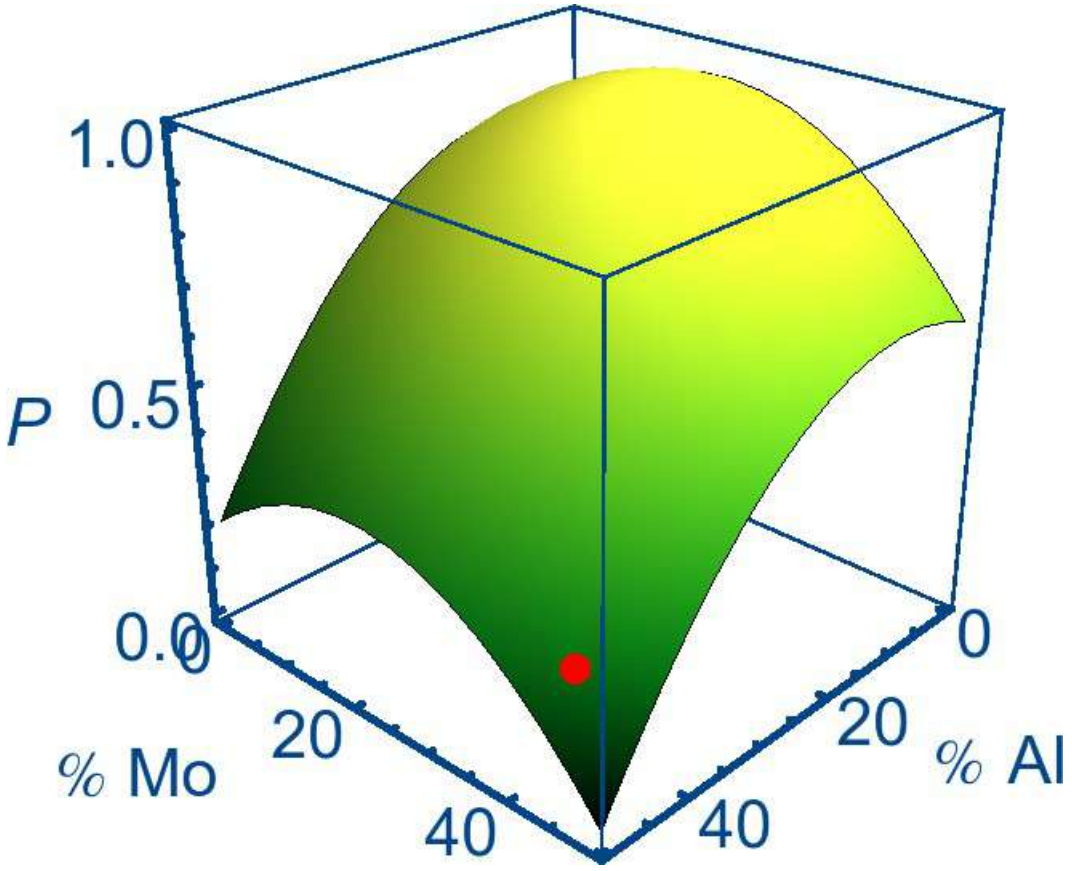
R.C. Reed, T. Tao & N. Warnken, Acta Materialia **57**, 5898 (2009)

Optimization – tradeoff diagrams

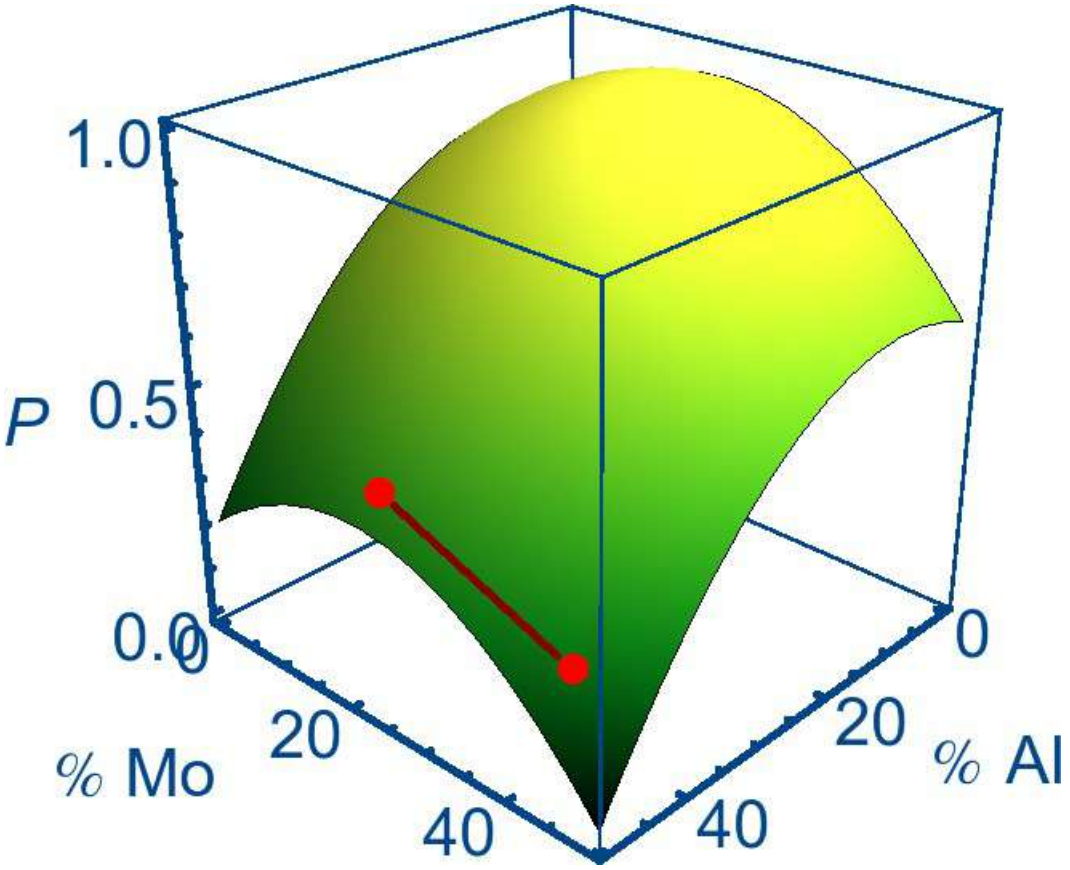
With 30 design variables, at 0.1% accuracy, and evaluation time of 1ms

$$1000^{30} = 10^{90} \rightarrow 3\times10^{79} \text{ years}$$

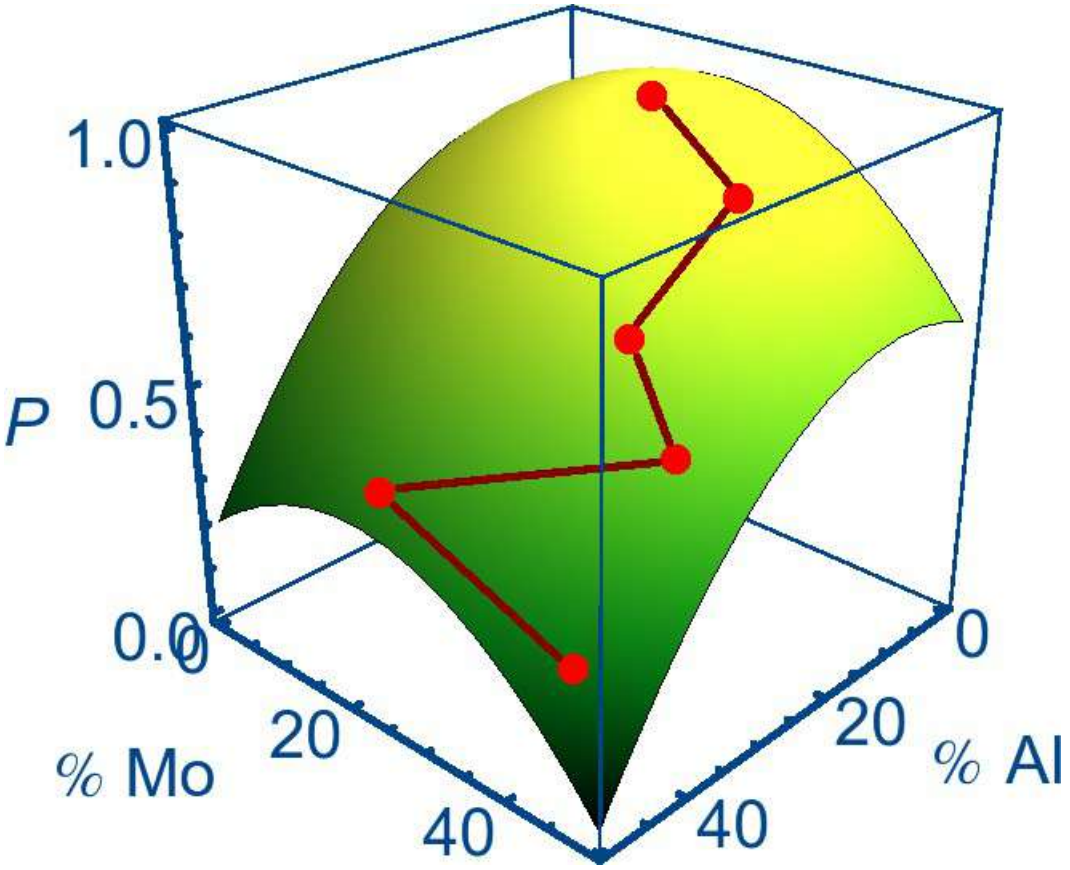
Optimization – replica exchange sampling



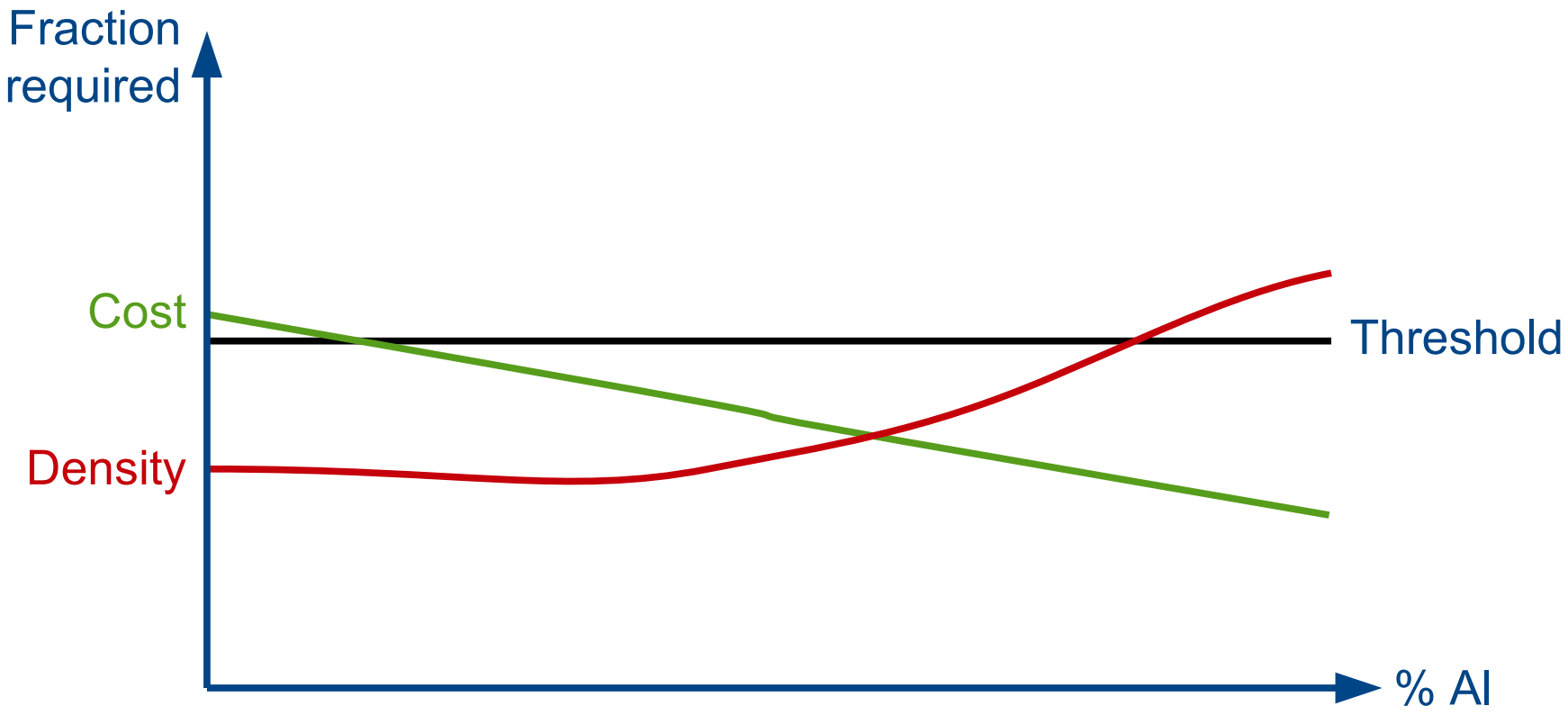
Optimization – replica exchange sampling



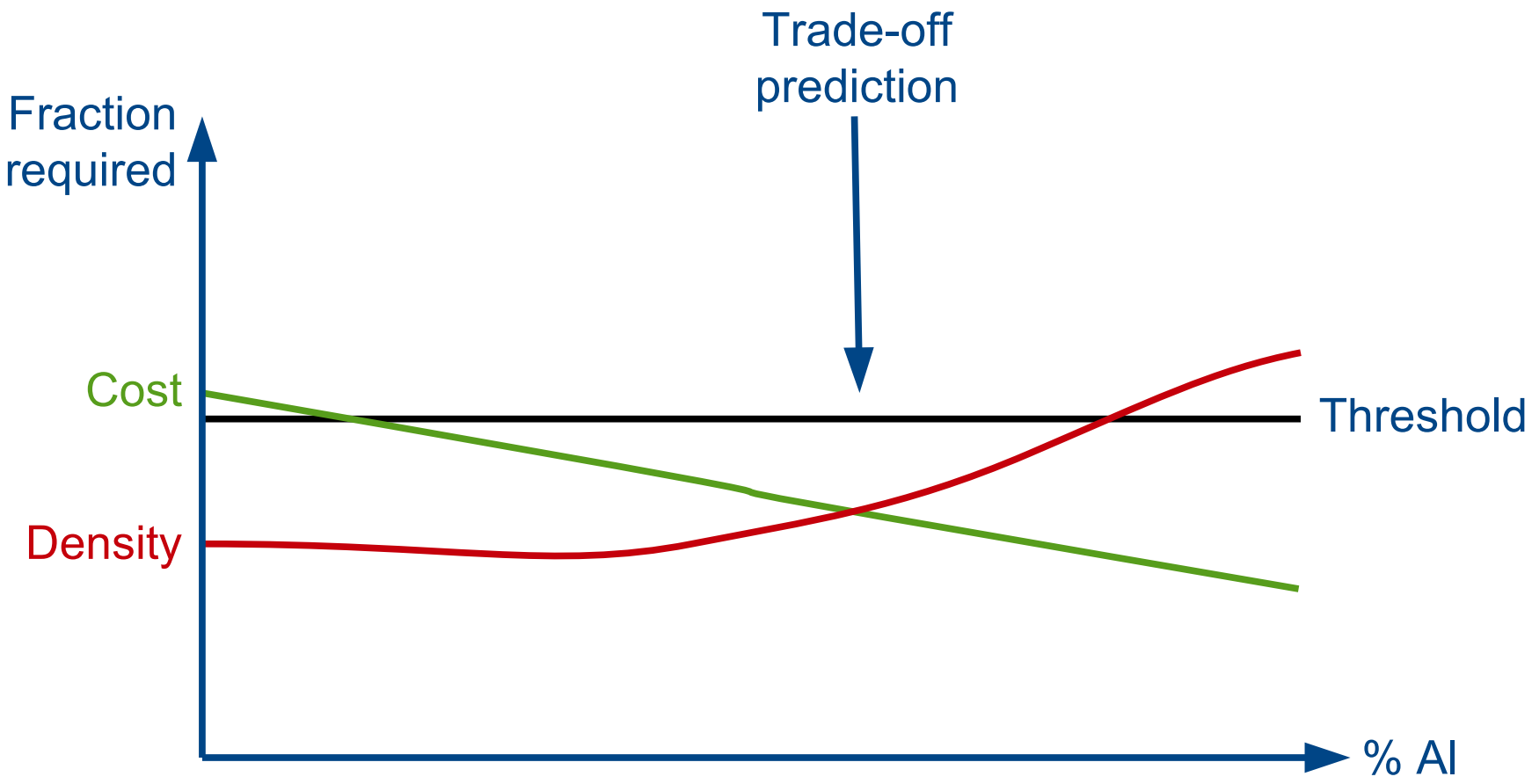
Optimization – replica exchange sampling



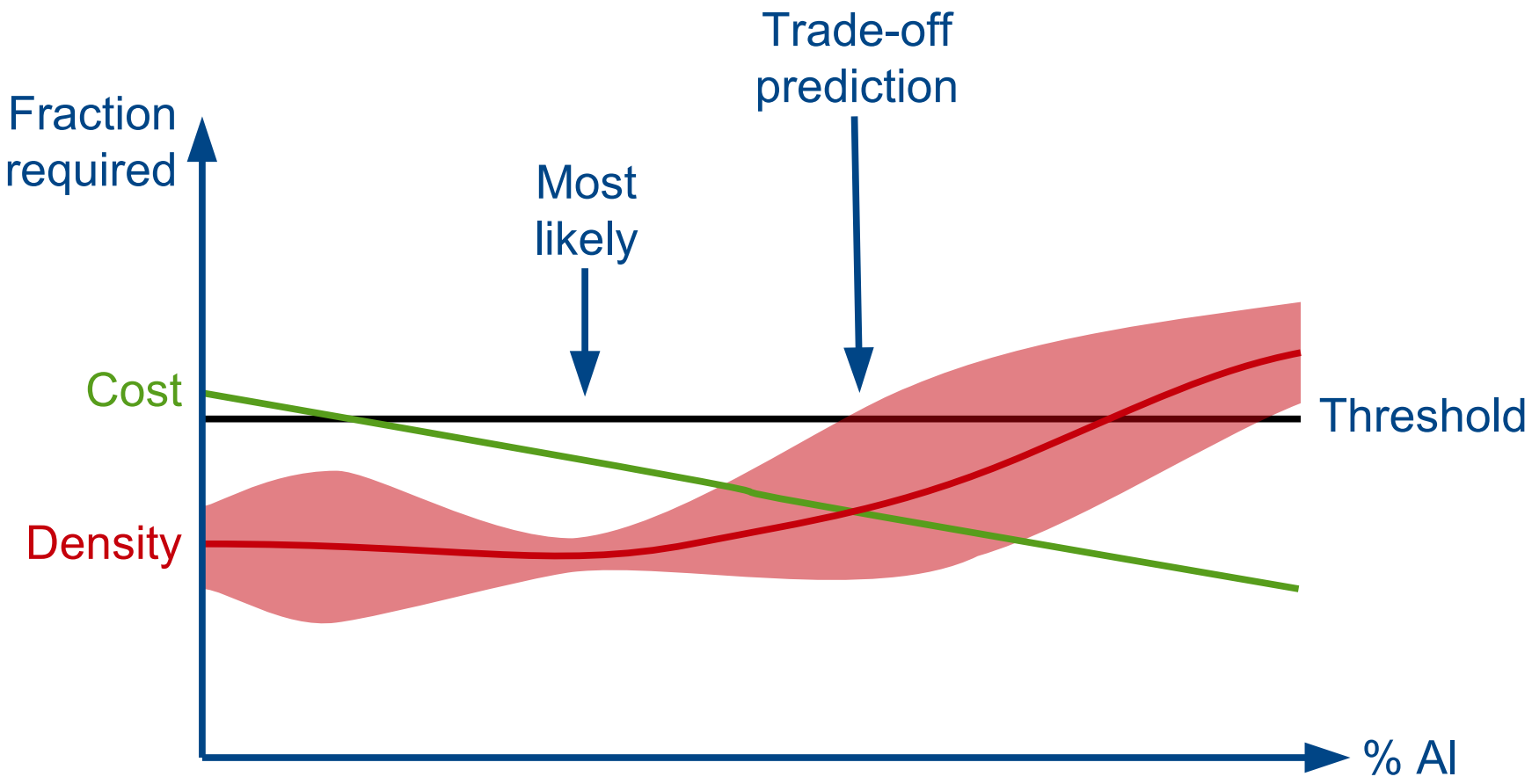
Optimization – probability



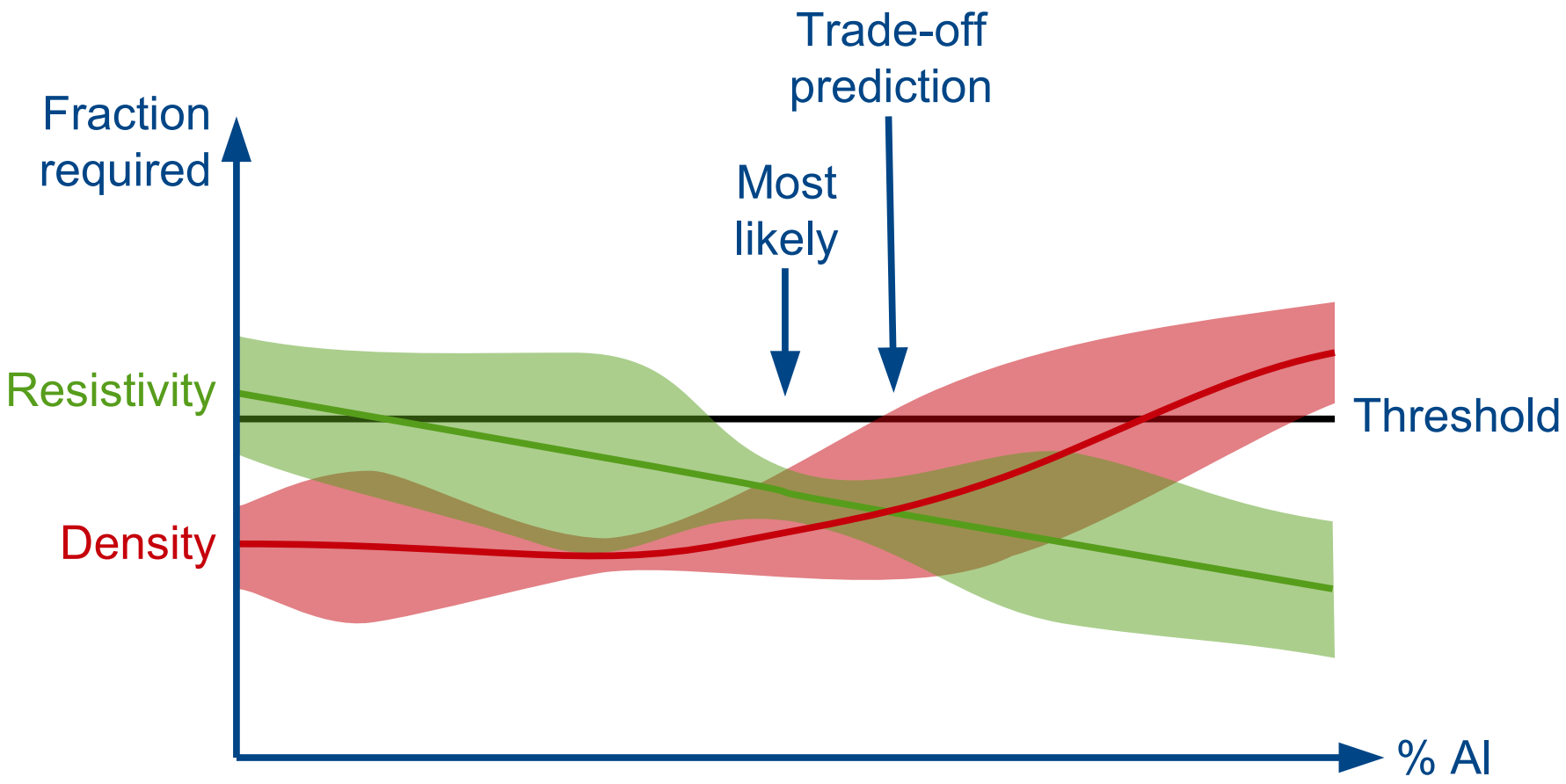
Optimization – probability



Optimization – probability



Optimization – probability

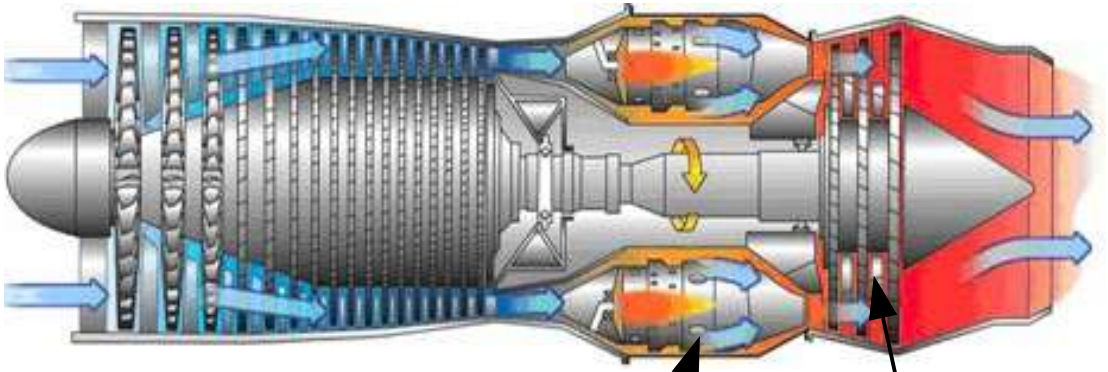


Optimization – tradeoff diagrams

With 10 specified properties,
each with probability of 0.5

0.5^{10} = 0.001 chance of success

Predicted alloys

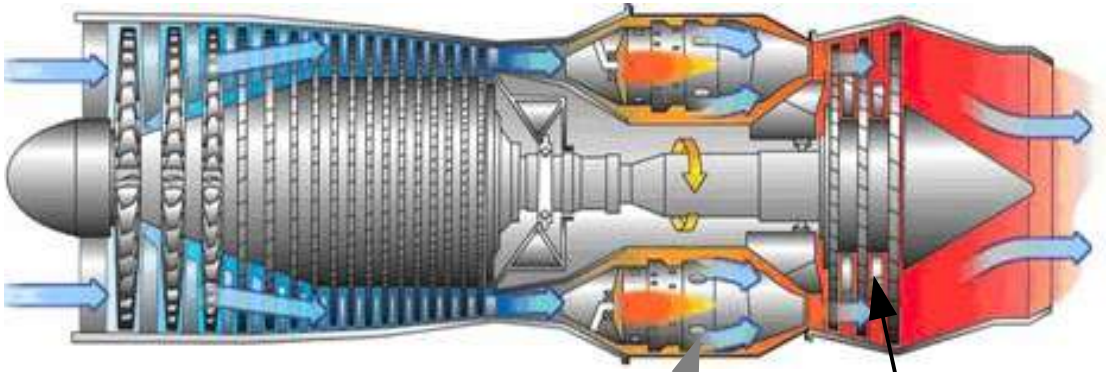


Combustor liner

2x disc alloy

2x forging hammer

Predicted alloys



Combustor liner

2x disc alloy

2x forging hammer

Case study: improved disc alloy



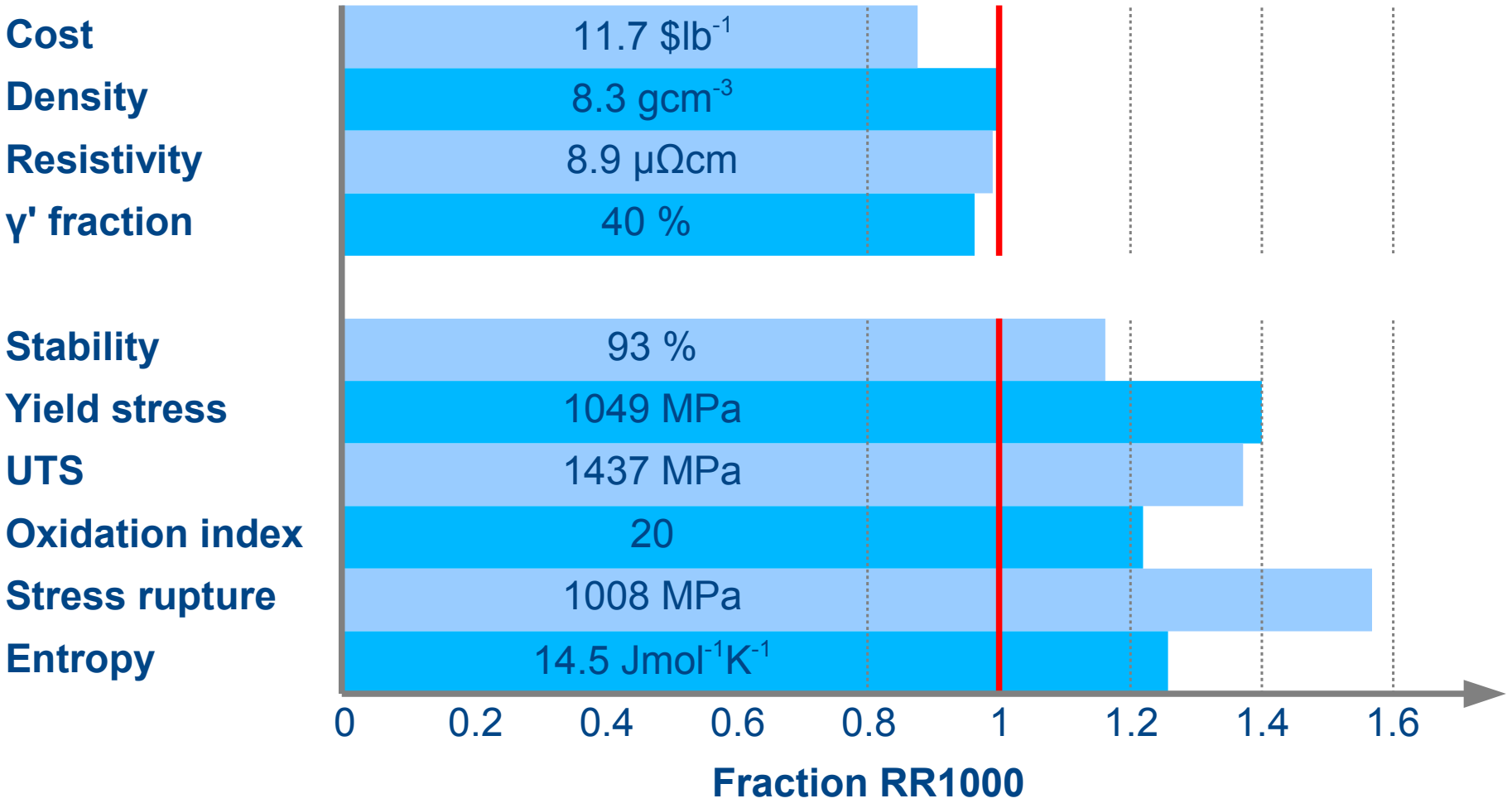






Ni	Cr	Co	Mo	Ti	Al	Ta	Hf	C	T	t
52	15	19	5	3.6	3	2	0.5	0.1	800	8

Case study: improved disc alloy



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

Case study: improved disc alloy

Ni

56

Cr

17

Co

1.0

Mo

4.0

Ti

1.5

Al

4.3

Ta

0.2

Hf

0.1

C

0.2

T

980

t

61

W

6.0

Mn

0.1

B

0.1

V

0.1

Si

0.1

Zr

0.2

Nb

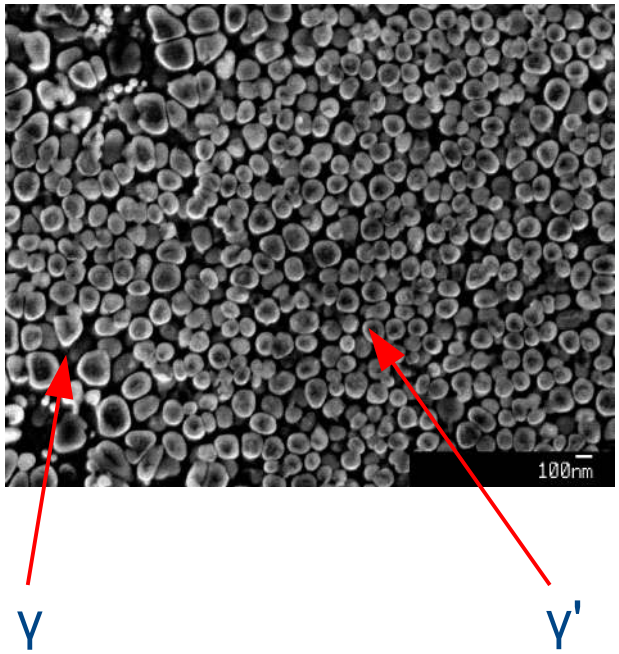
5.6

Fe

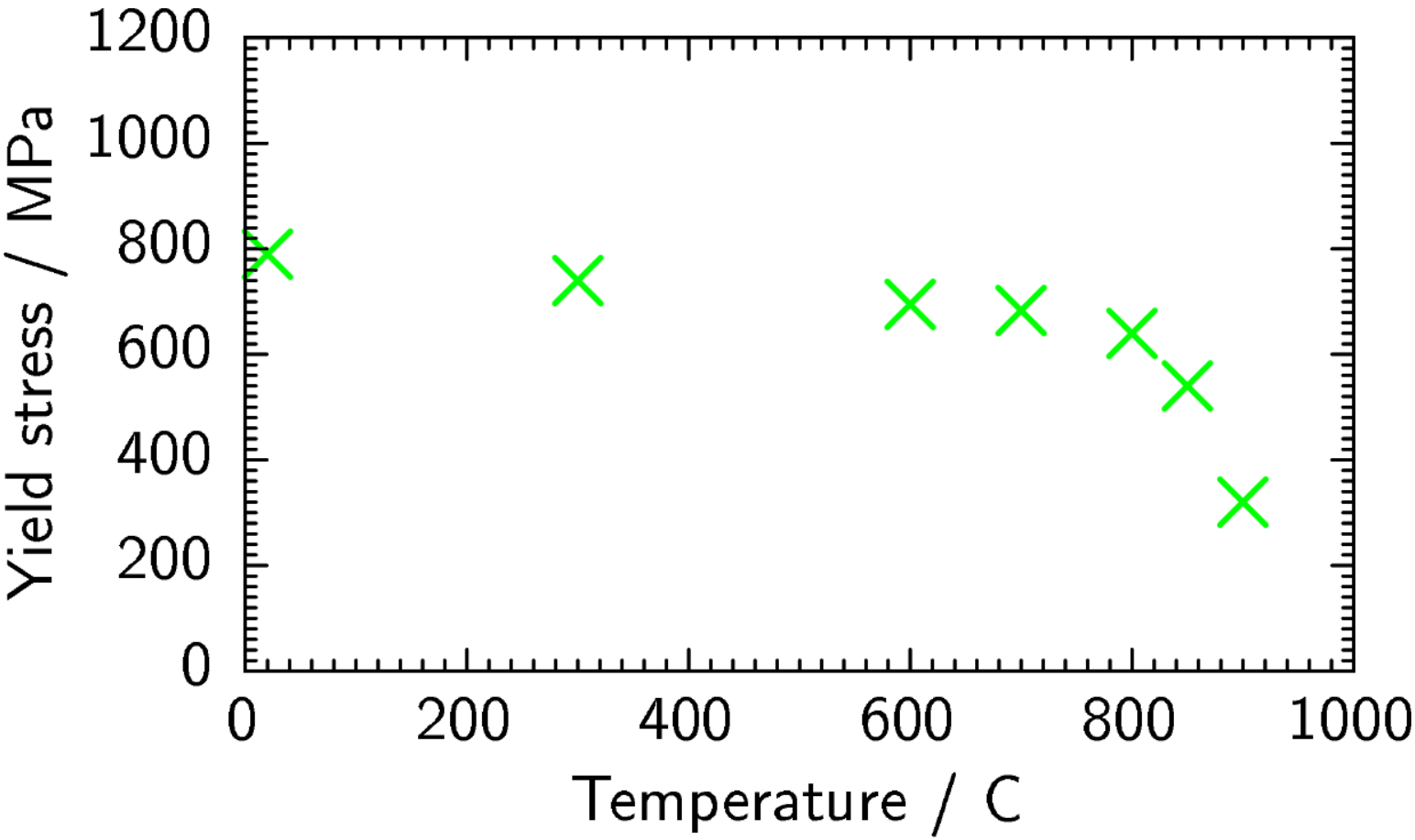
3.4

Electron micrograph – Ni disc alloy

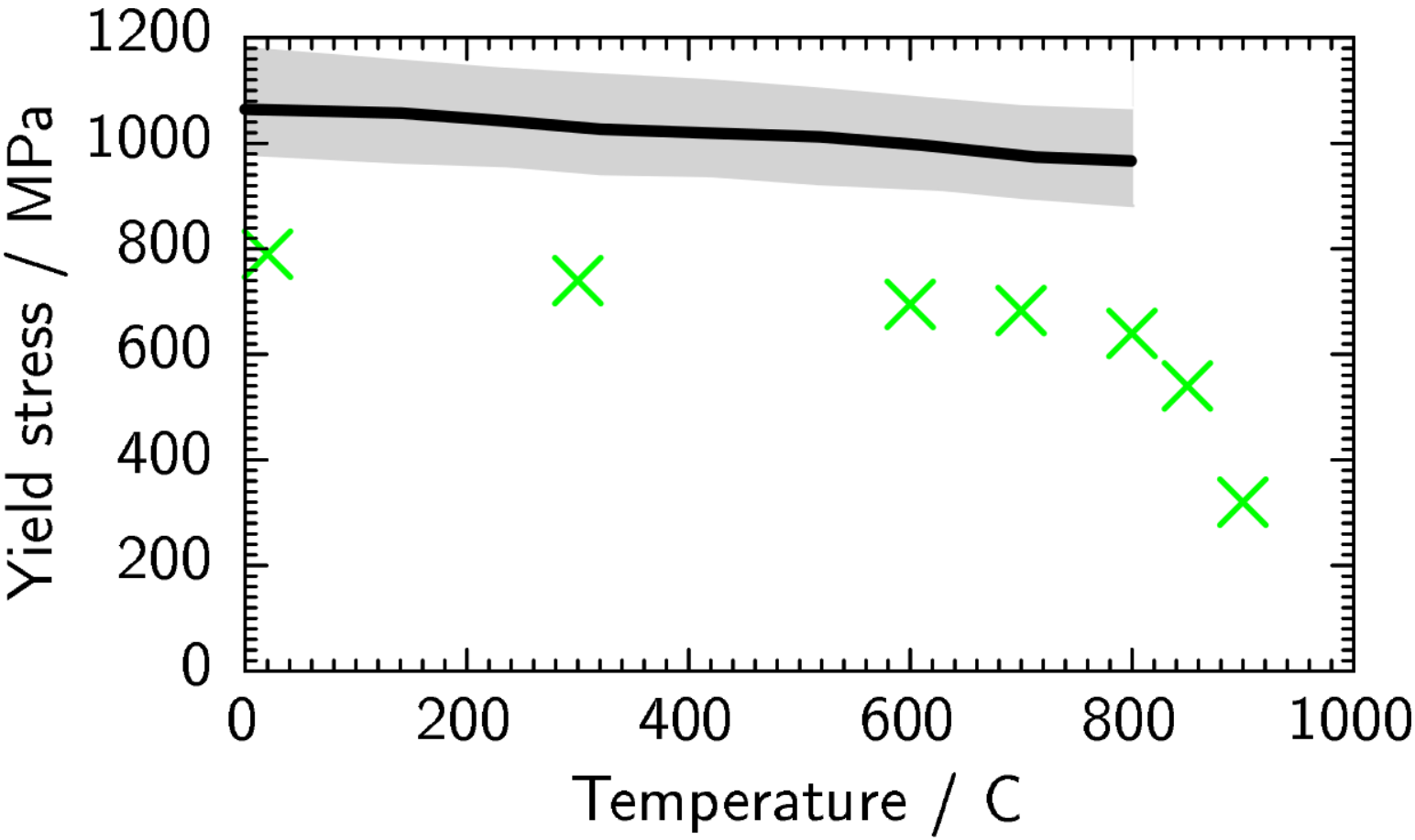
Ni disc alloy



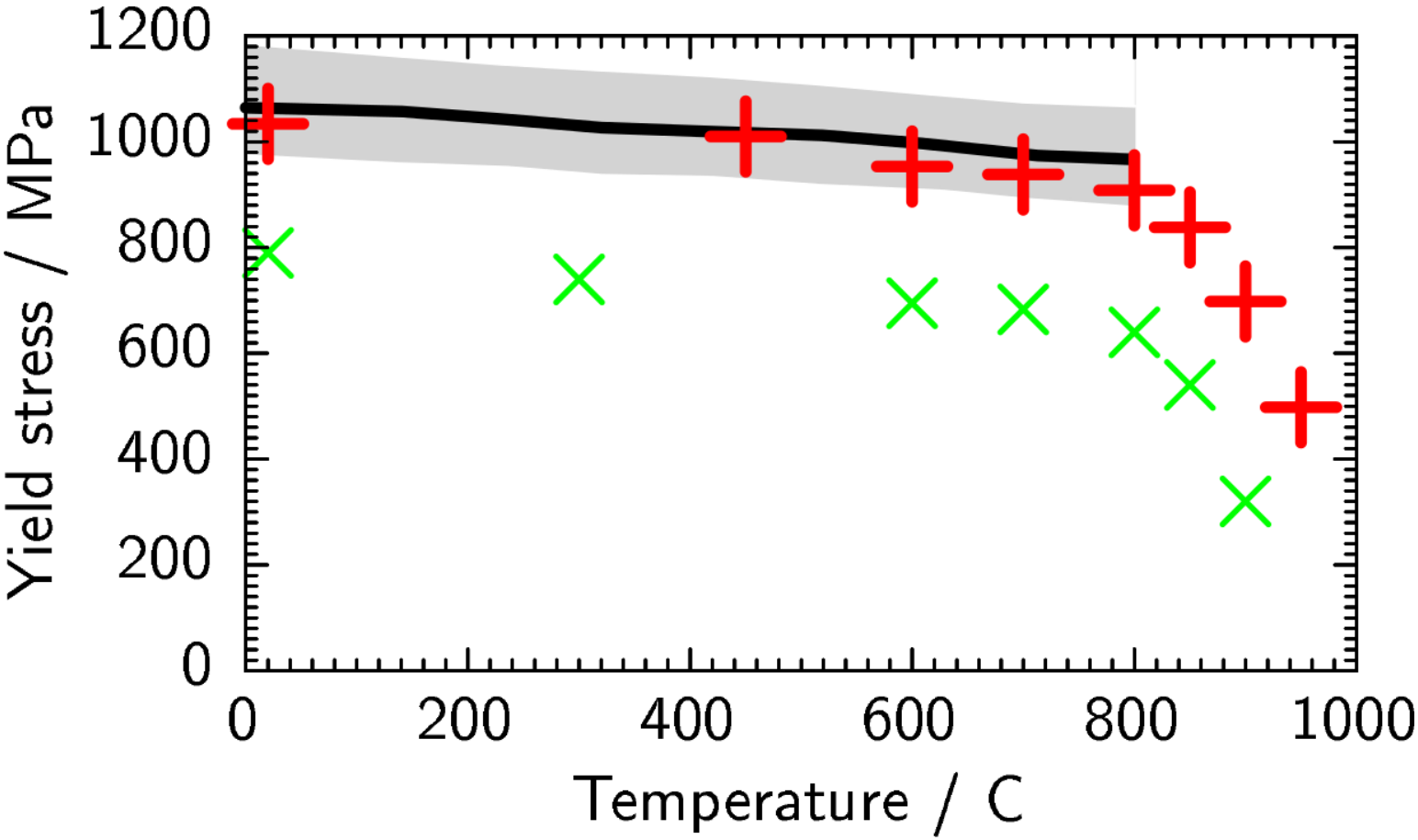
Yield stress



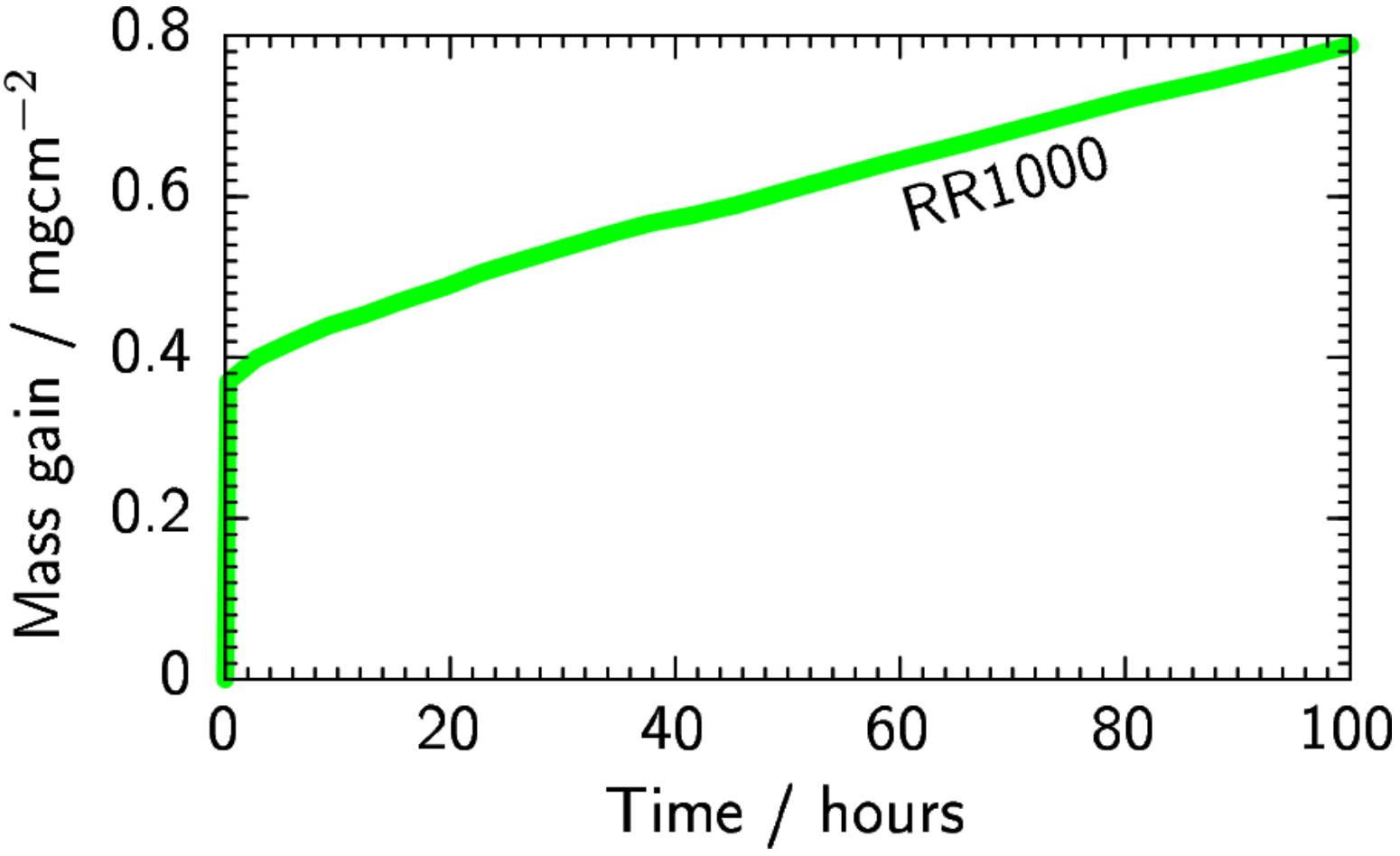
Yield stress



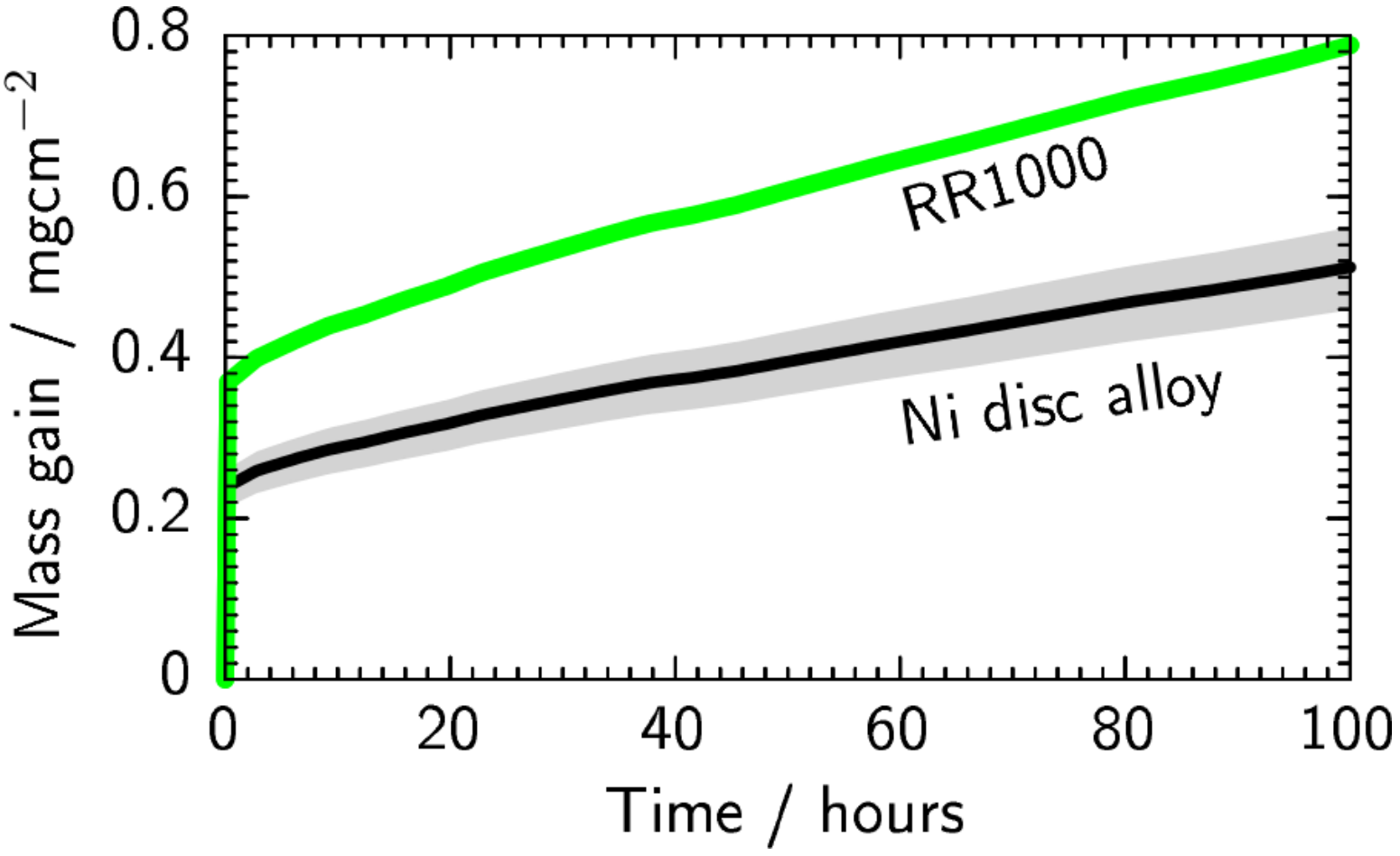
Yield stress



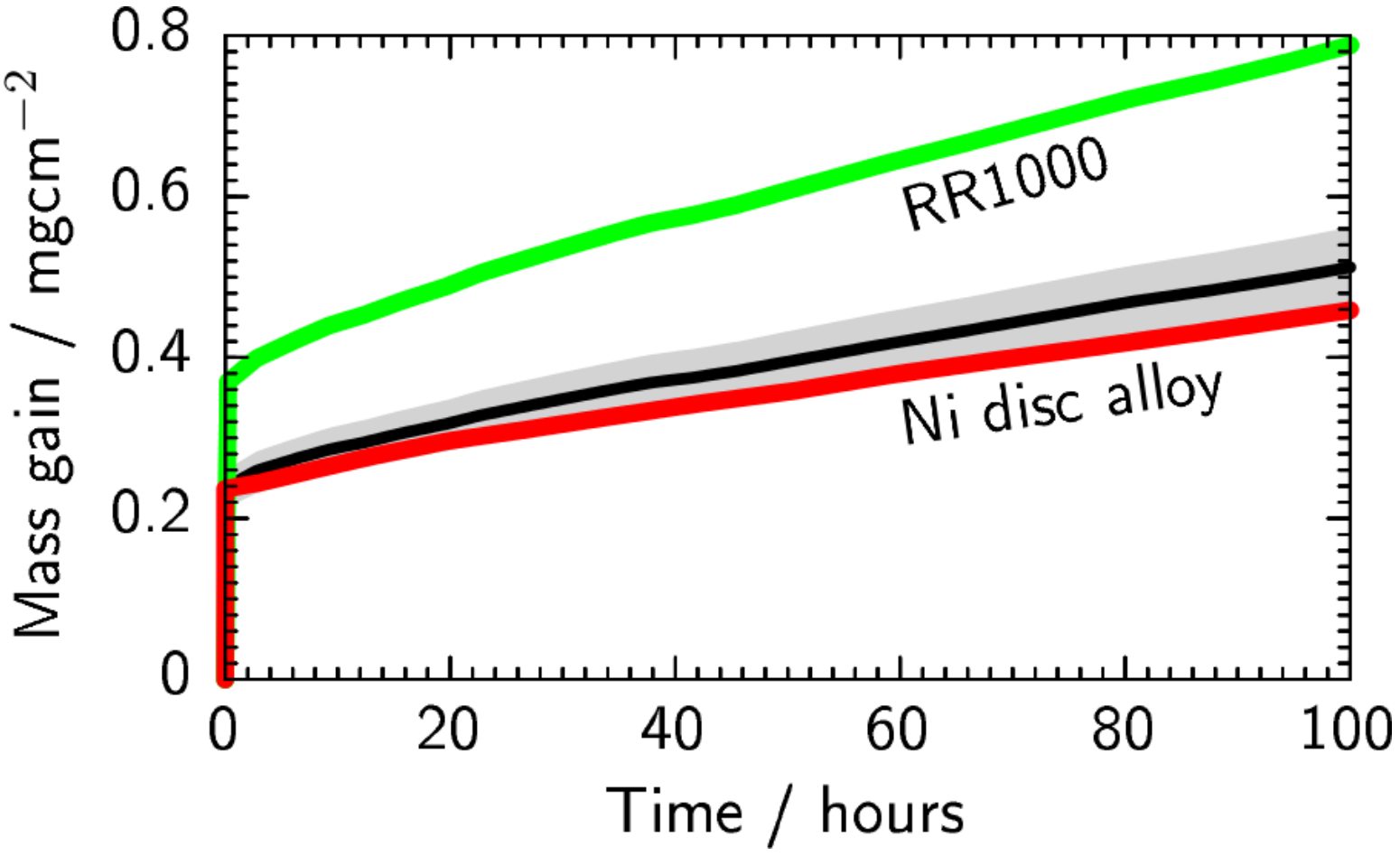
Oxidation



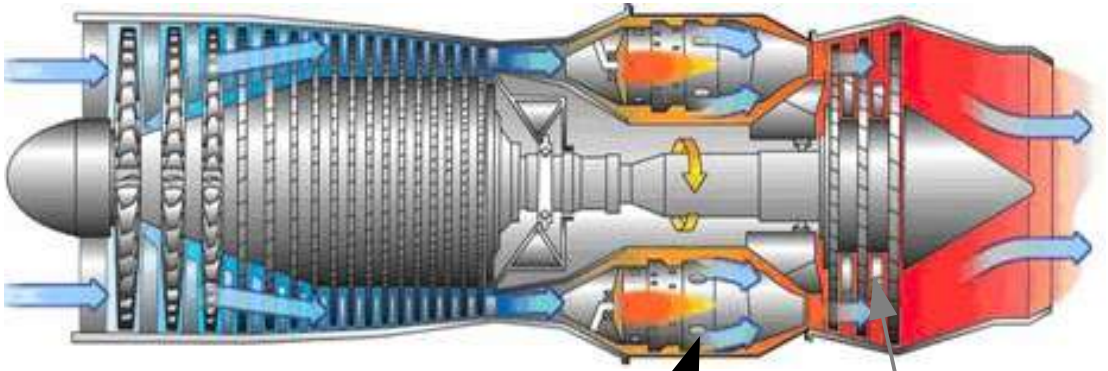
Oxidation


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

Predicted alloys

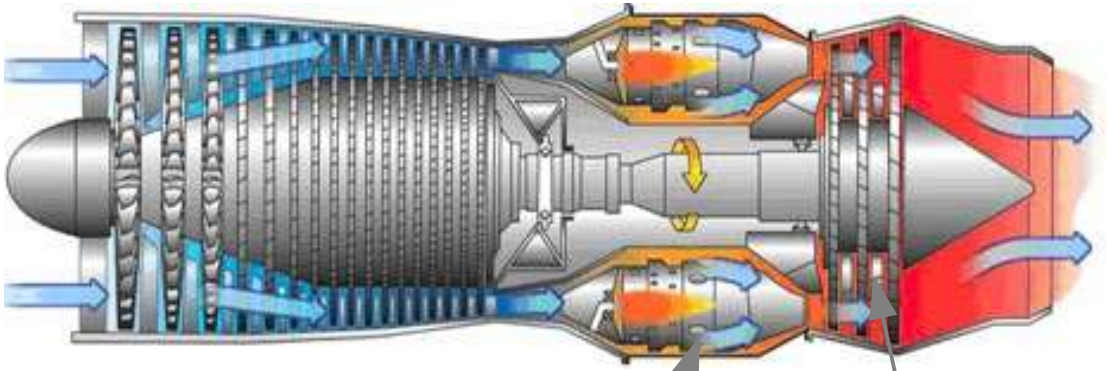


Combustor liner

2x disc alloy

2x forging hammer

Predicted alloys



Combustor liner

2x disc alloy

2x forging hammer

Case study: improved forging alloy

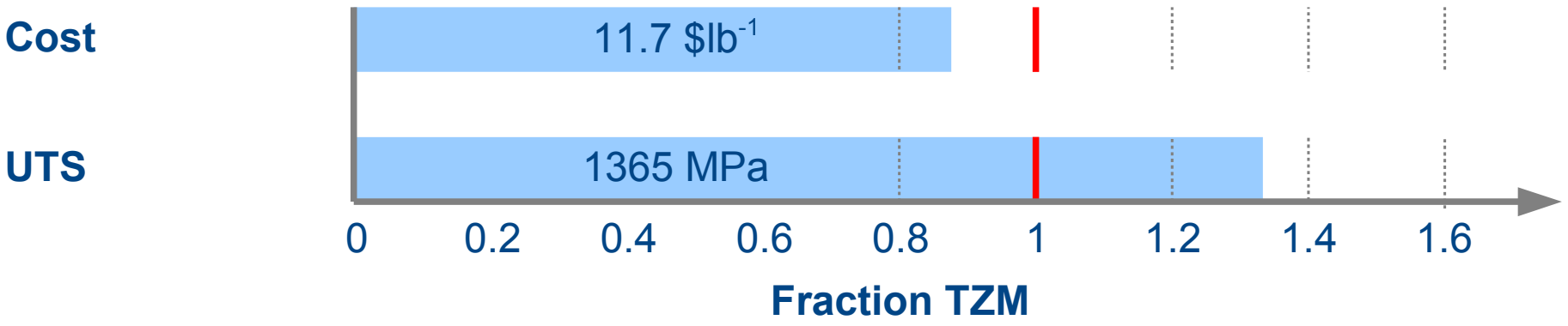






	Mo	Ti	C	Zr	Hf	W	Nb
TZM	99.4	0.5	0.02	0.08			

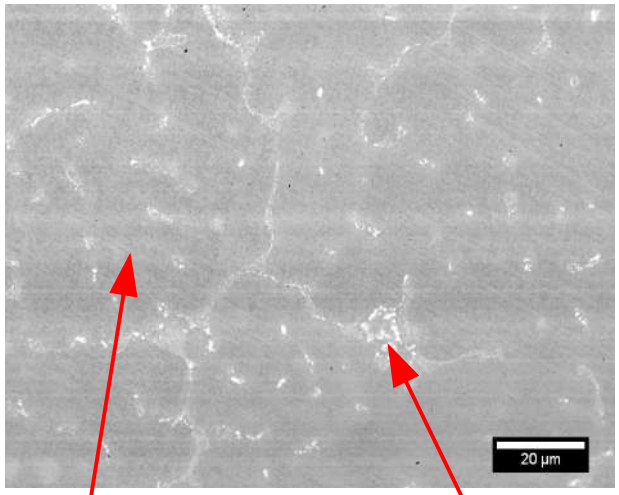
Case study: improved forging alloy



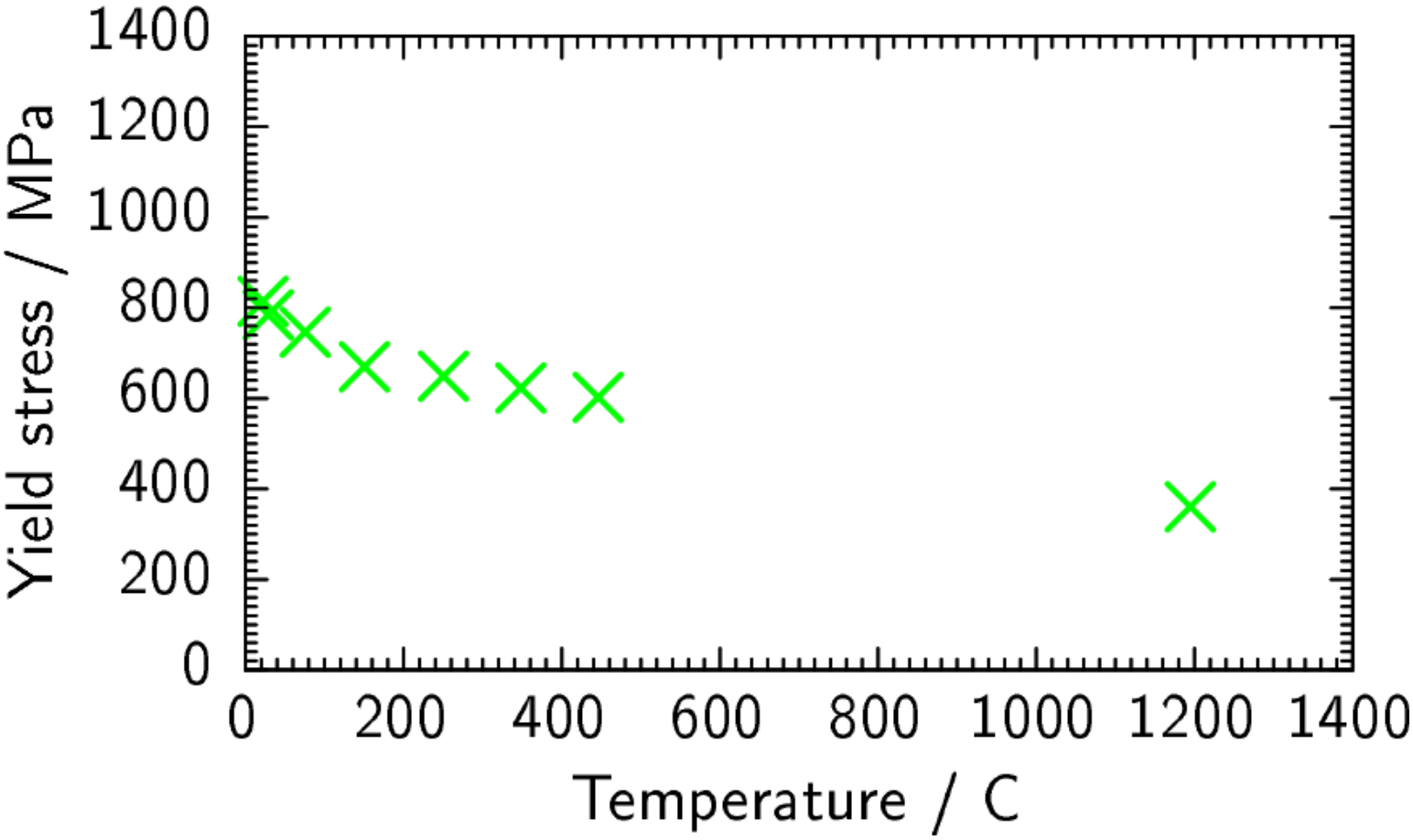
	Mo	Ti	C	Zr	Hf	W	Nb
TZM	99.4	0.5	0.02	0.08			
Optimal	82.7	1.0	0.2	0.9	9.0	0.5	5.7

Electron micrograph – Mo forging alloy

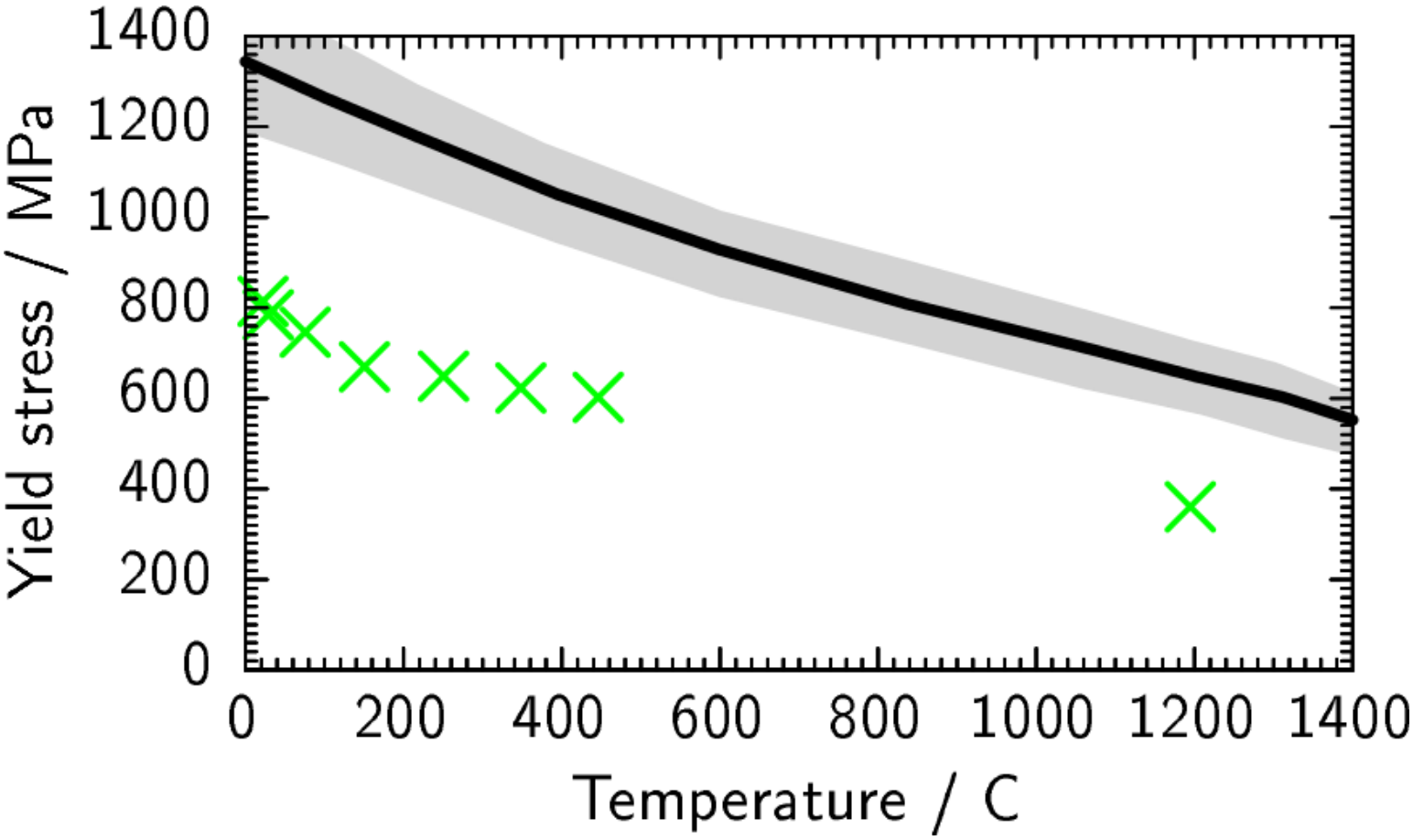
Mo forging alloy



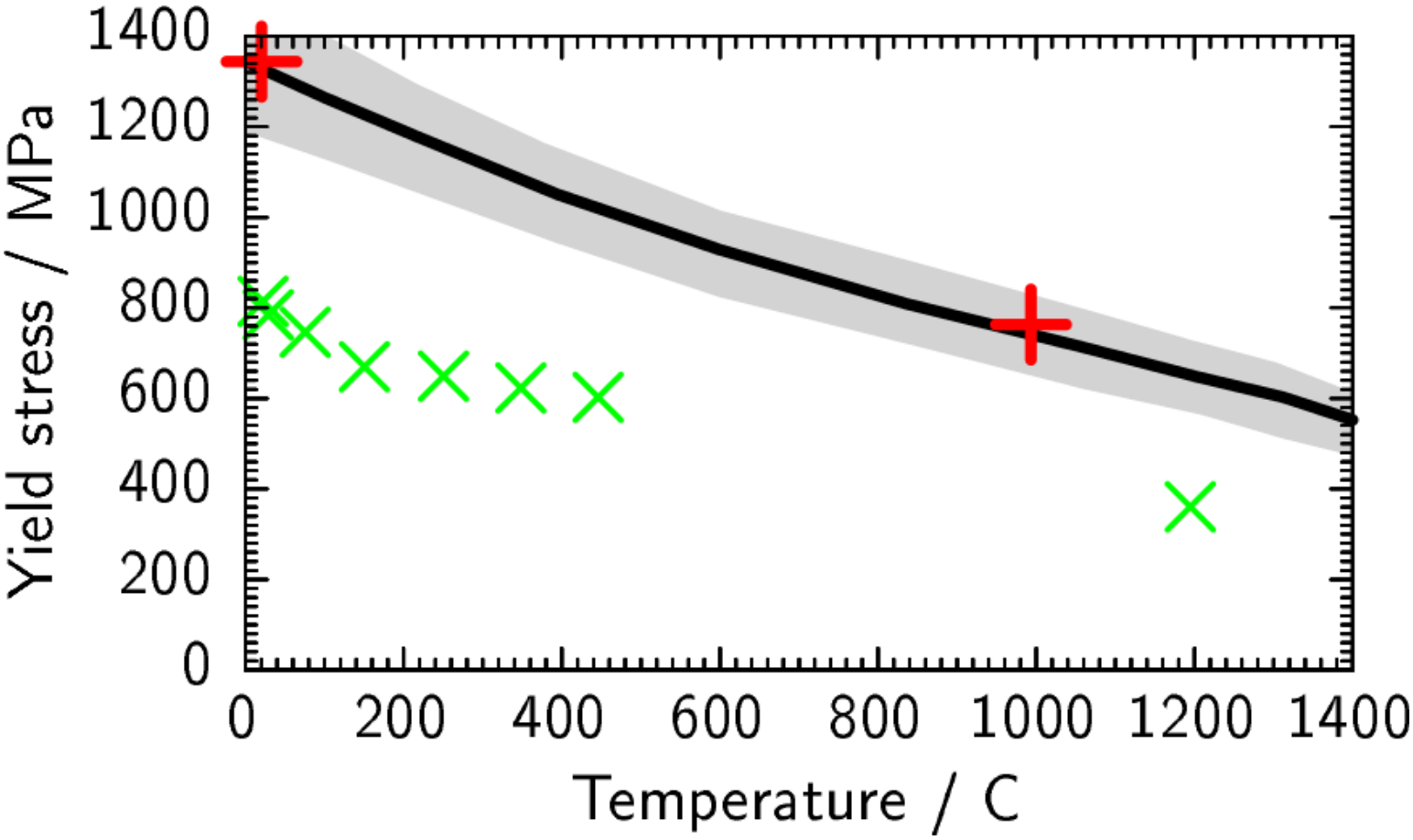
Yield stress



Yield stress

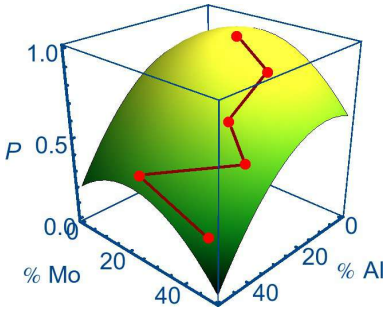


Yield stress

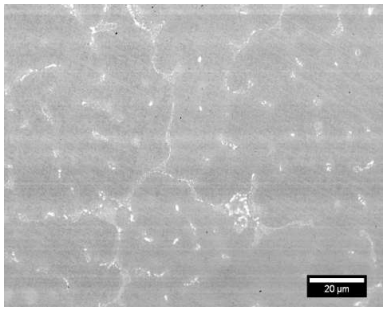


Concurrent materials design

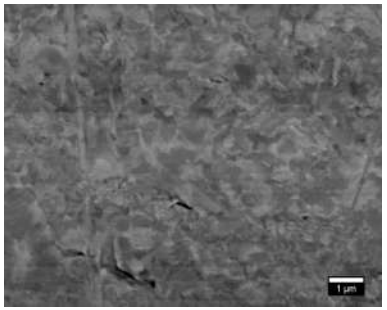
Discovery algorithm
Patent GB1302743.8 (2013)



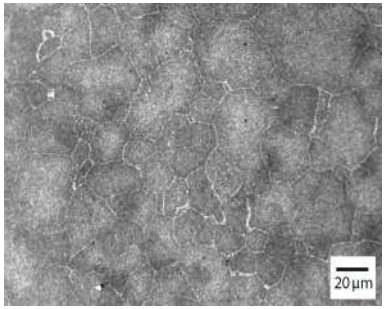
Mo-Hf forging alloy
Patent GB1307533.8 (2013)



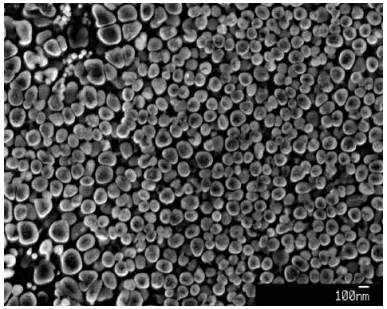
Mo-Nb forging alloy
Patent GB1307535.3 (2013)



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



Ni disc alloy
Rolls-Royce invention
NC12261 (2012)



Ni combustor liner
Rolls-Royce invention
NC13006 (2013)