

# Concurrent materials design

Gareth Conduit

Patent GB1302743.8 (2013)

Patent GB1307533.8 (2013)

Patent GB1307535.3 (2013)

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

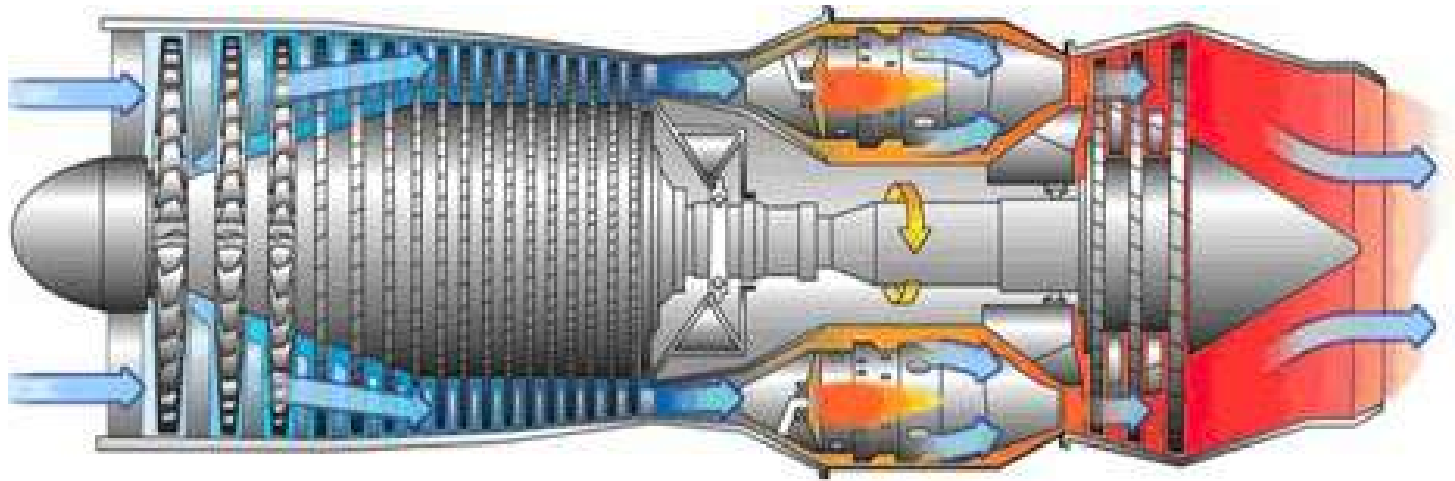
Submitted to Intermetallics (2013)

Rolls-Royce Group plc invention submission NC13006 (2013)

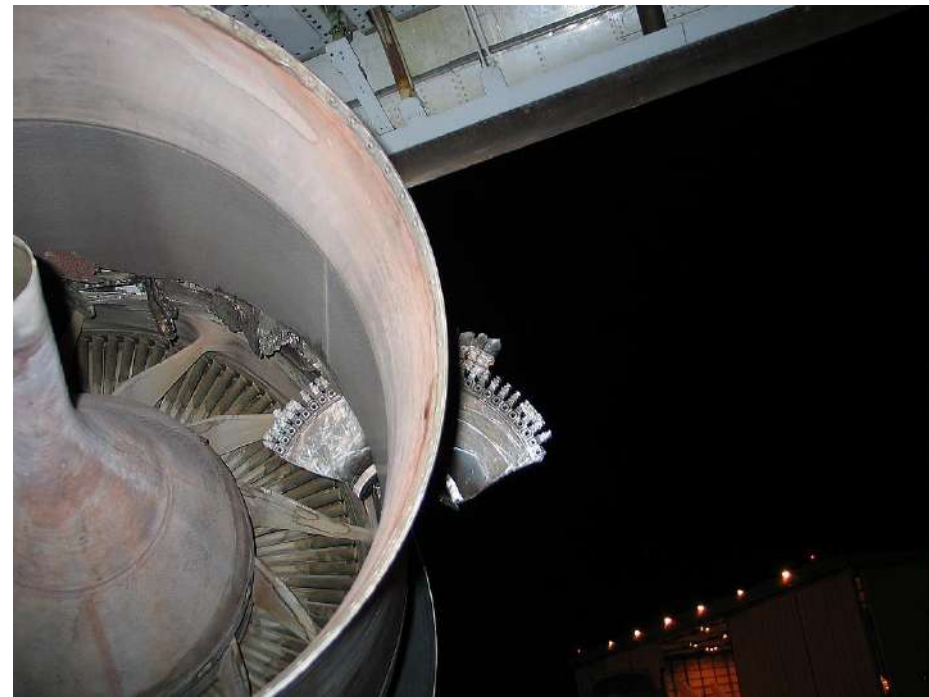
Rolls-Royce Group plc invention submission NC12261 (2012)

TCM Group, Department of Physics

# Jet engine



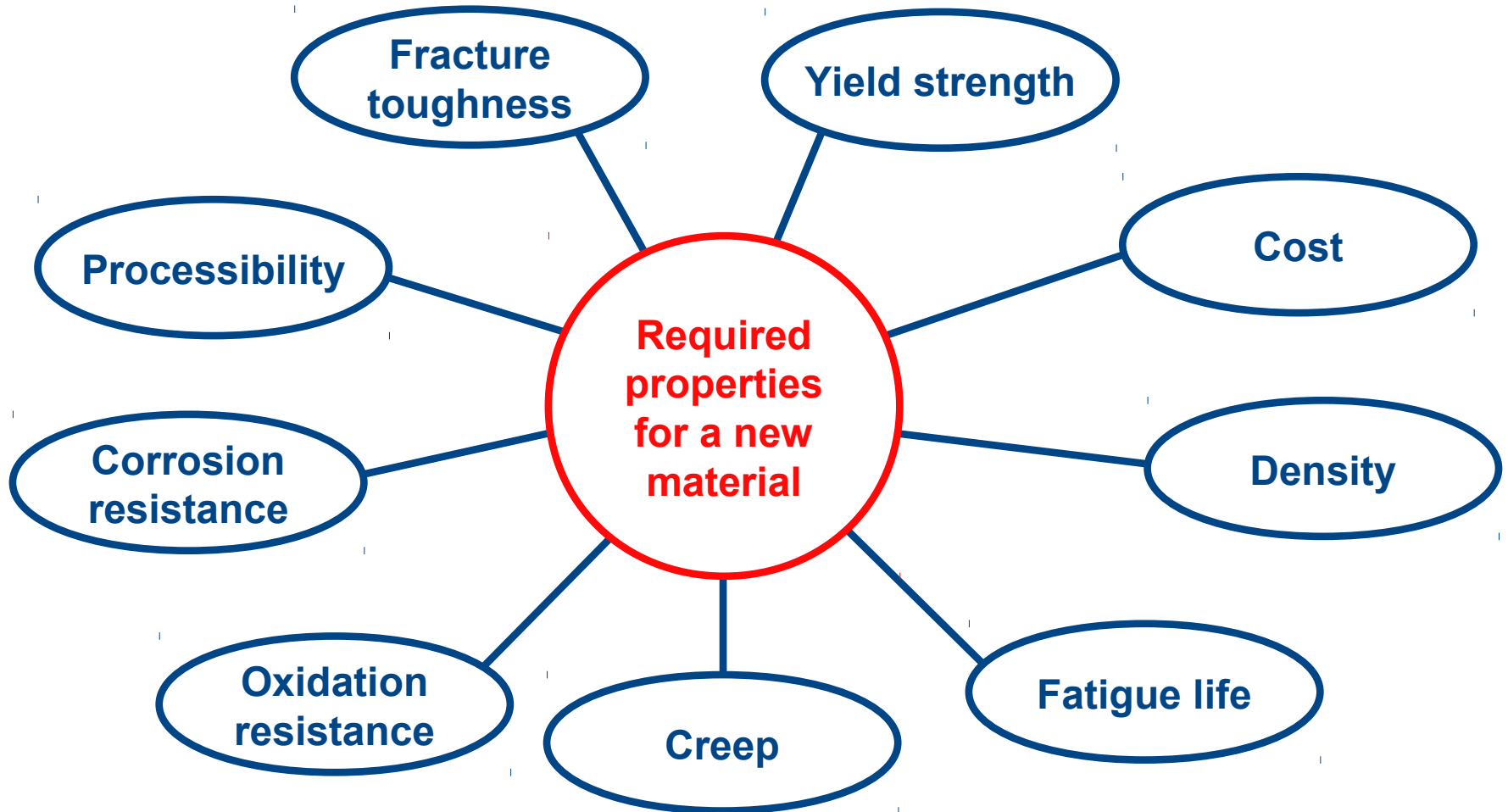
# Jet engine: disc failure



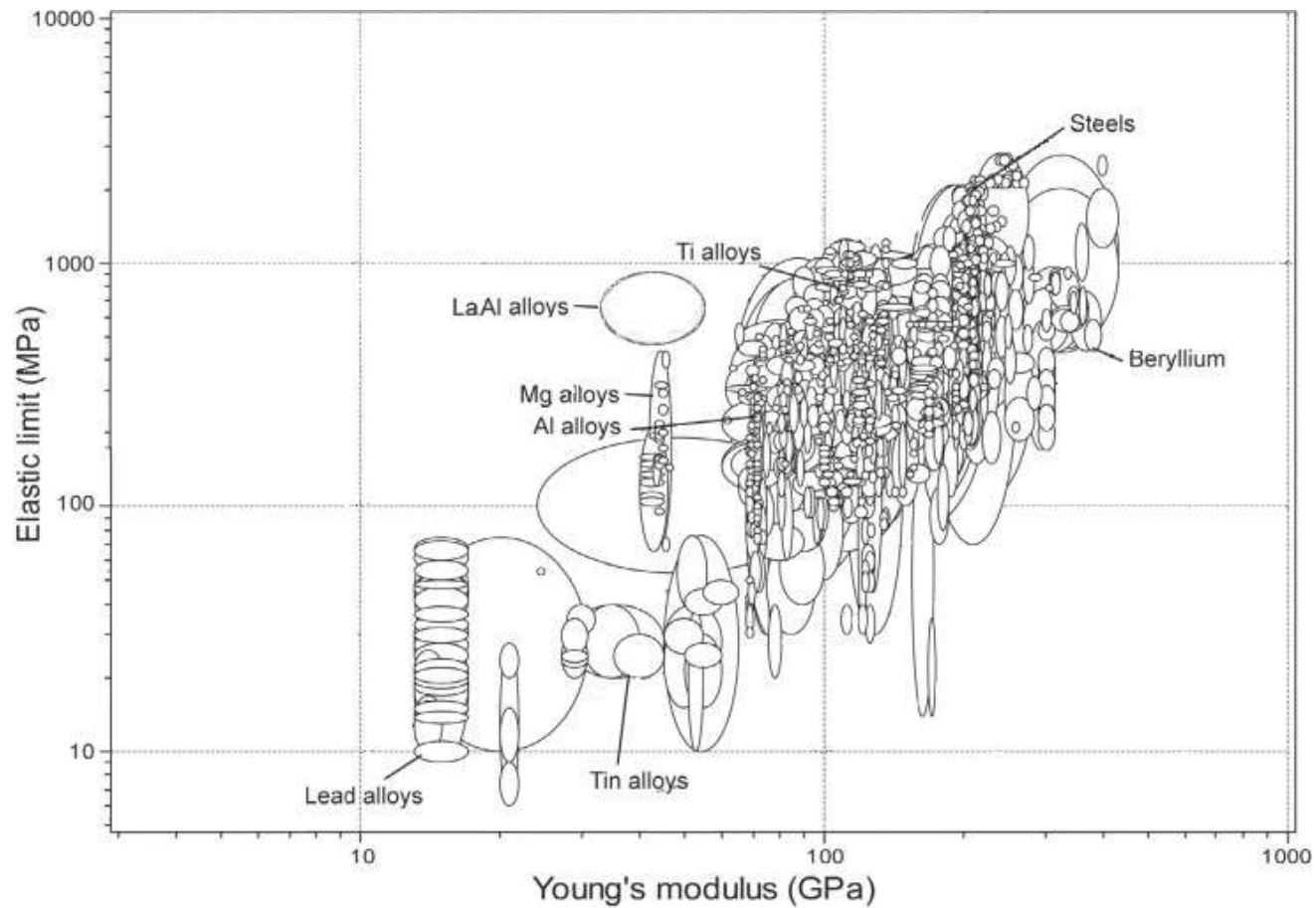
# Jet engine: bird strike



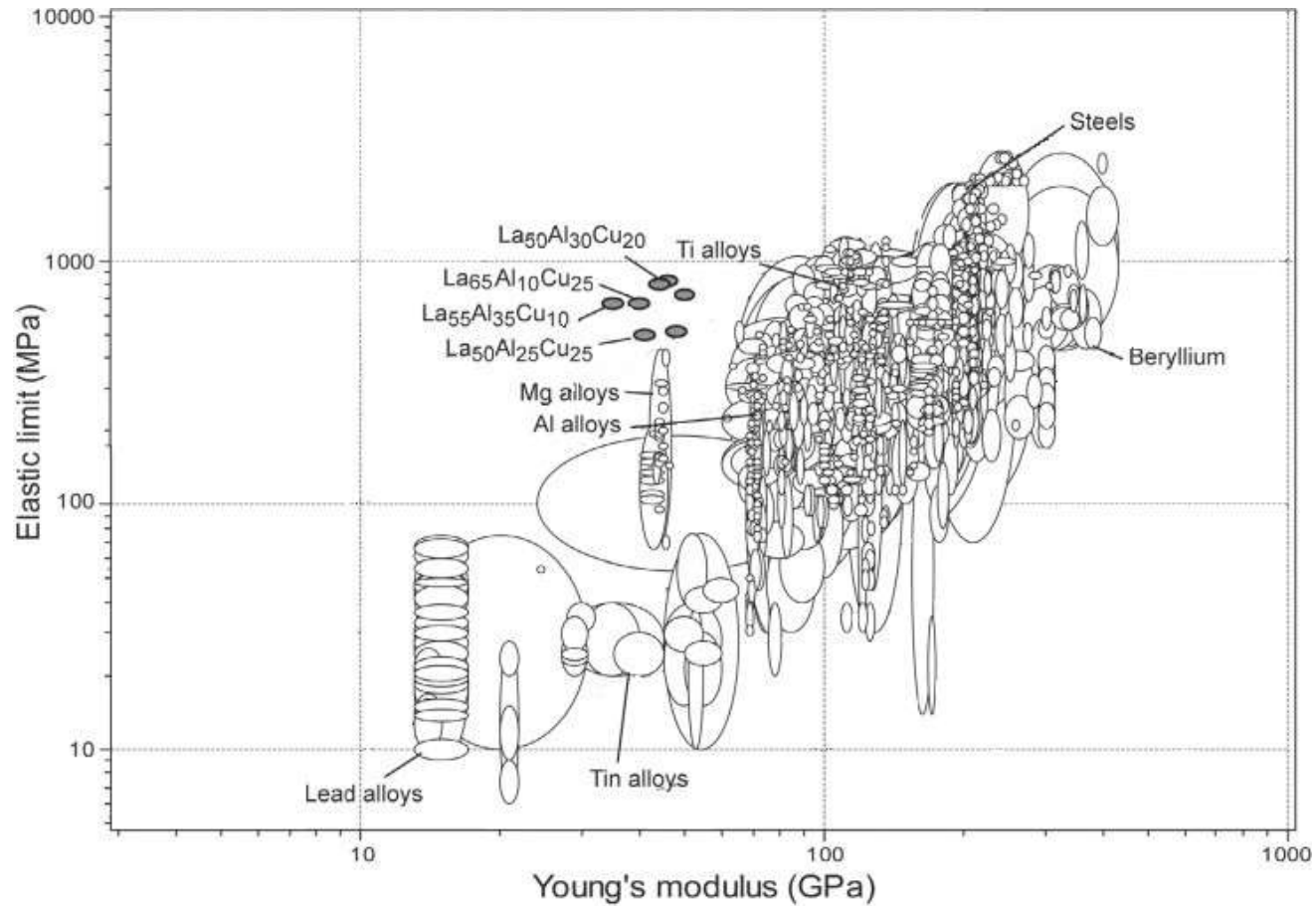
# Designing a new material – what is required ?



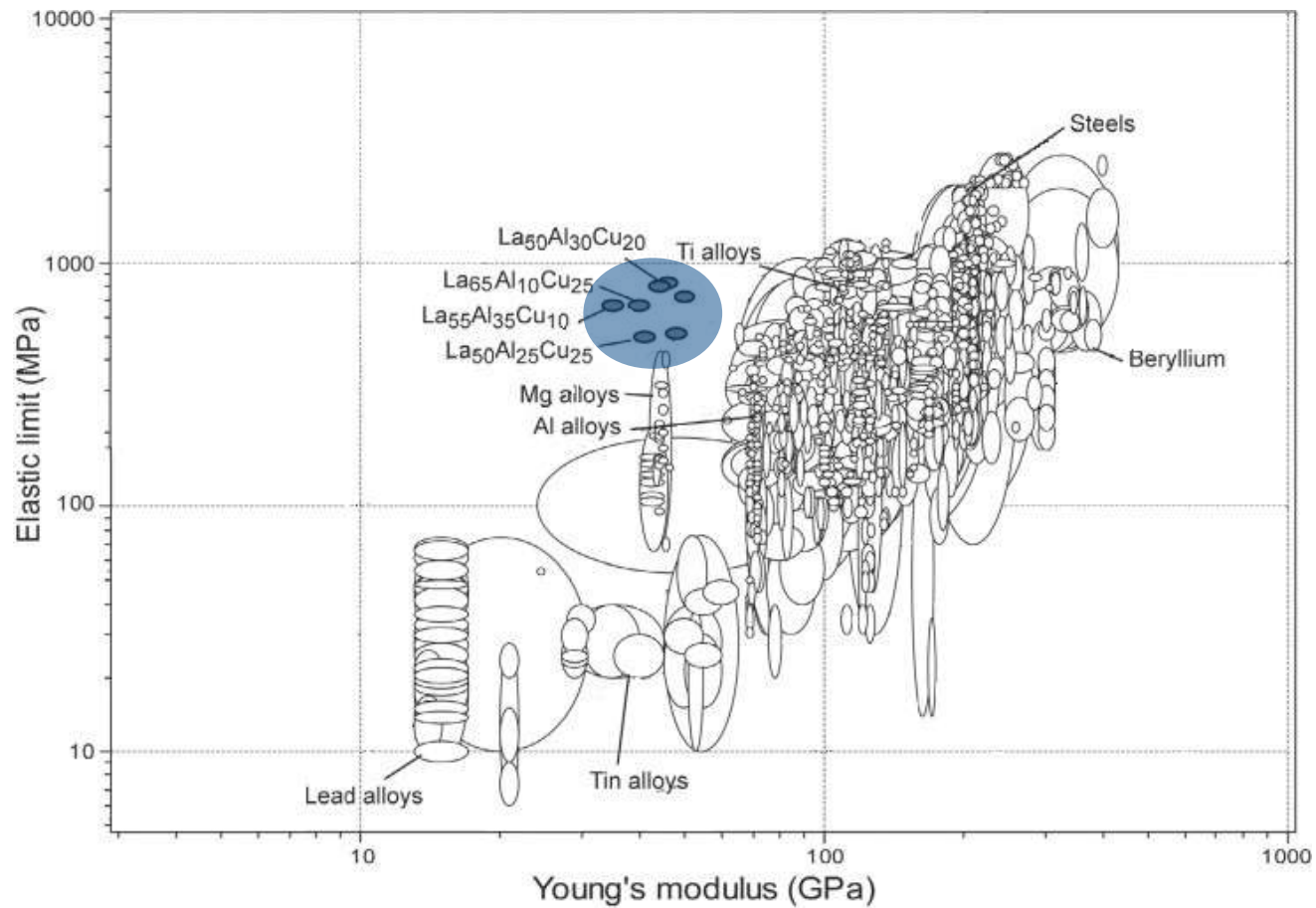
# Materials selection



# Materials selection



# Materials selection





# Materials selection

Guide the discovery of new materials

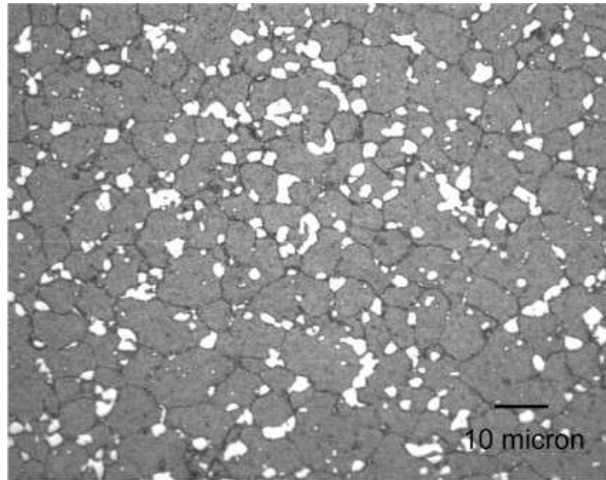
Concurrent materials design

Assess data quality

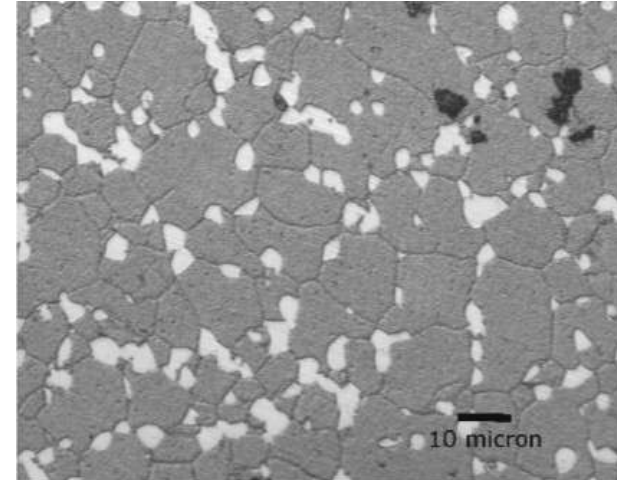
Estimate missing data

# Contemporary alloys

RR1000

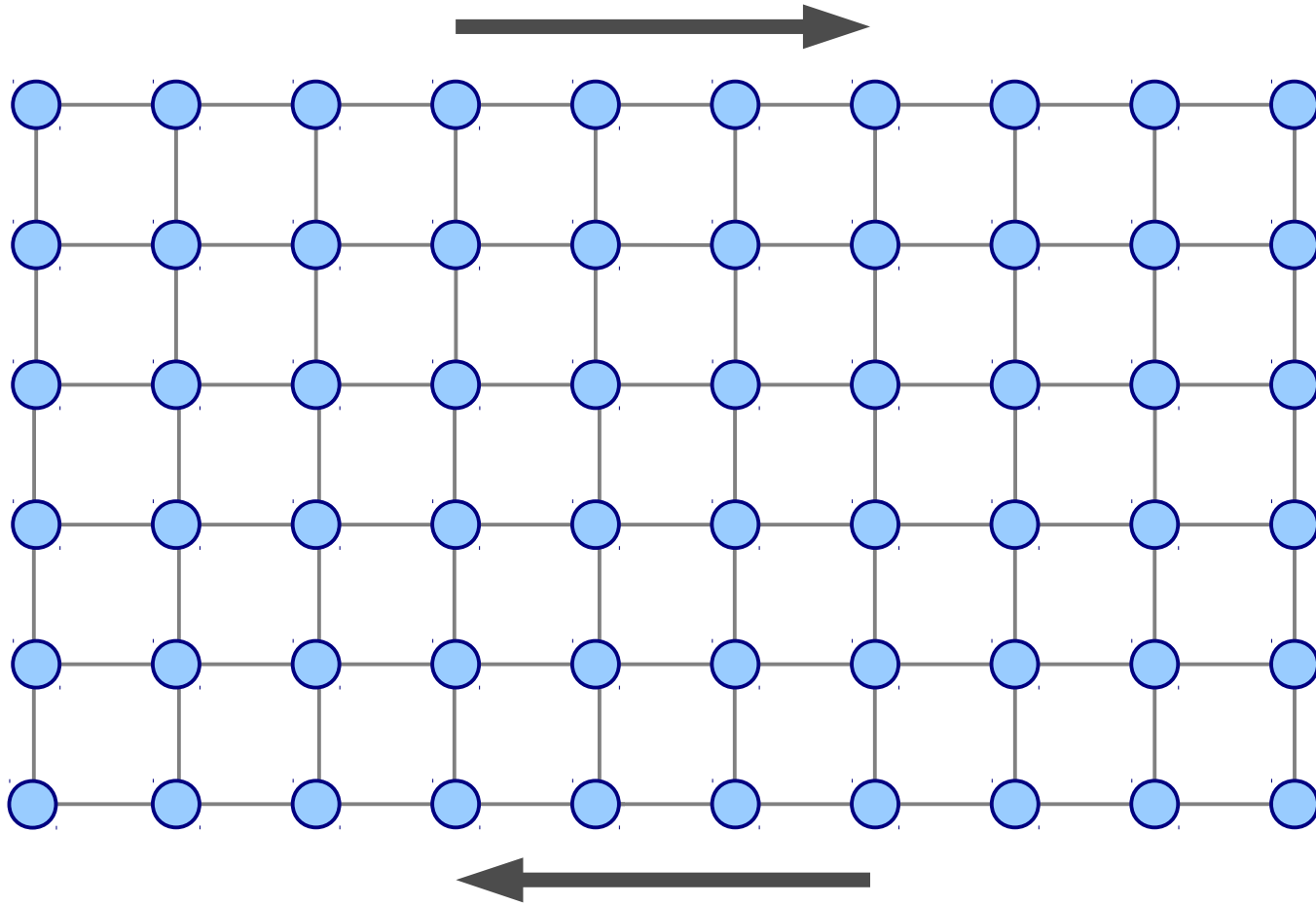


N18

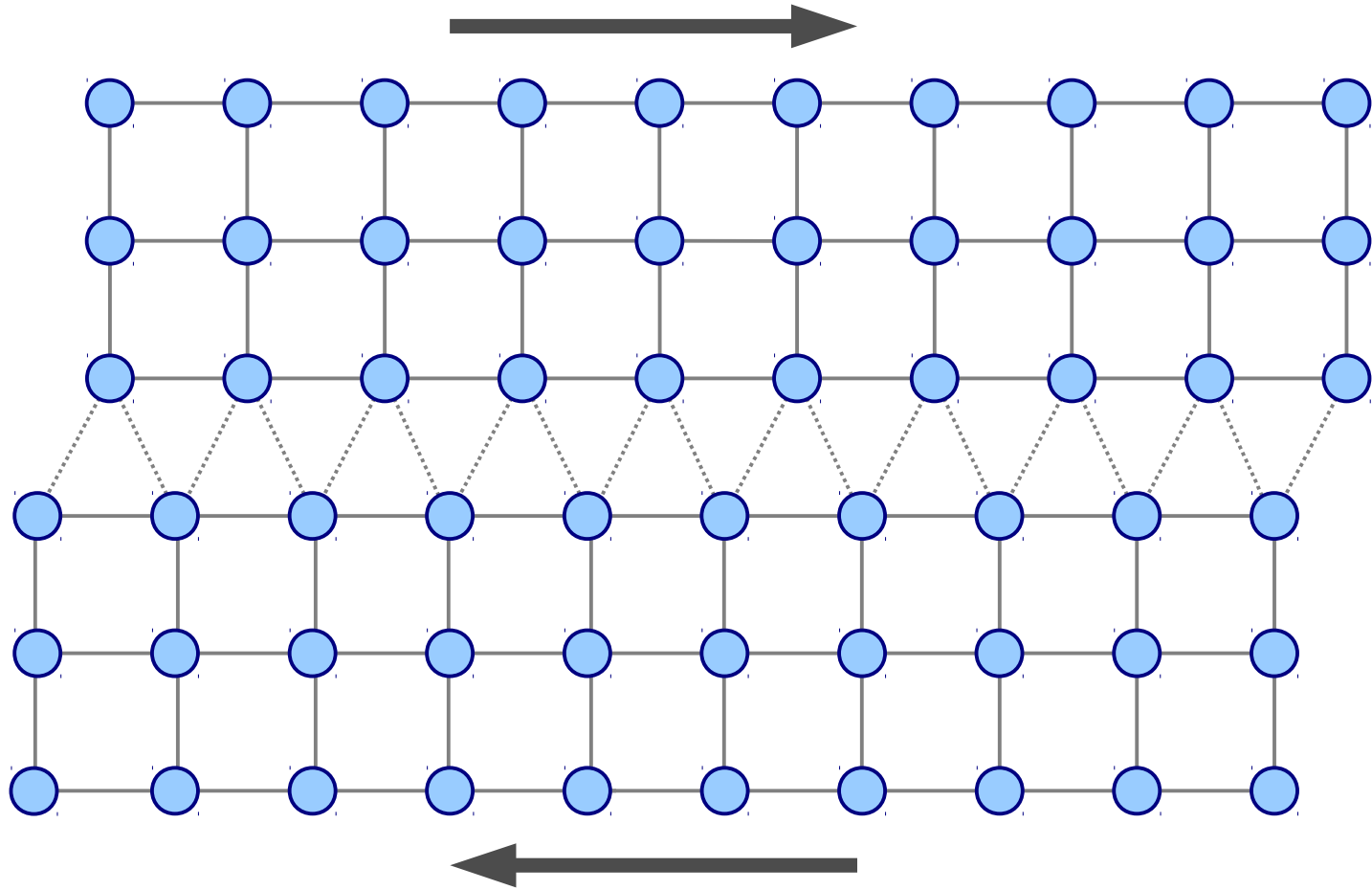


Alloy	Firm	Ni	Cr	Co	Mo	Ti	Al	C	Hf	Ta	W	Nb
Waspaloy	UTC	58	19	13	4	3	1.4					
N18	SNECMA	58	11.1	15.4	6.4	4.3	4.3	0.02	0.5			
Rene 88	General Elec.	56.5	16	13	4	3.7	2.1	0.03			4	0.7
RR1000	Rolls Royce	52.4	15	18.5	5	3.6	3	0.03	0.5	2		

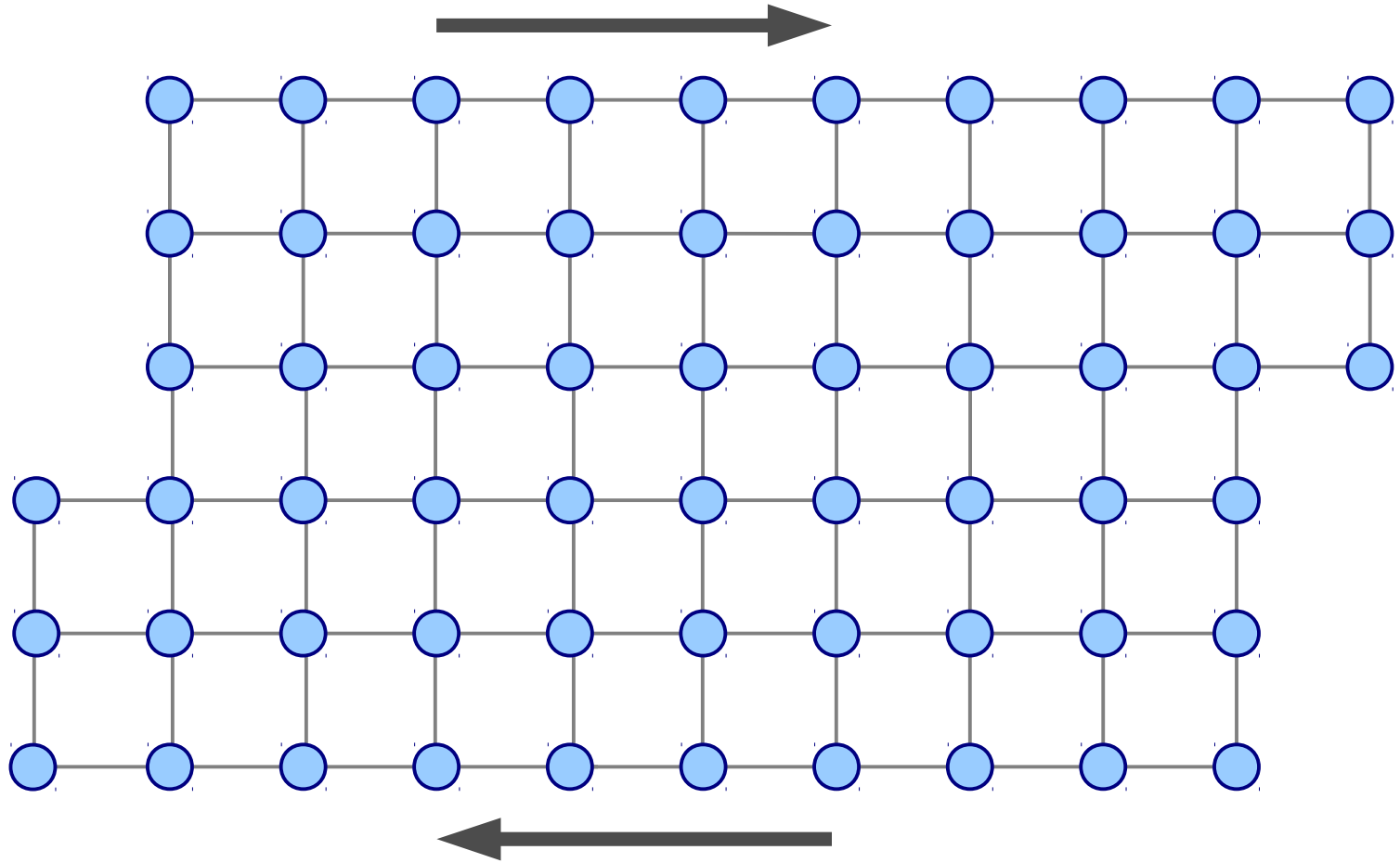
# Creep



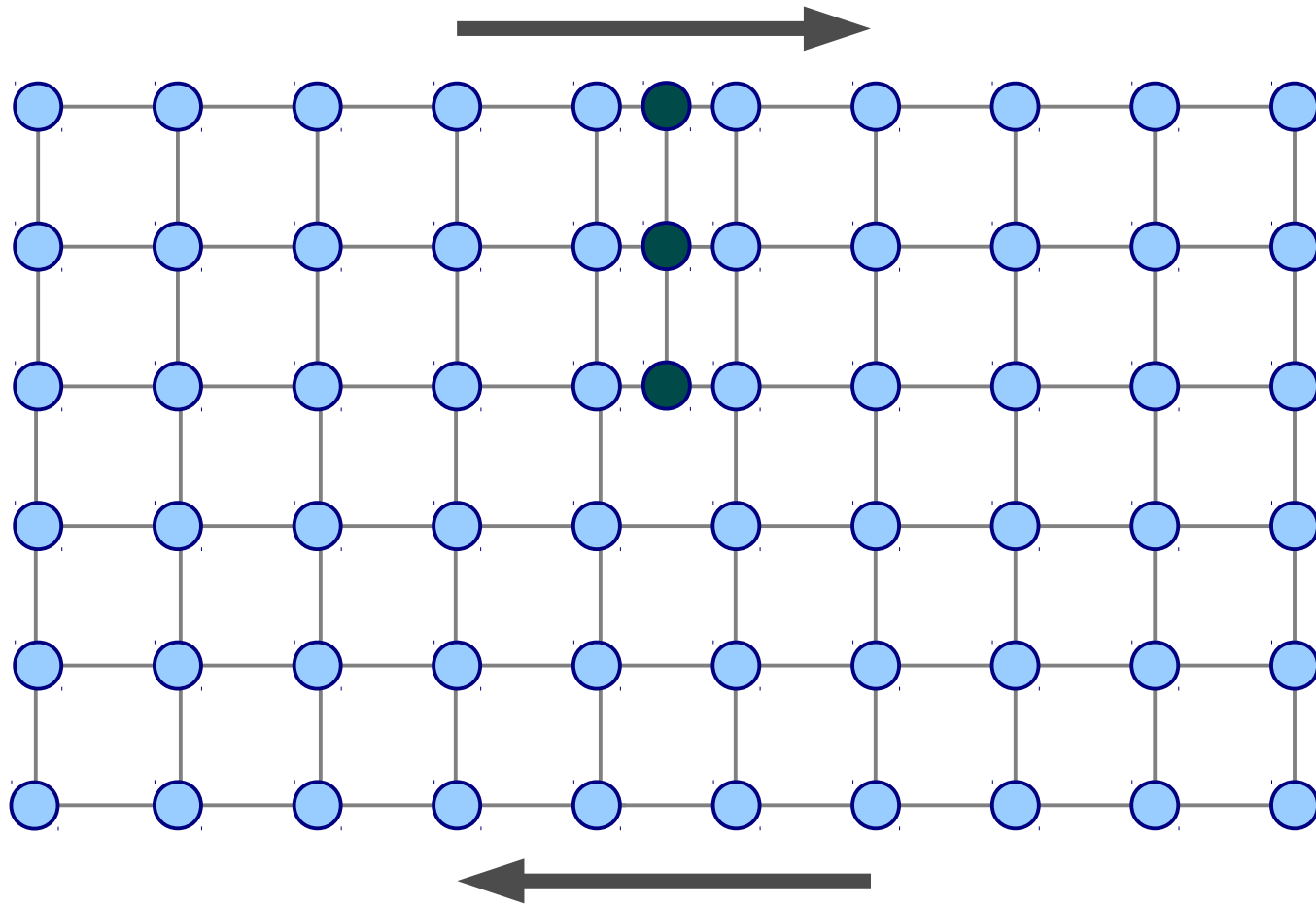
# Creep



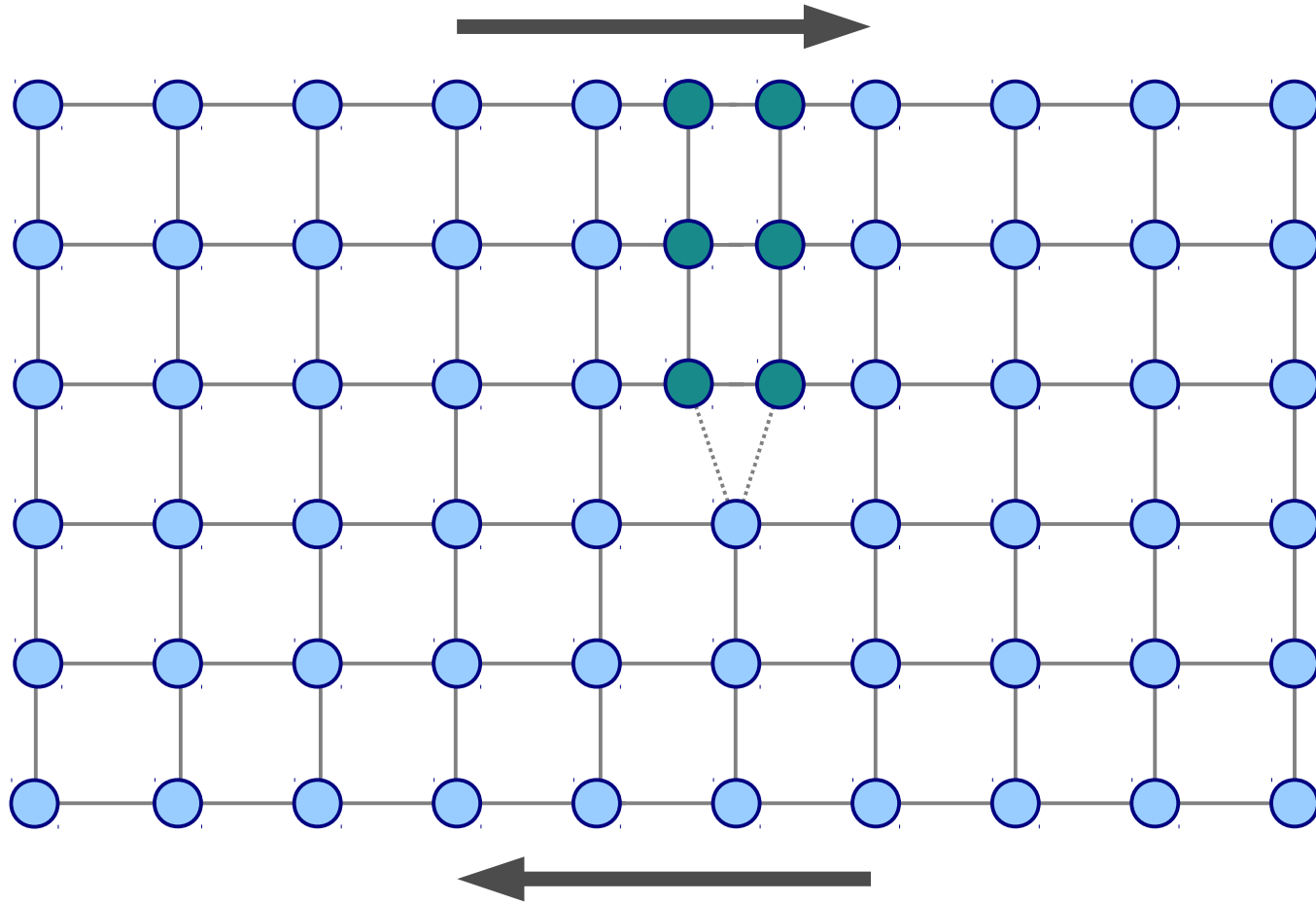
# Creep



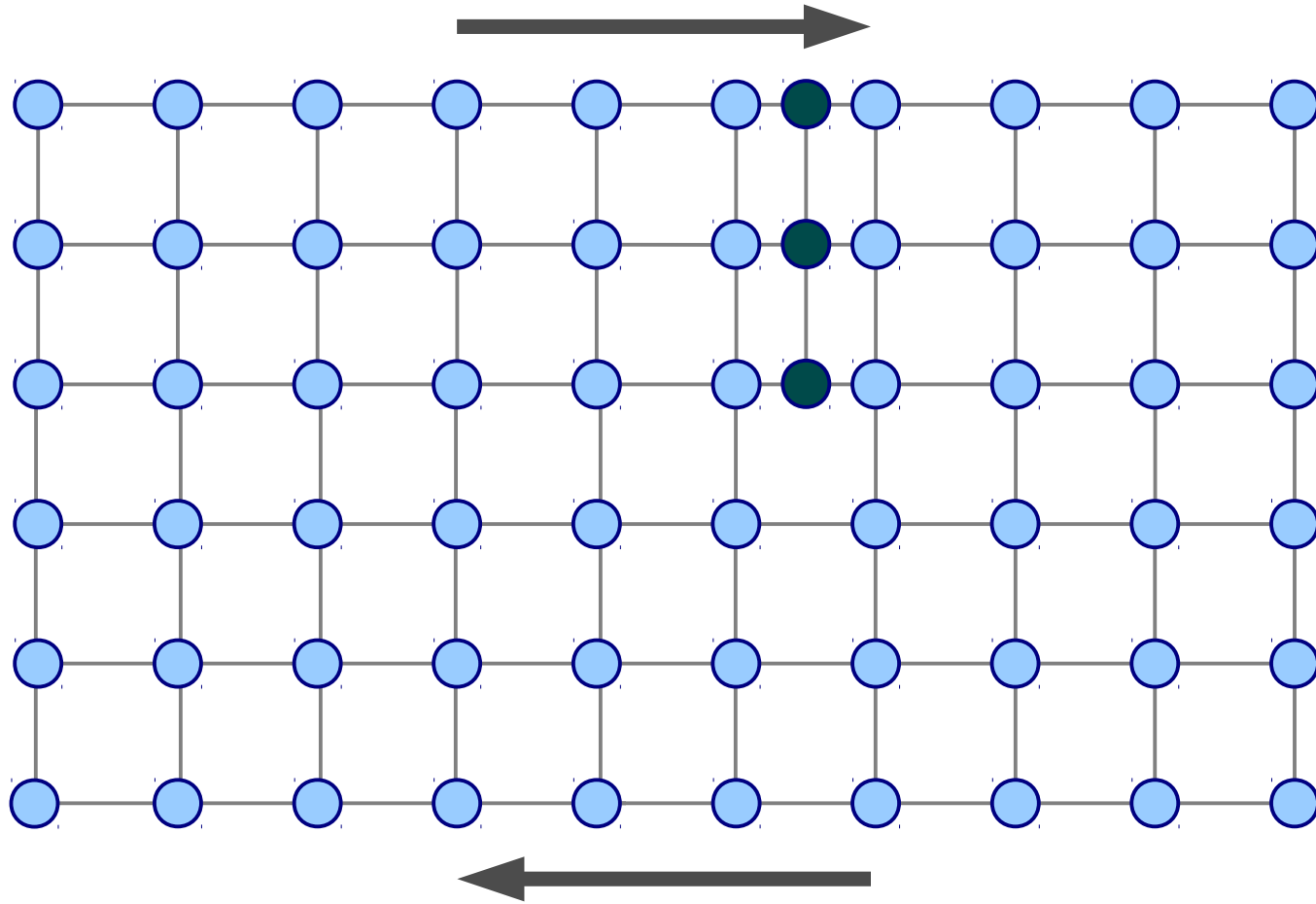
# Creep



# Creep

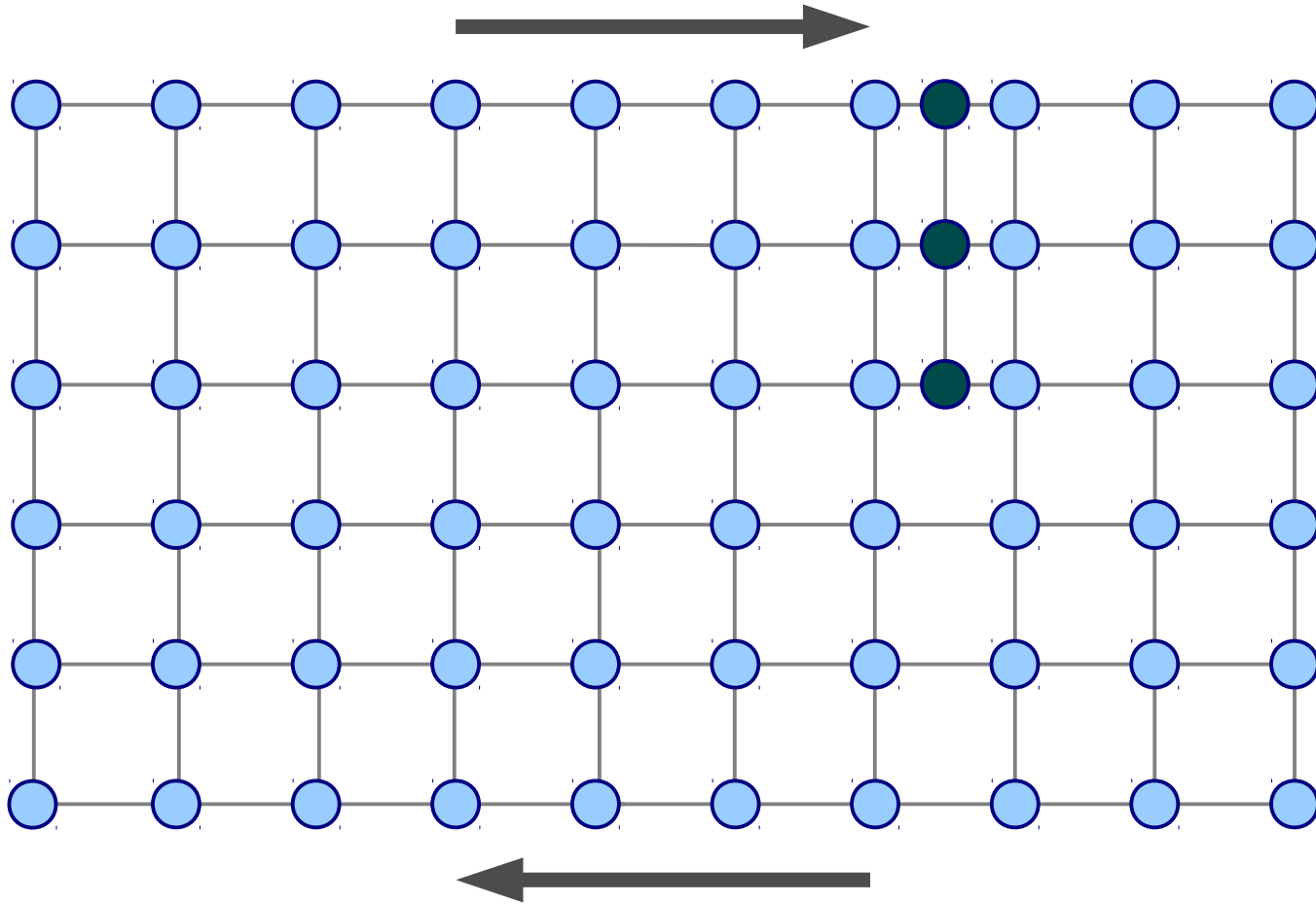


# Creep

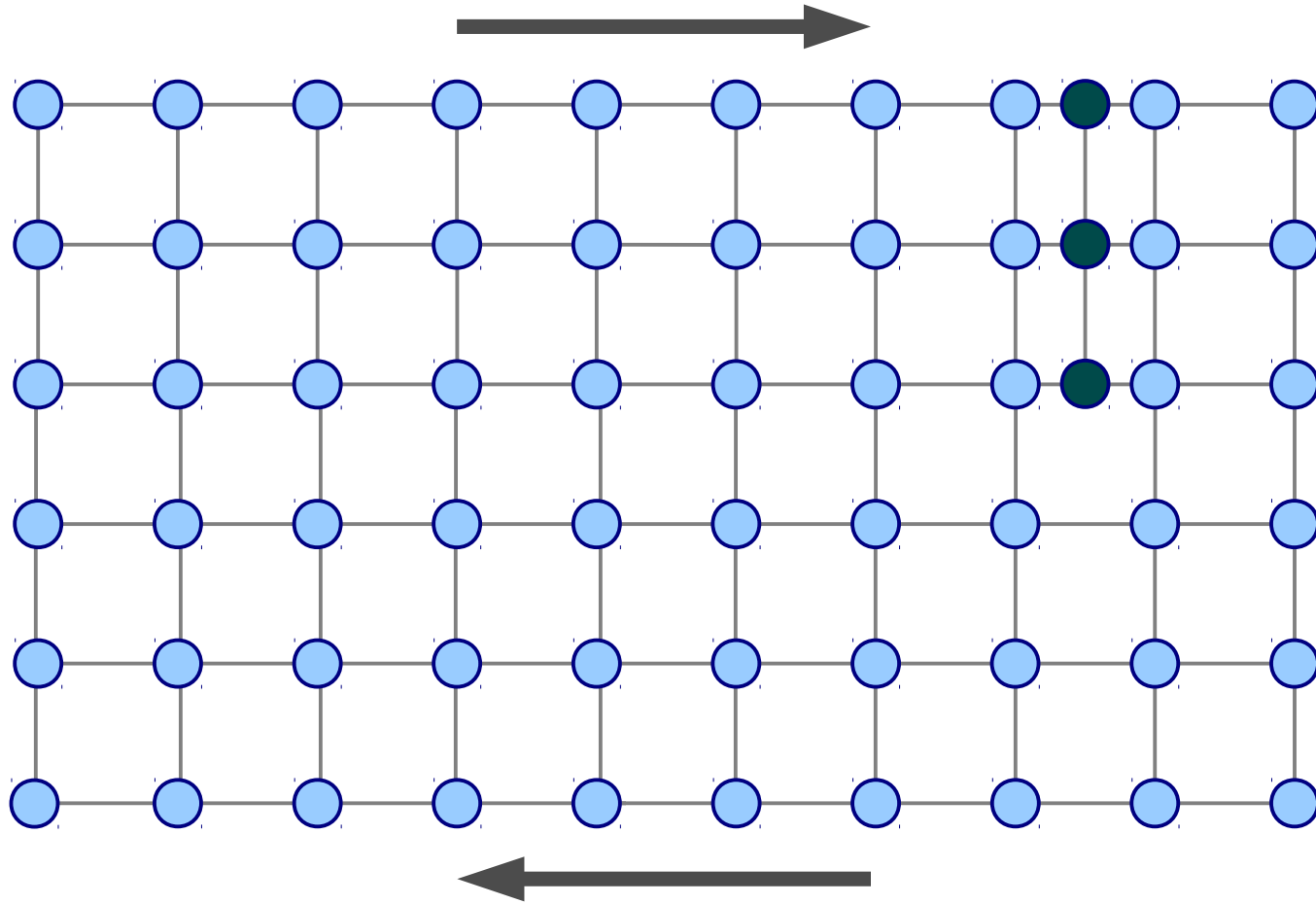




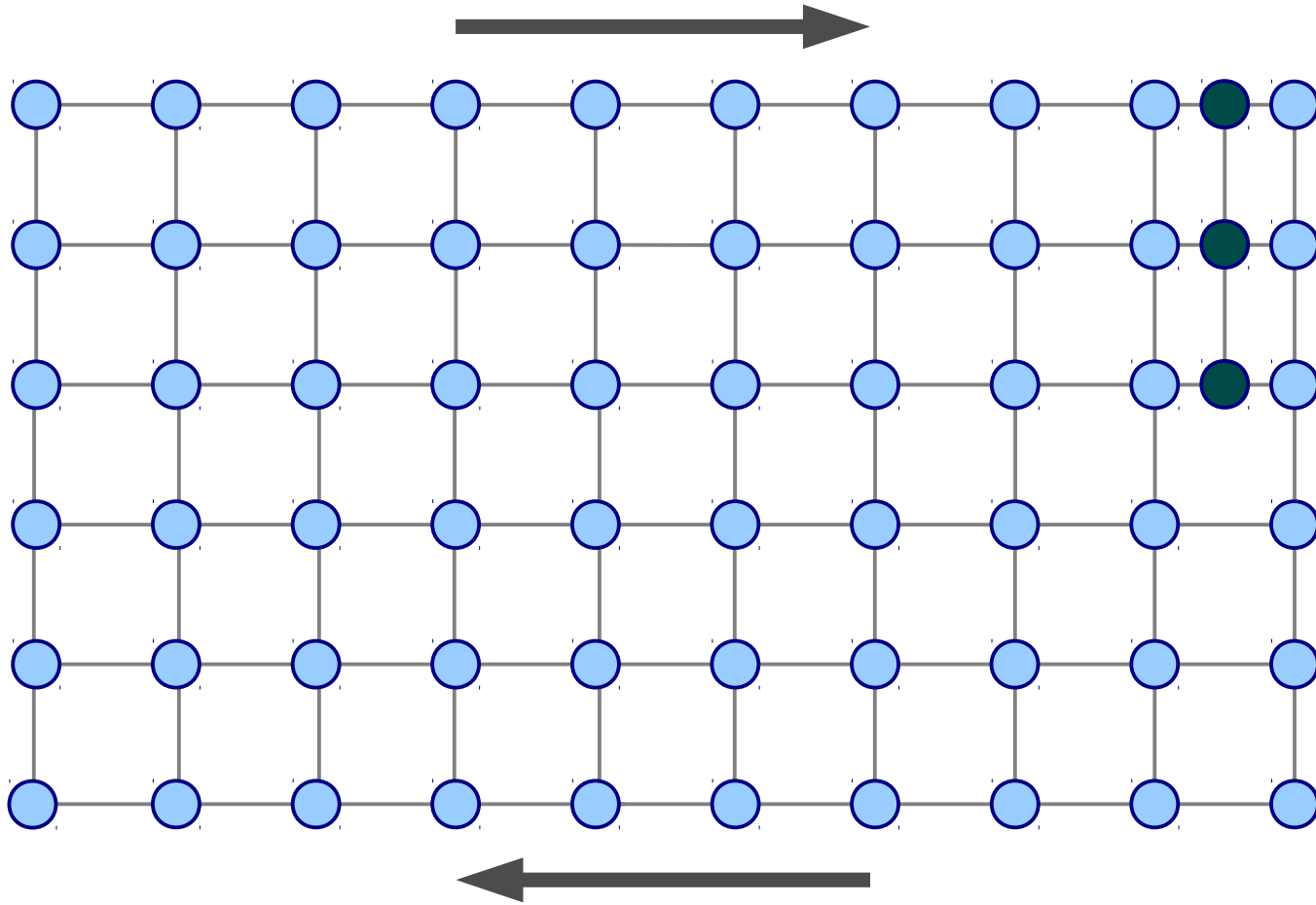
# Creep



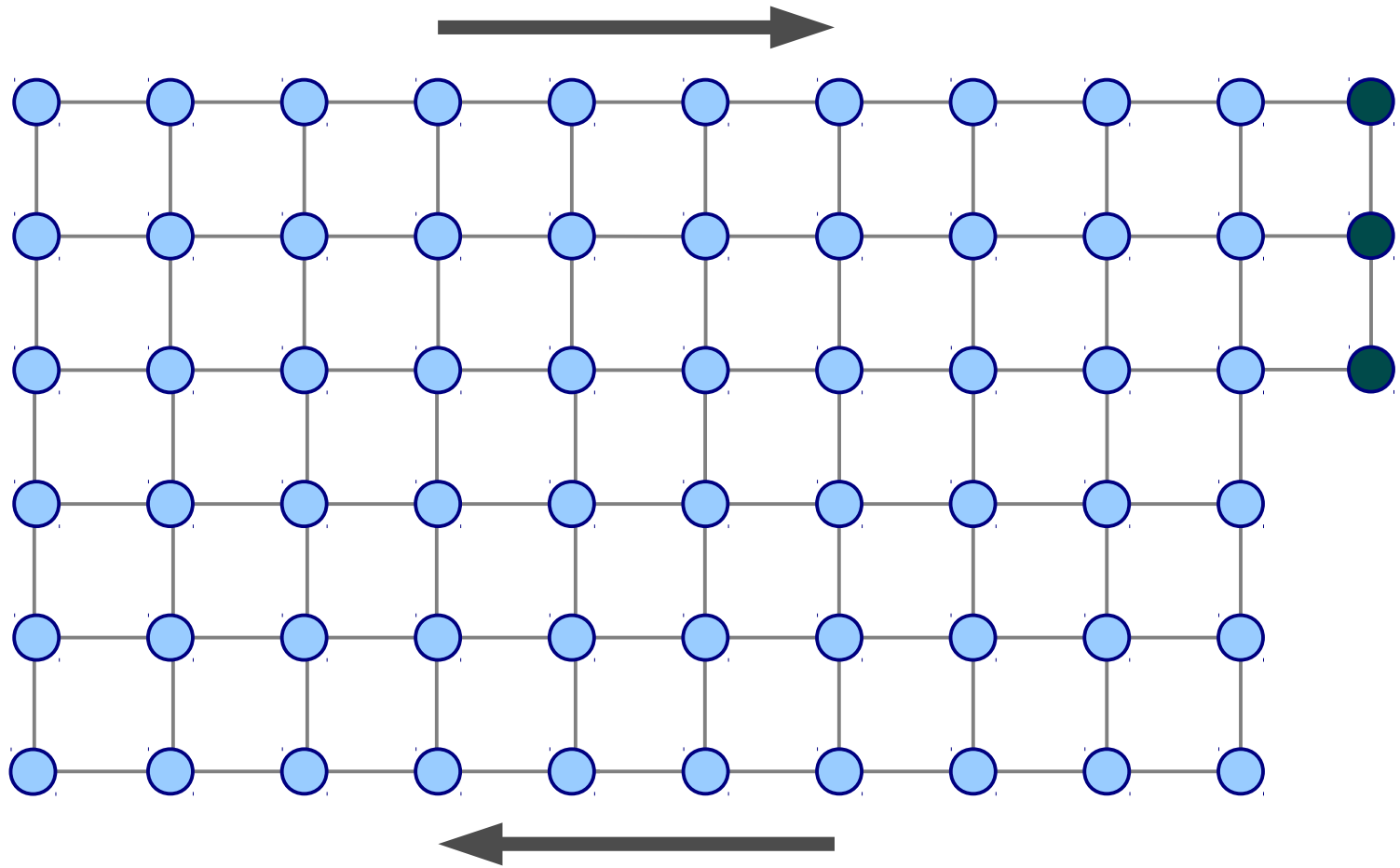
# Creep



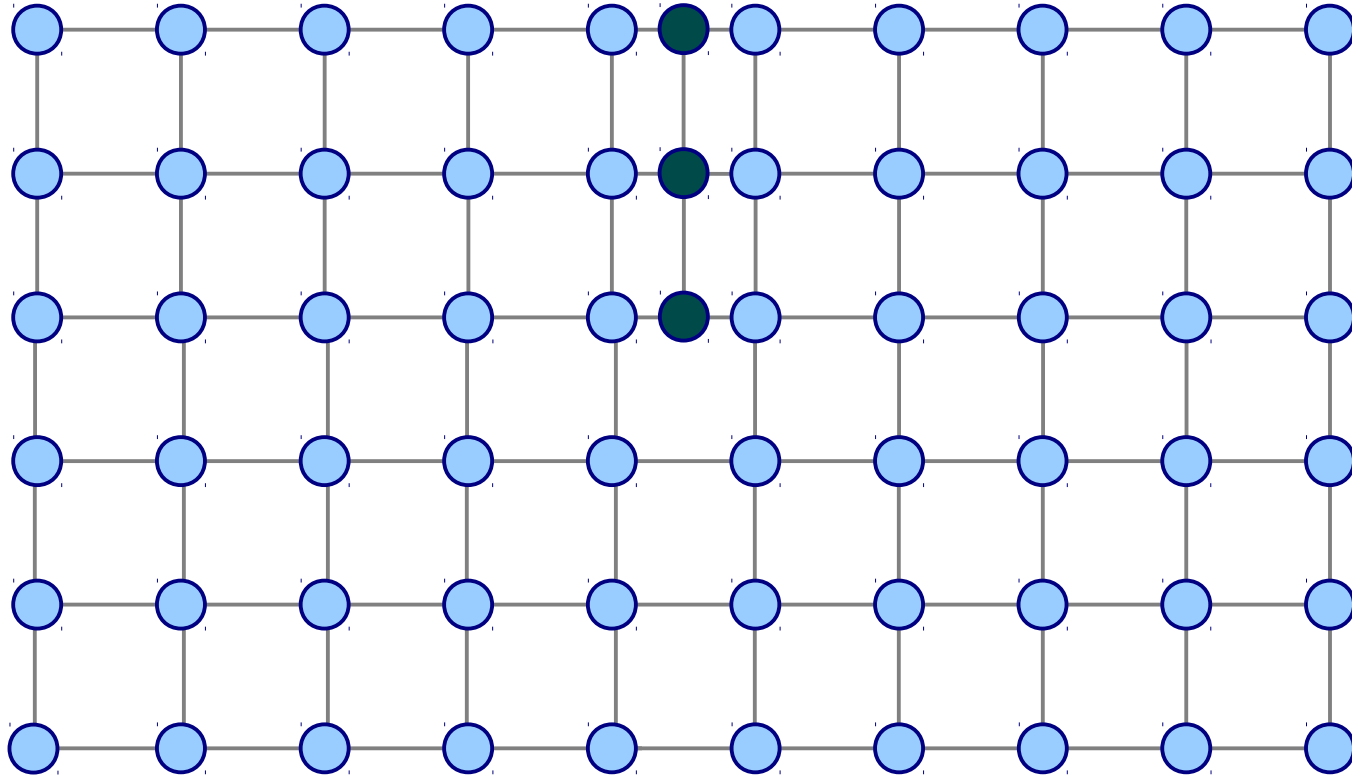
# Creep



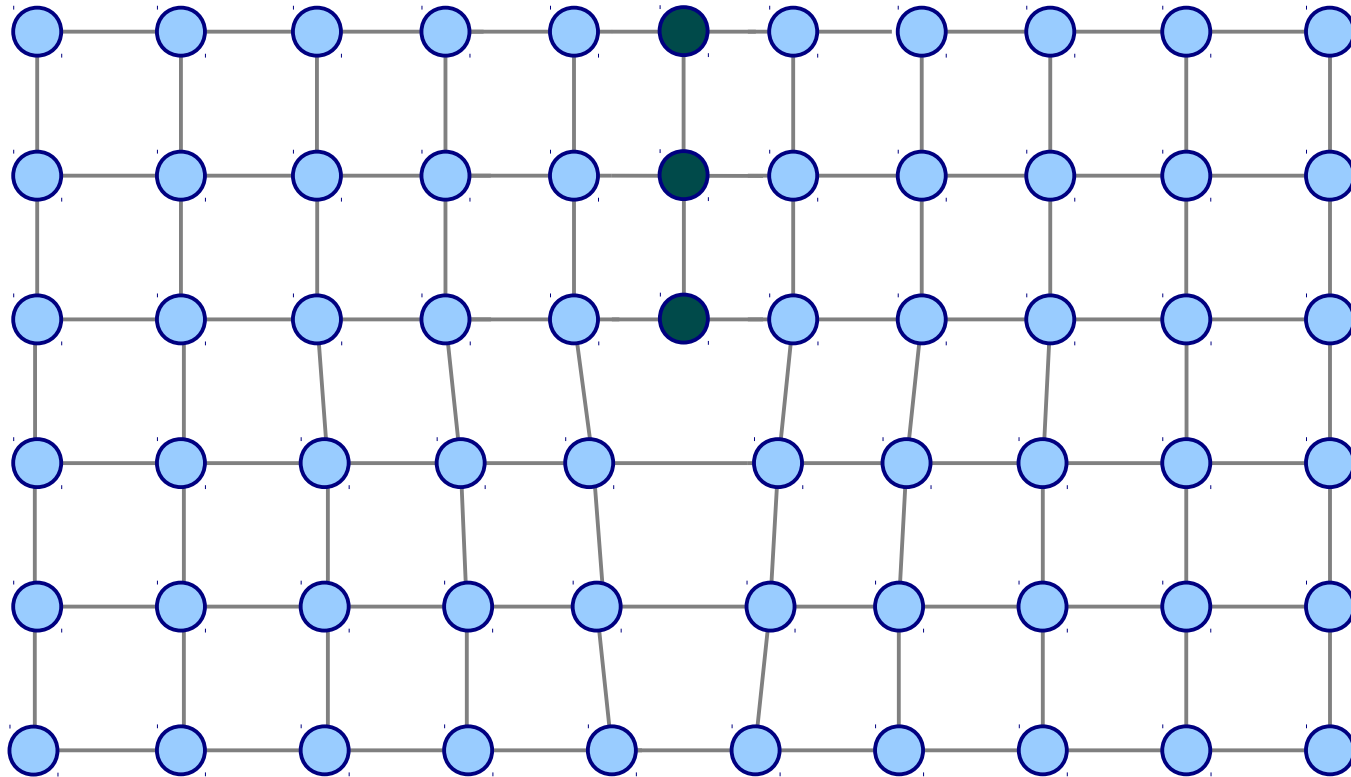
# Creep



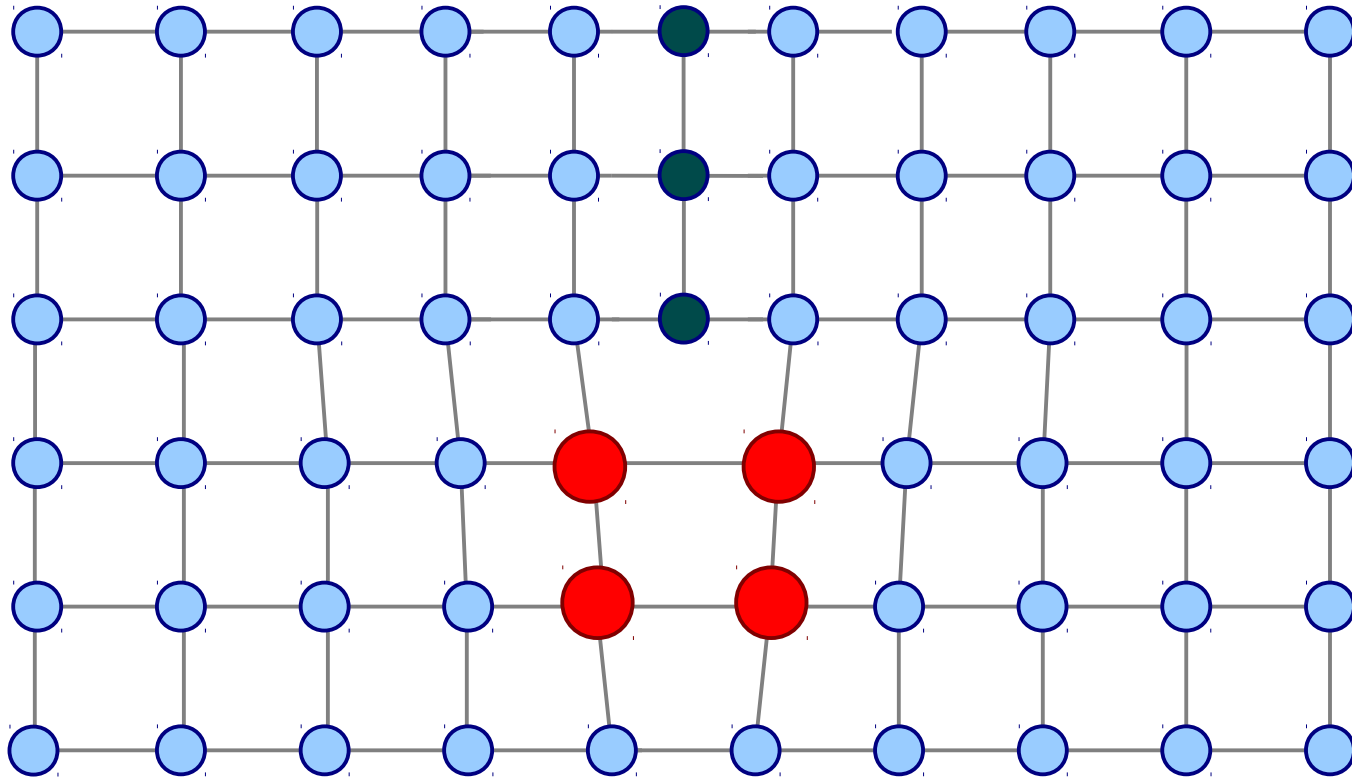
# Solution hardening



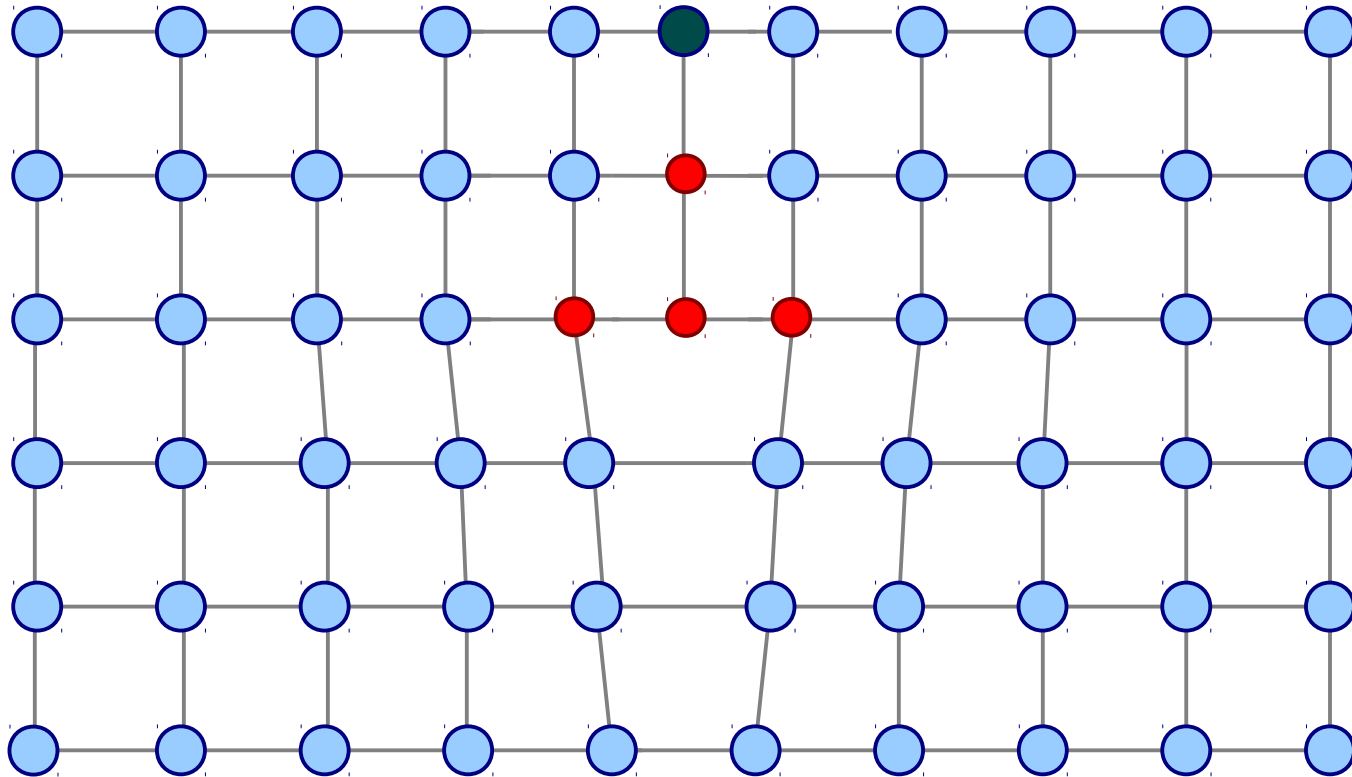
# Solution hardening



# Solution hardening

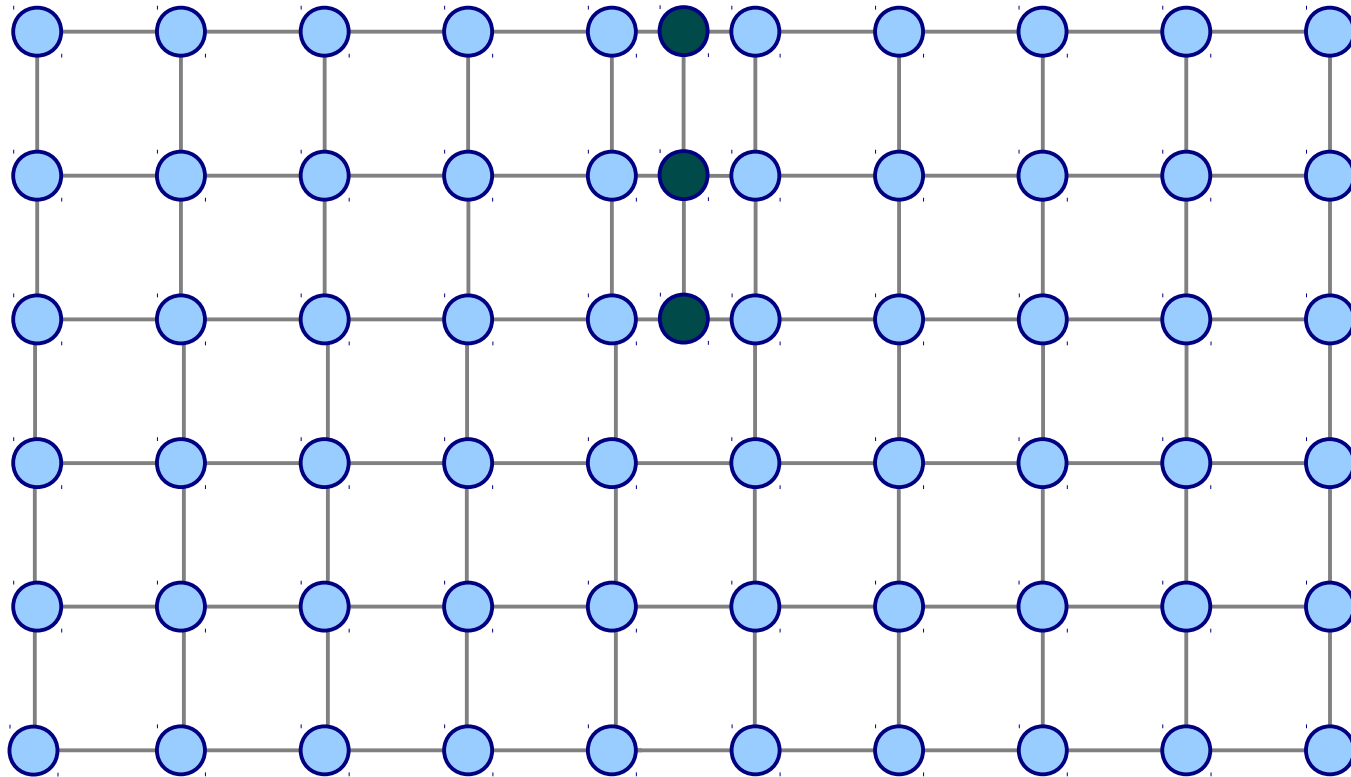


# Solution hardening

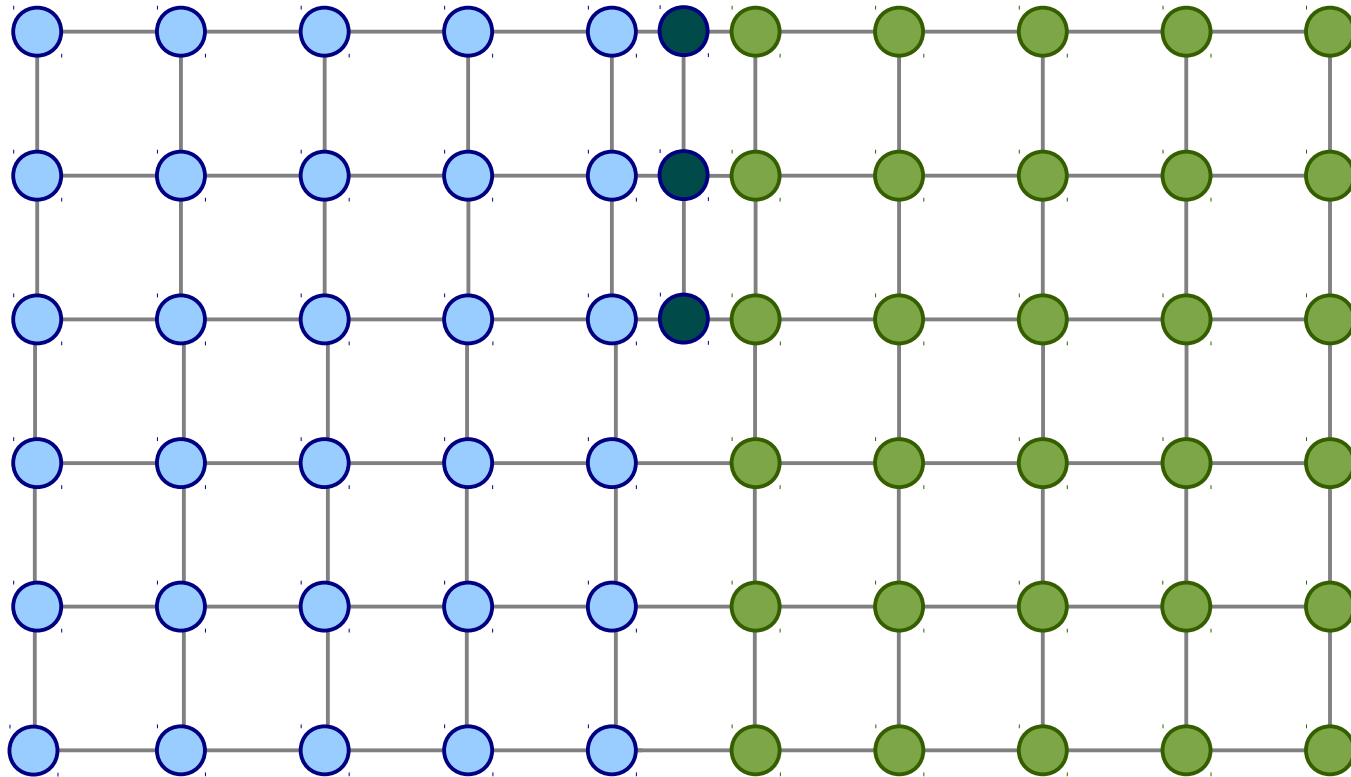




# Precipitate hardening

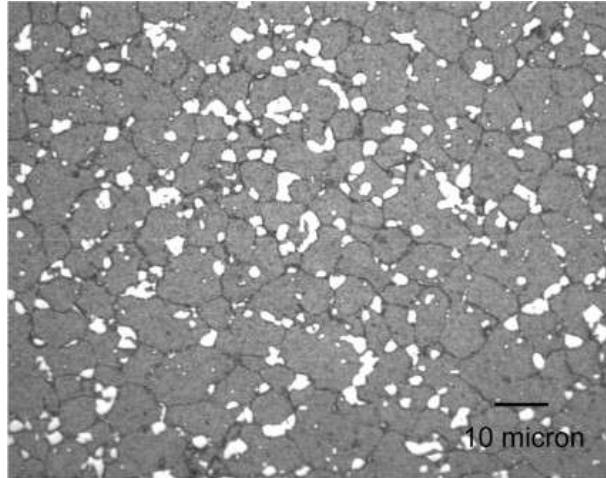


# Precipitate hardening

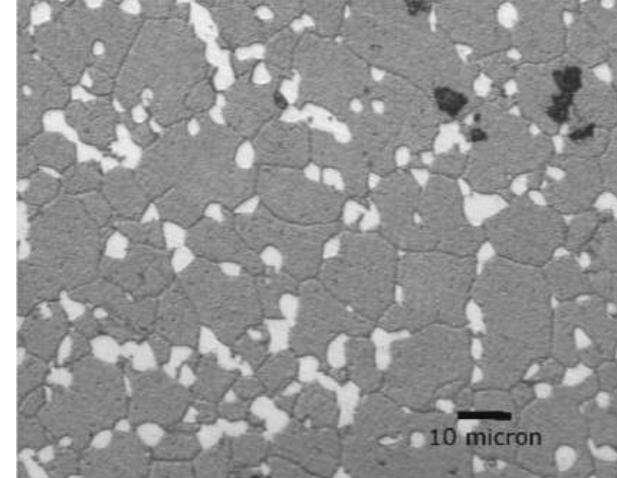


# Contemporary alloys

RR1000



N18



Alloy	Firm	Ni	Cr	Co	Mo	Ti	Al	C	Hf	Ta	W	Nb
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# Properties

Cost  $\text{\$lb}^{-1}$

$\gamma'$  fraction

Stability

Density  $\text{gcm}^{-3}$

Yield stress MPa

UTS MPa

Oxidation index

Stress rupture MPa

Resistivity  $\mu\Omega\text{cm}$

Entropy  $\text{Jmol}^{-1}\text{K}^{-1}$

Low cycle fatigue

High cycle fatigue

Weldability

Creep model

# Properties

Cost \$lb<sup>-1</sup>

γ' fraction

Stability

Density gcm<sup>-3</sup>

Yield stress MPa

UTS MPa

Oxidation index

Stress rupture MPa

Resistivity μΩcm

Entropy Jmol<sup>-1</sup>K<sup>-1</sup>

Low cycle fatigue

High cycle fatigue

Weldability

Creep model

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

# Properties

Collect data for yield stress from 2248 alloys

Cost  $\$/\text{lb}^{-1}$

$\gamma'$  fraction

Stability

Density  $\text{gcm}^{-3}$

**Yield stress MPa**

UTS MPa

Oxidation index

Stress rupture MPa

Resistivity  $\mu\Omega\text{cm}$

Entropy  $\text{Jmol}^{-1}\text{K}^{-1}$

Low cycle fatigue

High cycle fatigue

Weldability

Creep model

# Properties

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

Collect data for yield stress from 2248 alloys



Generate neural network model

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

# Properties

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

**Collect data for yield stress from 2248 alloys**



**Generate neural network model**

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



**Calculate uncertainty in neural network model**



# Properties

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

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

Calculate uncertainty in neural network model



# Properties

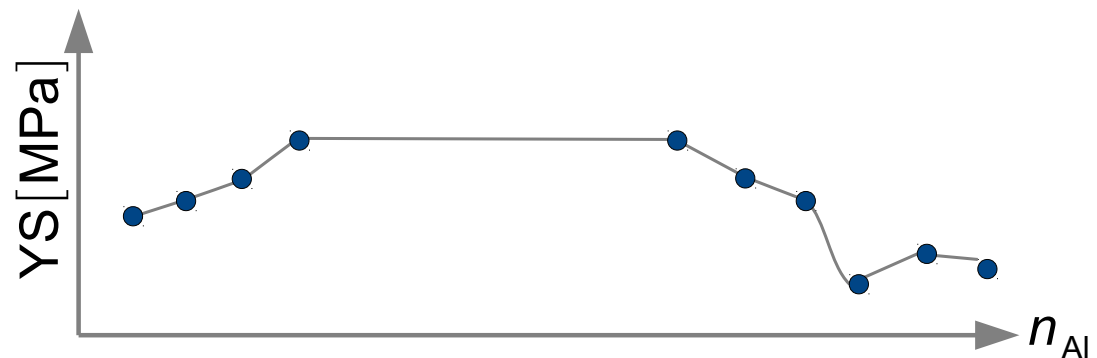
Cost \$lb<sup>-1</sup>  
γ' fraction  
Stability  
Density gcm<sup>-3</sup>  
**Yield stress MPa**  
UTS MPa  
Oxidation index  
Stress rupture MPa  
Resistivity μΩcm  
Entropy Jmol<sup>-1</sup>K<sup>-1</sup>  
Low cycle fatigue  
High cycle fatigue  
Weldability  
Creep model

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Calculate uncertainty in neural network model



# Properties

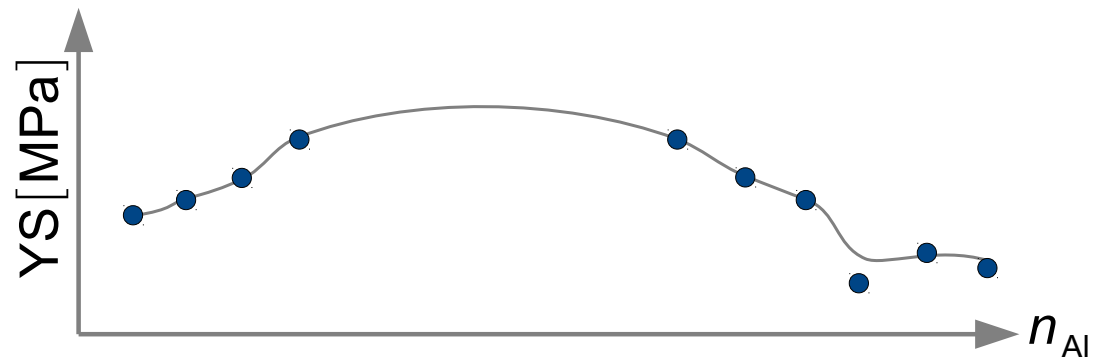
Cost \$lb<sup>-1</sup>  
γ' fraction  
Stability  
Density gcm<sup>-3</sup>  
**Yield stress MPa**  
UTS MPa  
Oxidation index  
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Calculate uncertainty in neural network model



# Properties

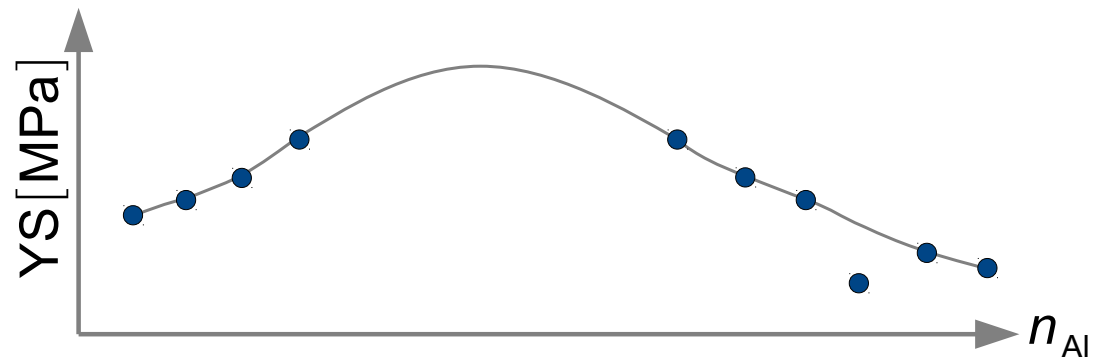
Cost \$lb<sup>-1</sup>  
γ' fraction  
Stability  
Density gcm<sup>-3</sup>  
**Yield stress MPa**  
UTS MPa  
Oxidation index  
Stress rupture MPa  
Resistivity μΩcm  
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Calculate uncertainty in neural network model



# Properties

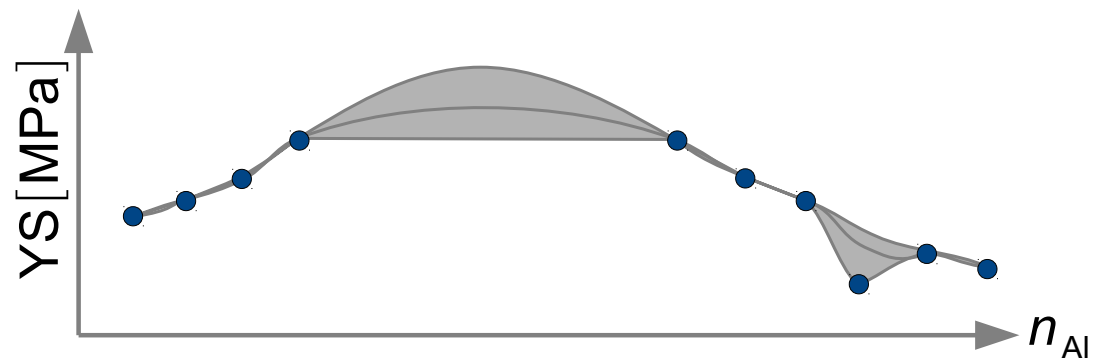
Cost \$lb<sup>-1</sup>  
γ' fraction  
Stability  
Density gcm<sup>-3</sup>  
**Yield stress MPa**  
UTS MPa  
Oxidation index  
Stress rupture MPa  
Resistivity μΩcm  
Entropy Jmol<sup>-1</sup>K<sup>-1</sup>  
Low cycle fatigue  
High cycle fatigue  
Weldability  
Creep model

Collect data for yield stress from 2248 alloys

Generate neural network model

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

Calculate uncertainty in neural network model



# Properties

Calculate grid of

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

Cost \$lb<sup>-1</sup>

$\gamma'$  fraction

Stability

Density gcm<sup>-3</sup>

Yield stress MPa

UTS MPa

Oxidation index

Stress rupture MPa

Resistivity  $\mu\Omega\text{cm}$

Entropy Jmol<sup>-1</sup>K<sup>-1</sup>

Low cycle fatigue

High cycle fatigue

Weldability

Creep model

# Properties

Cost \$lb<sup>-1</sup>  
 $\gamma'$  fraction  
Stability  
Density gcm<sup>-3</sup>  
Yield stress MPa  
UTS MPa  
Oxidation index  
Stress rupture MPa  
Resistivity  $\mu\Omega\text{cm}$   
Entropy Jmol<sup>-1</sup>K<sup>-1</sup>  
Low cycle fatigue  
High cycle fatigue  
Weldability  
Creep model

Calculate grid of

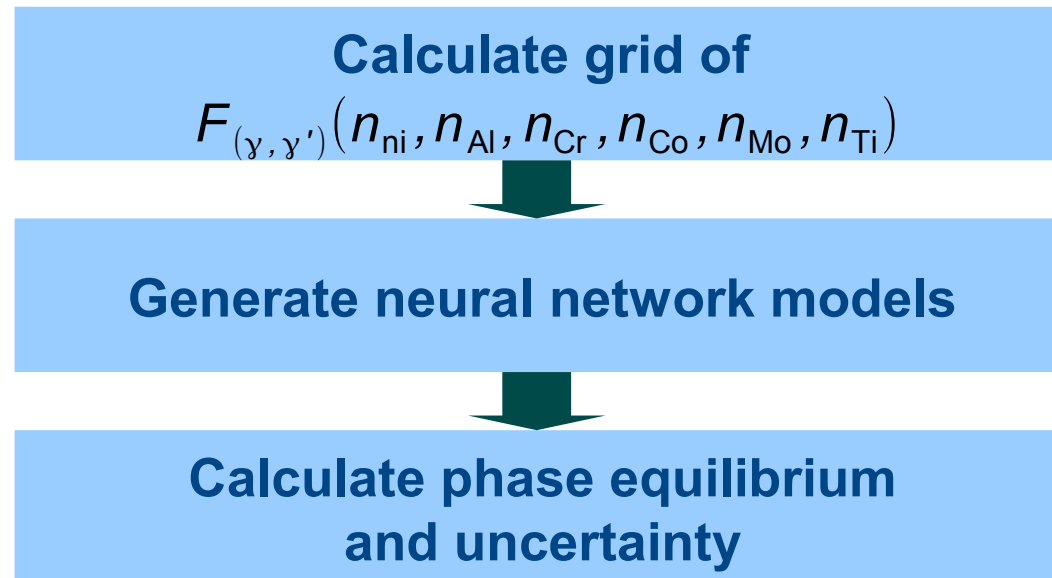
$$F_{(\gamma, \gamma')} (n_{\text{Ni}}, n_{\text{Al}}, n_{\text{Cr}}, n_{\text{Co}}, n_{\text{Mo}}, n_{\text{Ti}})$$



Generate neural network models

# Properties

Cost \$lb<sup>-1</sup>  
 $\gamma'$  fraction  
Stability  
Density gcm<sup>-3</sup>  
Yield stress MPa  
UTS MPa  
Oxidation index  
Stress rupture MPa  
Resistivity  $\mu\Omega\text{cm}$   
Entropy Jmol<sup>-1</sup>K<sup>-1</sup>  
Low cycle fatigue  
High cycle fatigue  
Weldability  
Creep model





# Properties

Cost \$lb<sup>-1</sup>

$\gamma'$  fraction

Stability

Density gcm<sup>-3</sup>

Yield stress MPa

UTS MPa

Oxidation index

Stress rupture MPa

Resistivity  $\mu\Omega\text{cm}$

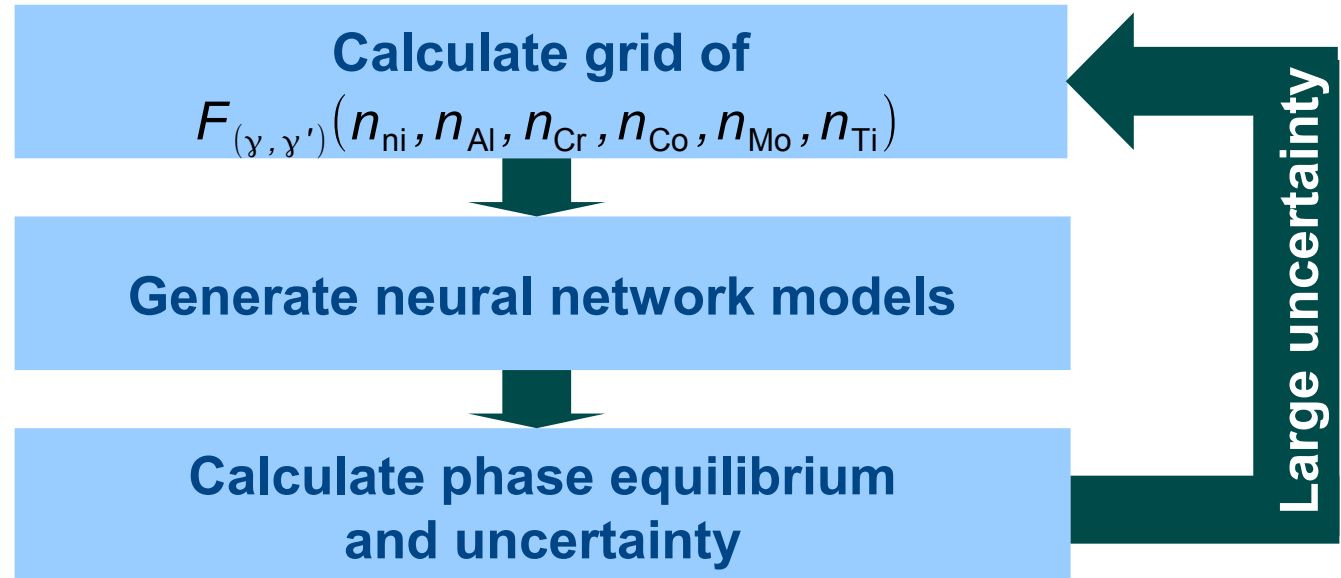
Entropy Jmol<sup>-1</sup>K<sup>-1</sup>

Low cycle fatigue

High cycle fatigue

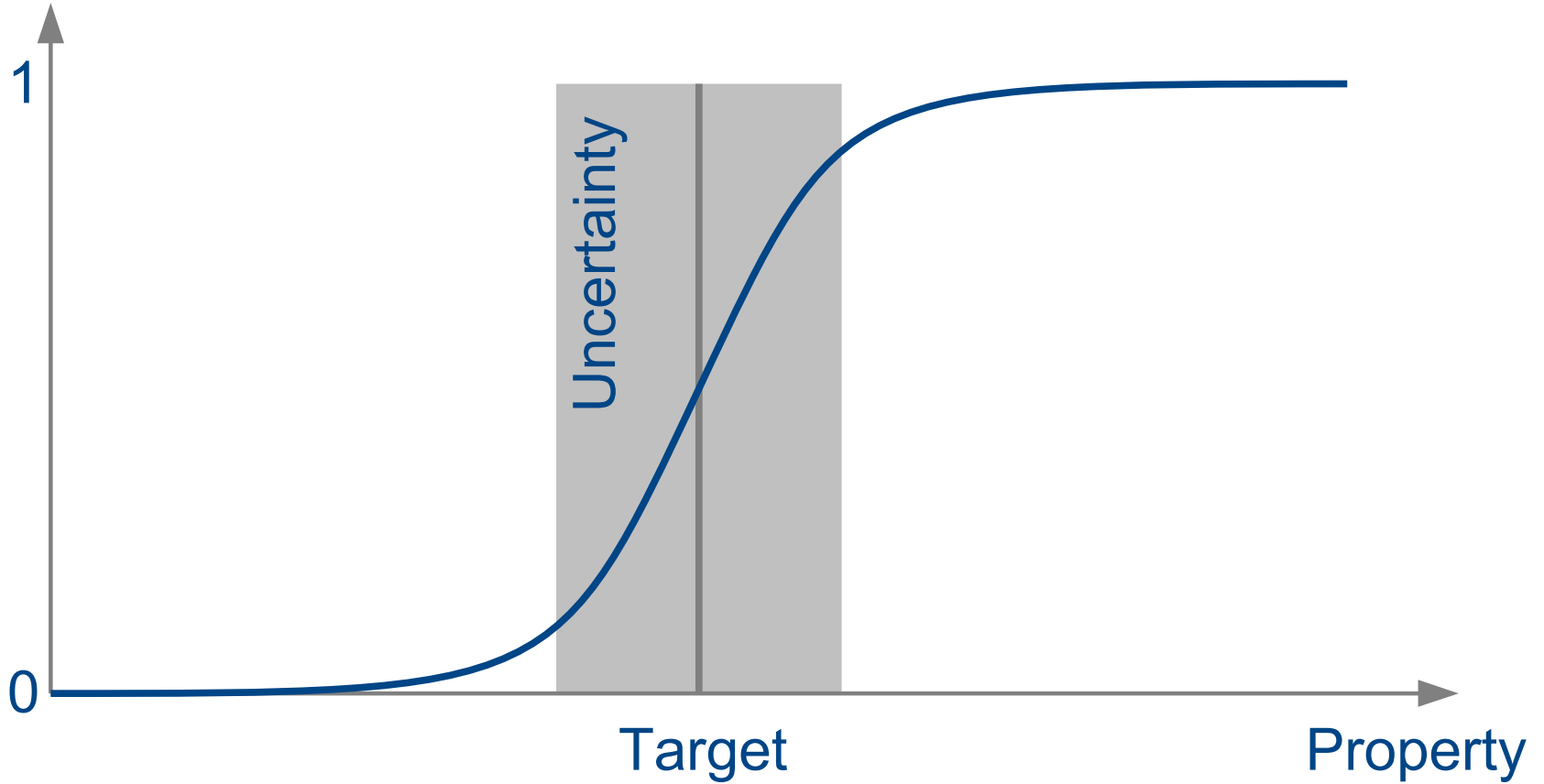
Weldability

Creep model



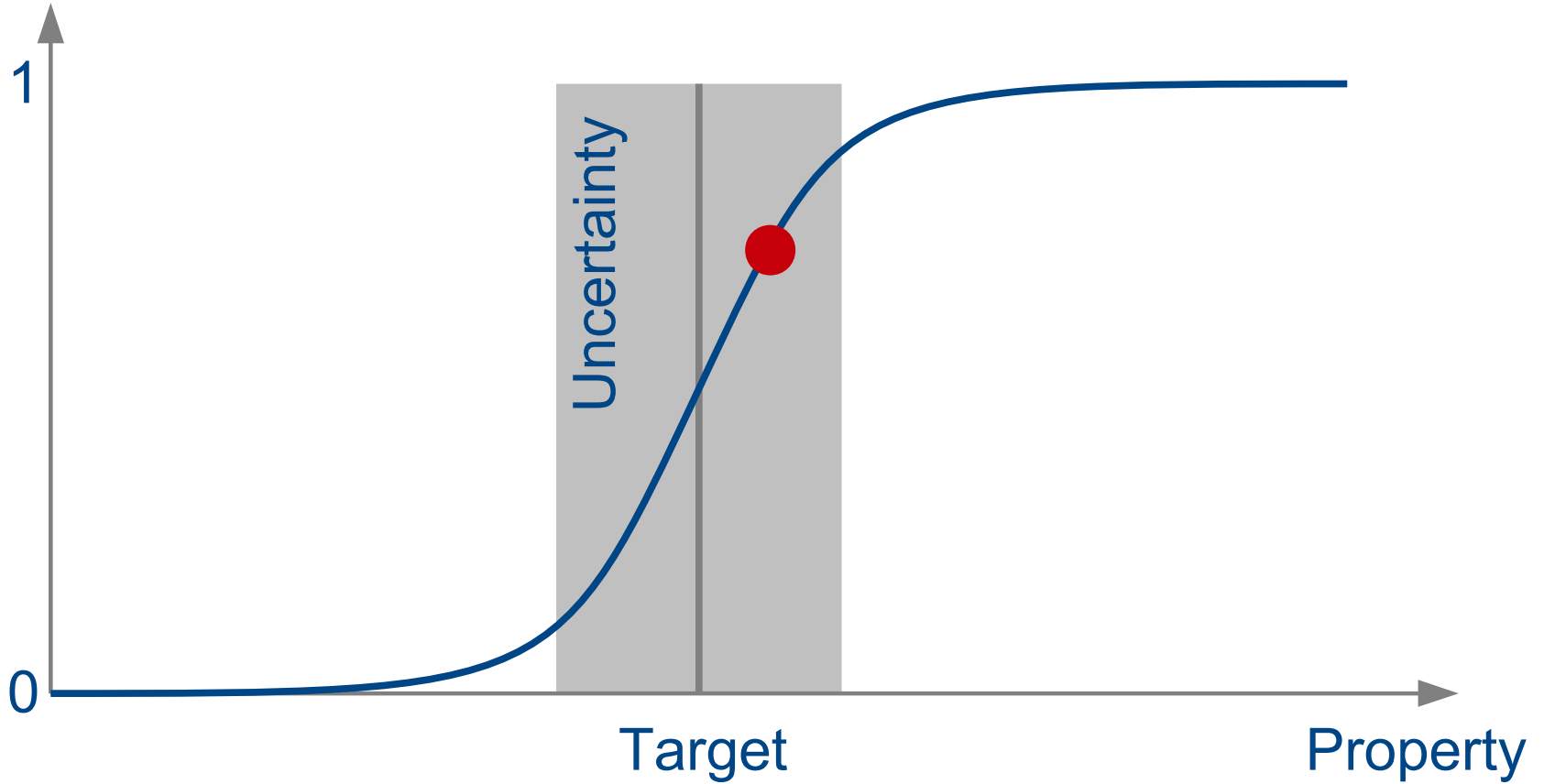
# Probability

Probability



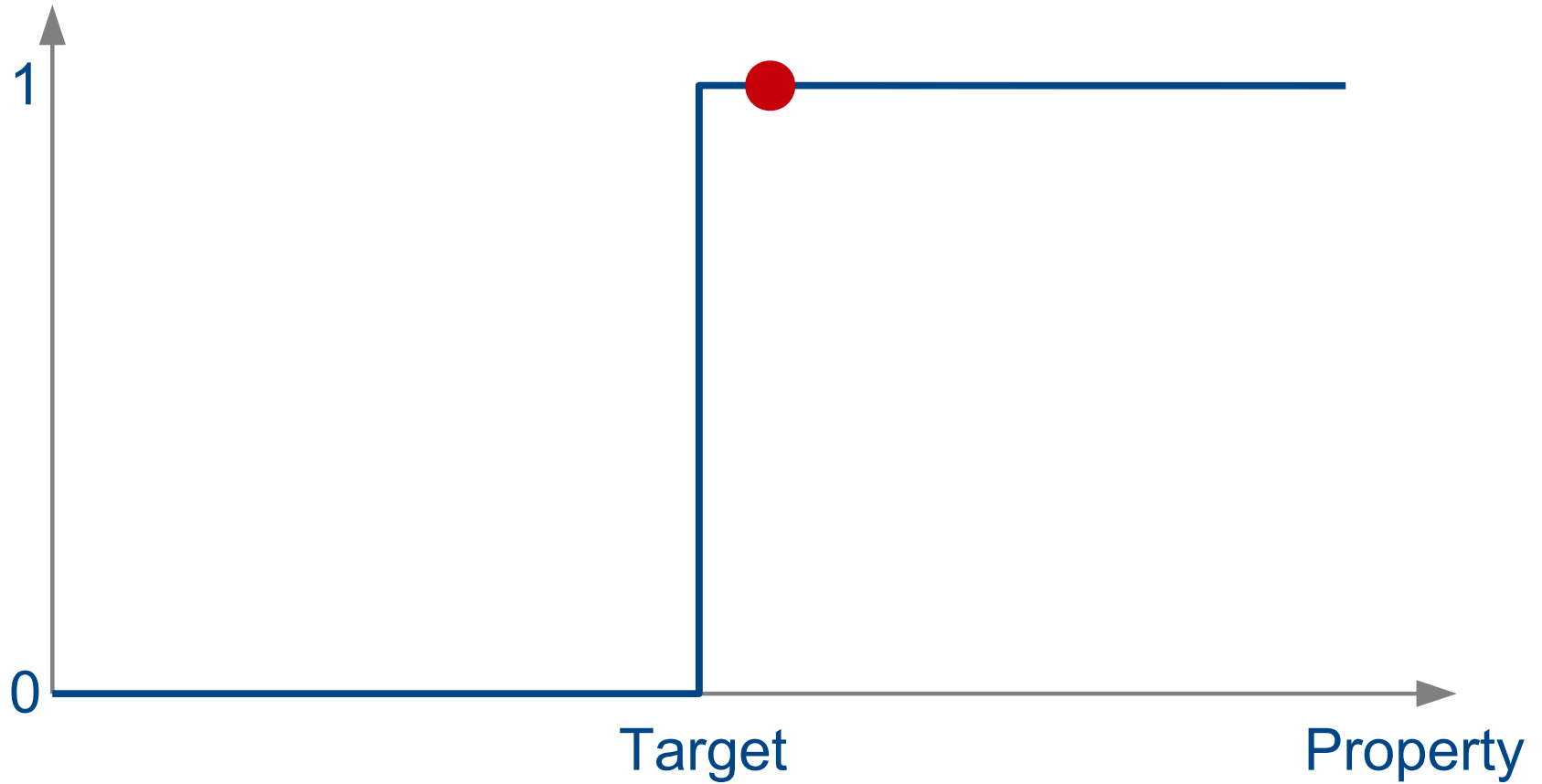
# Probability

Probability

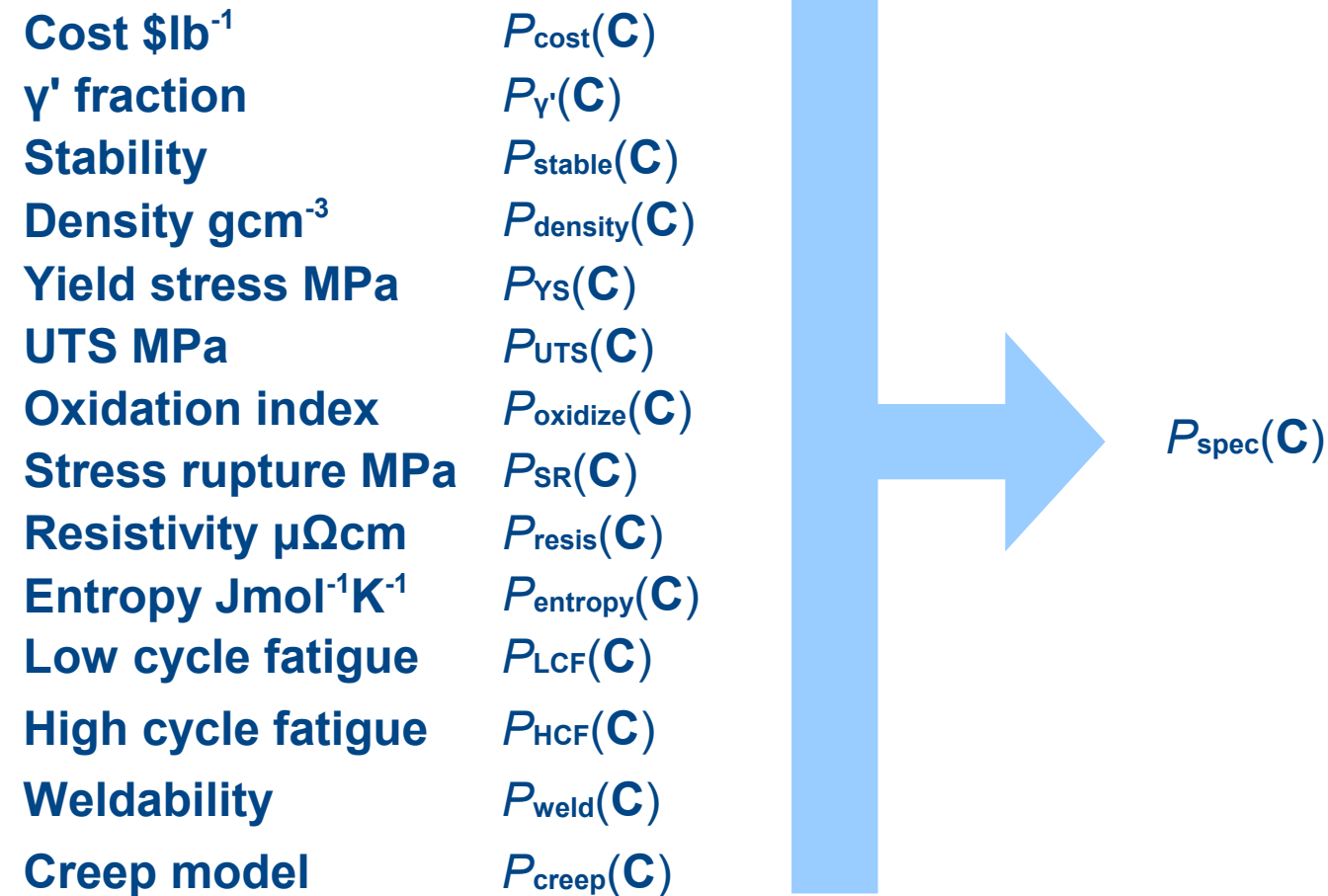


# Probability

Probability



# 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**



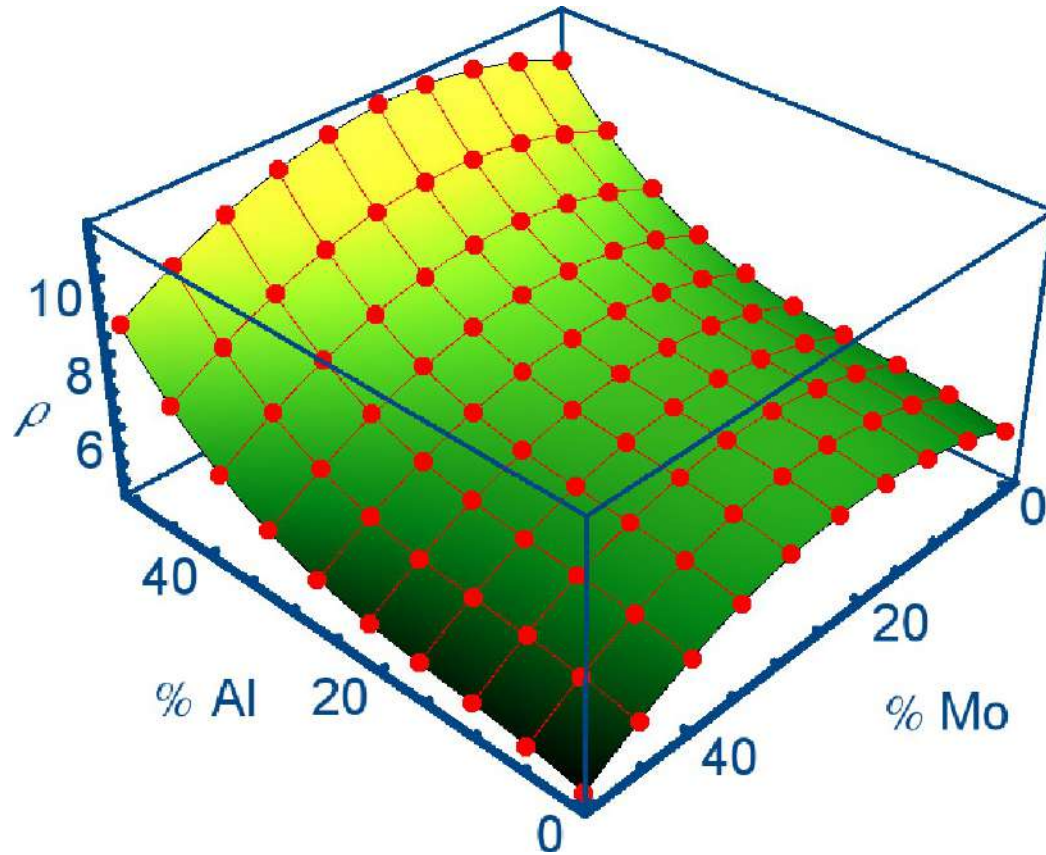
**Ni**



**Heat  
treatment**



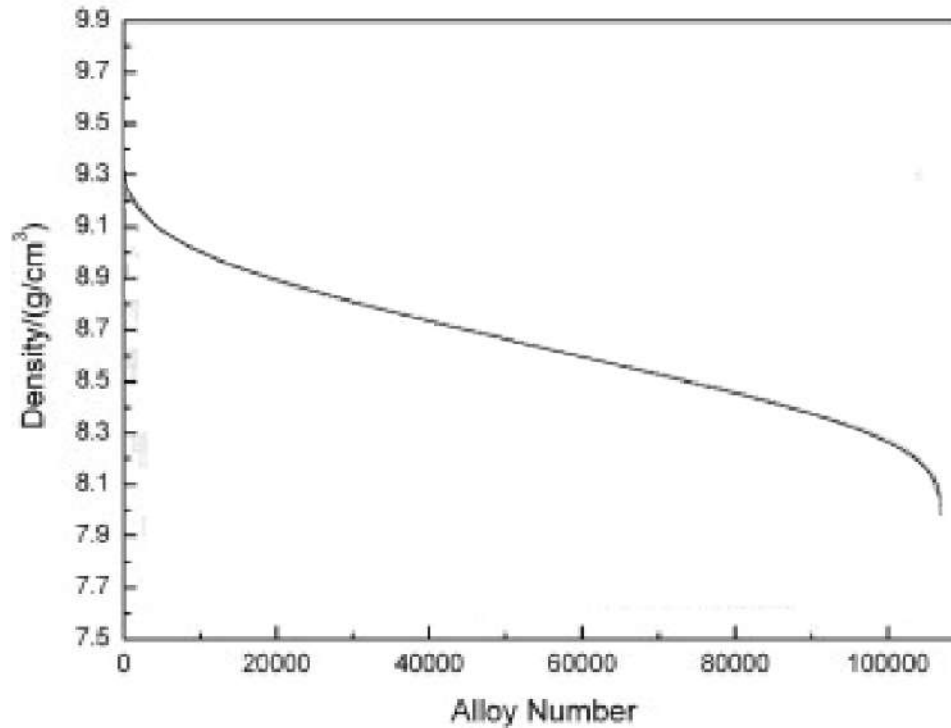
# Optimization – tradeoff diagrams



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

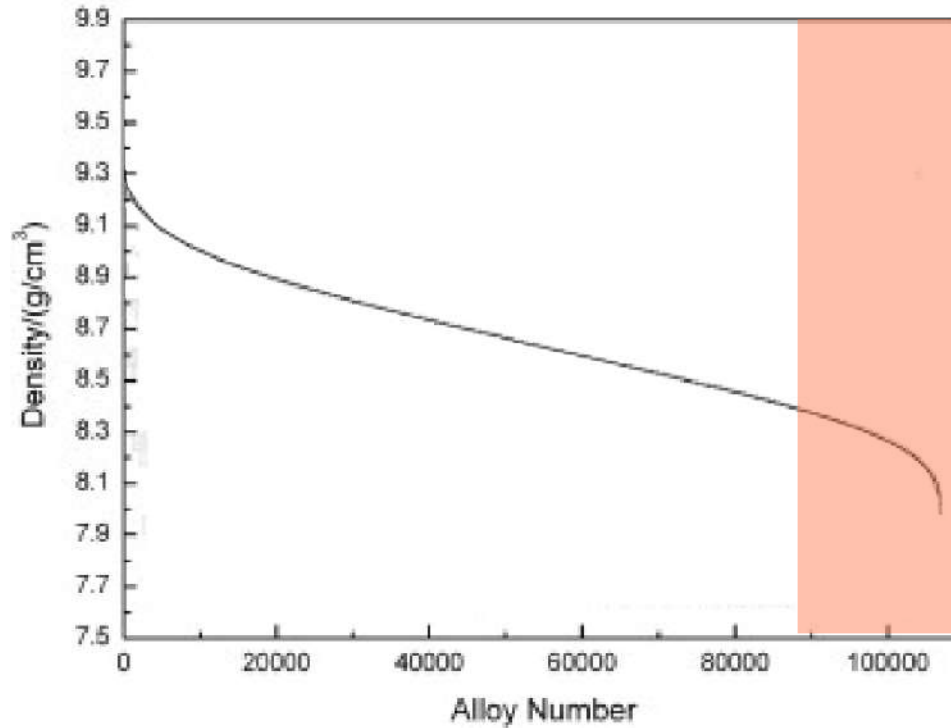


# Optimization – tradeoff diagrams



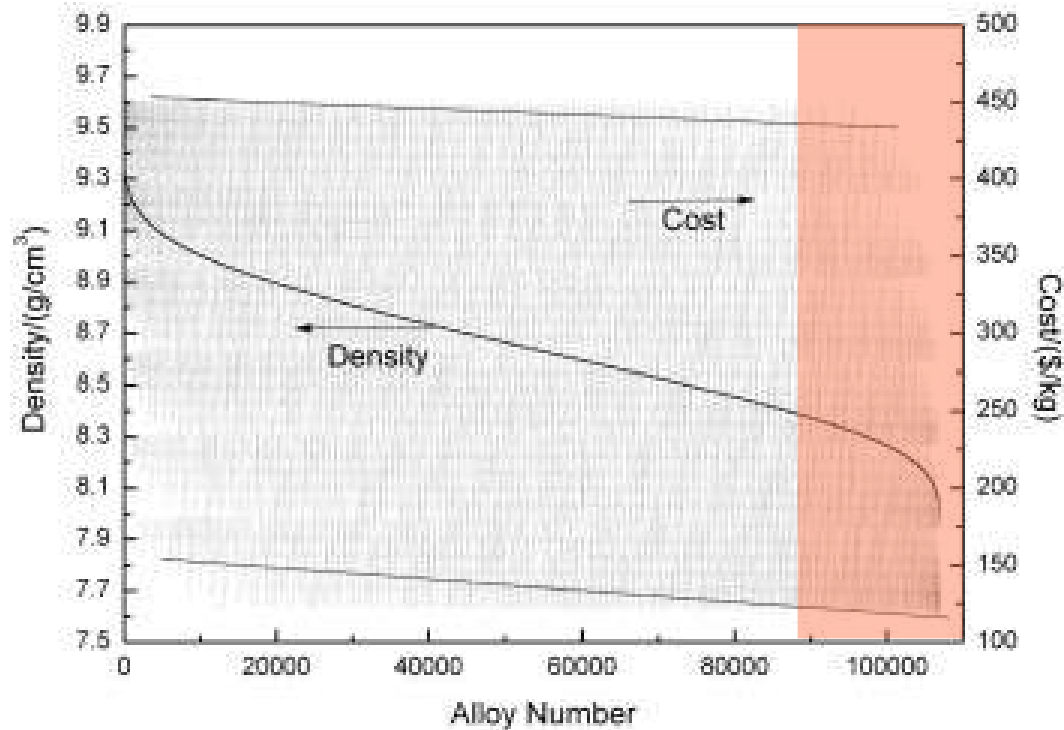
R.C. Reed, T. Tao & N. Warnken, *Acta Materialia* **57**, 5898 (2009)

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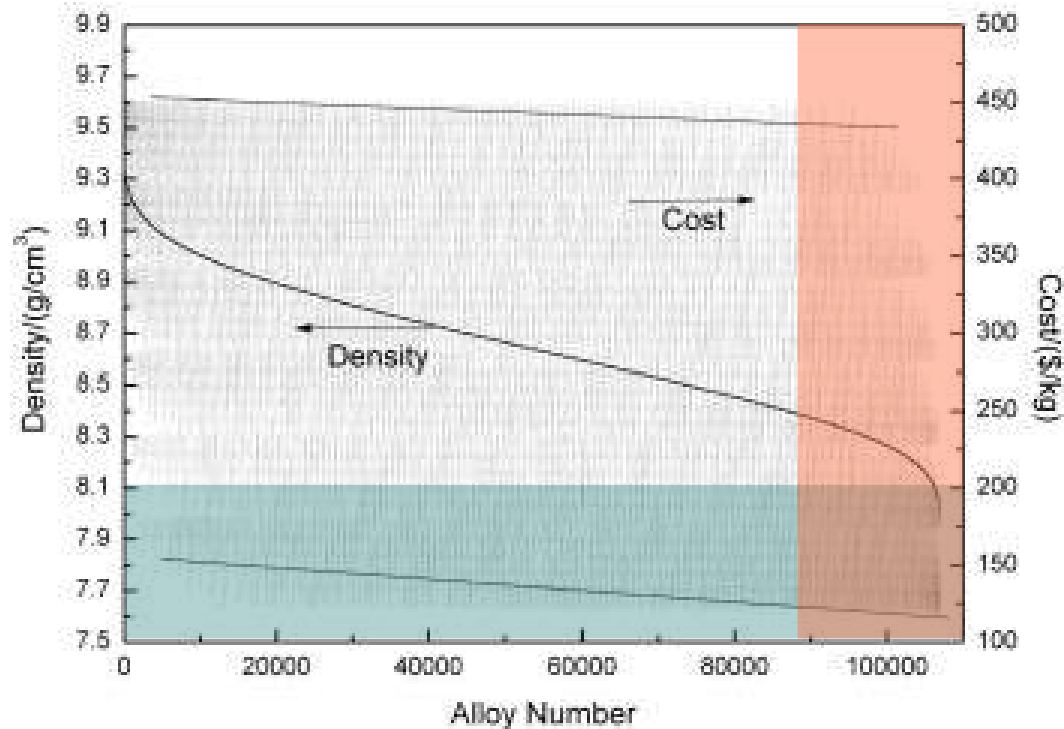
R.C. Reed, T. Tao & N. Warnken, *Acta Materialia* **57**, 5898 (2009)

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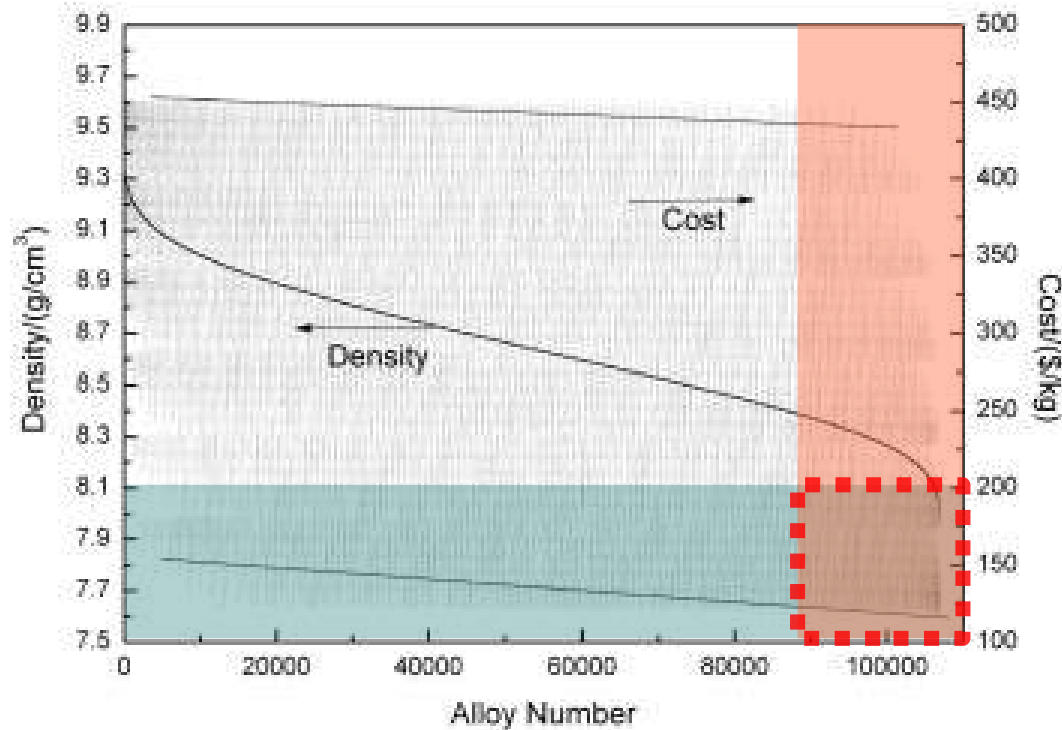
R.C. Reed, T. Tao & N. Warnken, *Acta Materialia* **57**, 5898 (2009)

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# Optimization – tradeoff diagrams



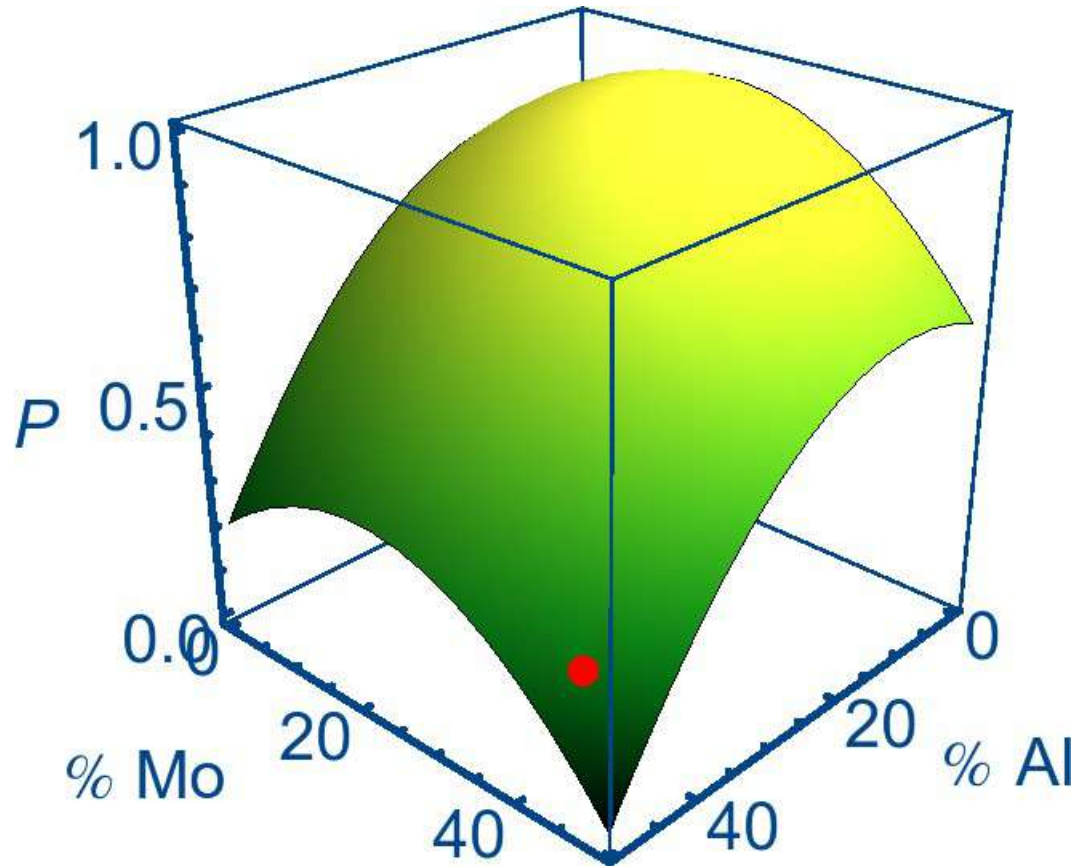
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# Optimization – tradeoff diagrams

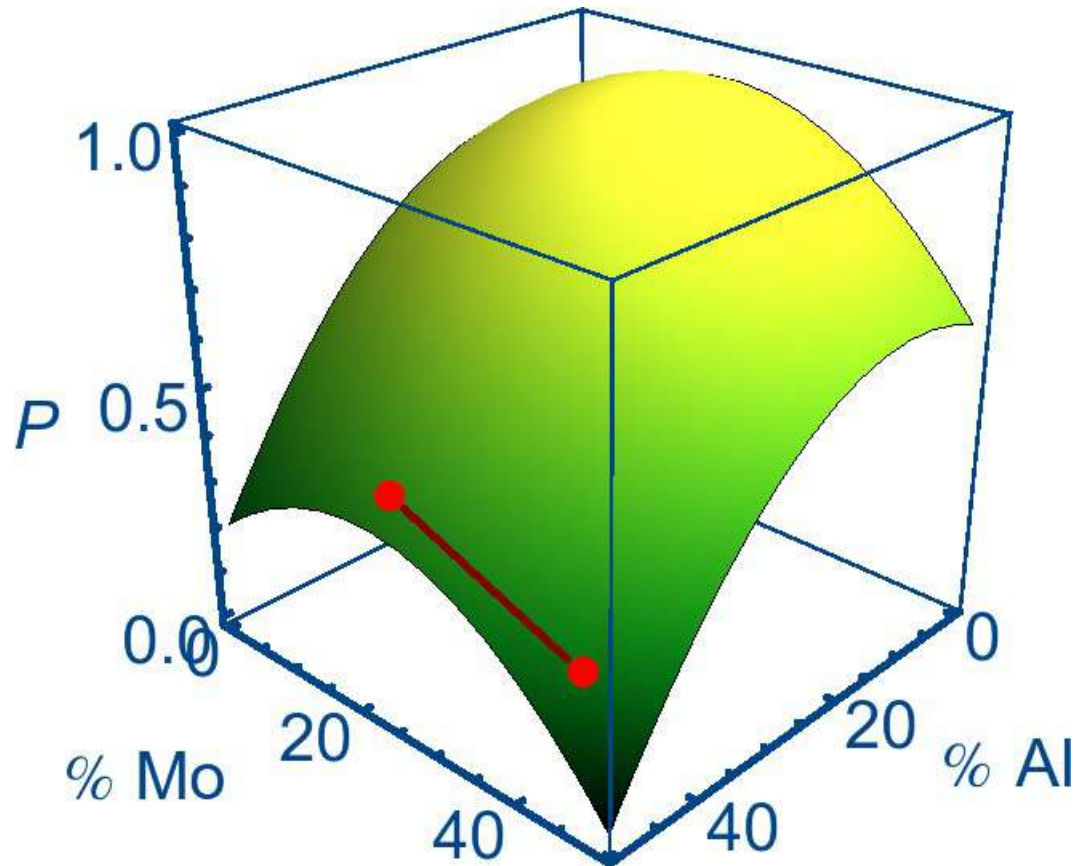
30 design variables, at 0.1% accuracy,  
and evaluation time of 1ms

$$1000^{30} = 3 \times 10^{79} \text{ years}$$

# Optimization – replica exchange sampling

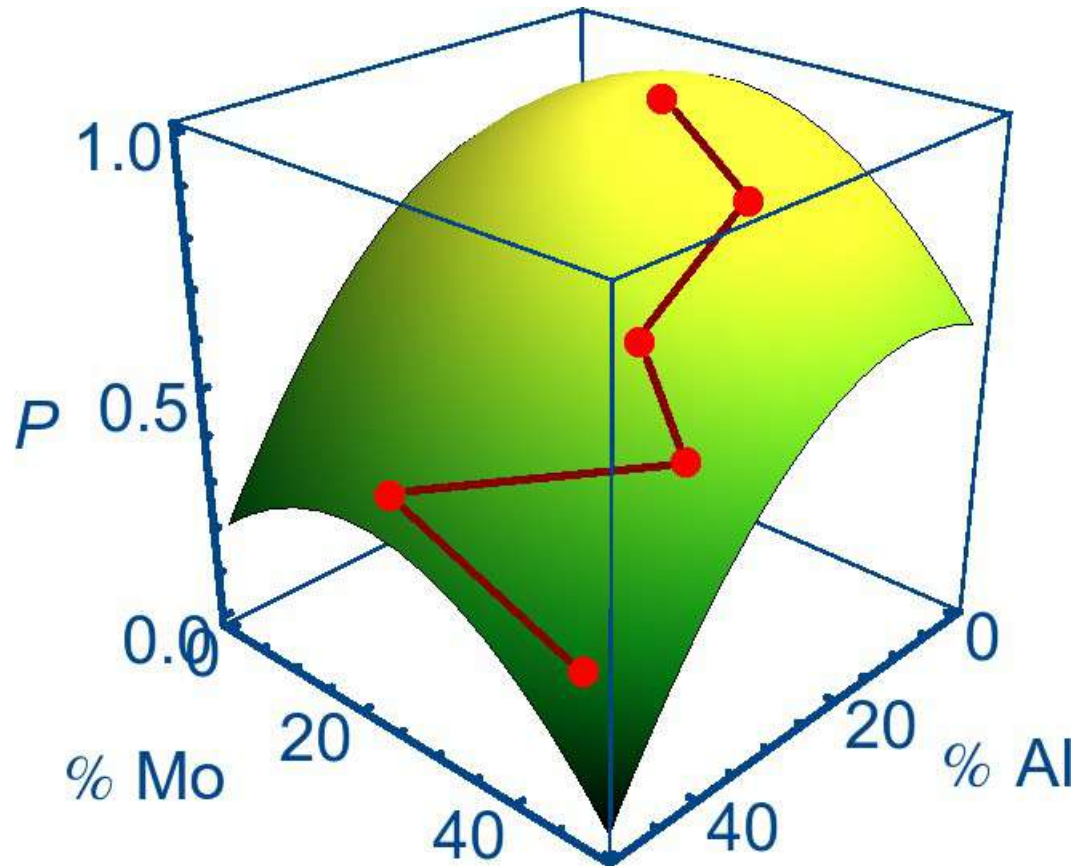


# Optimization – replica exchange sampling

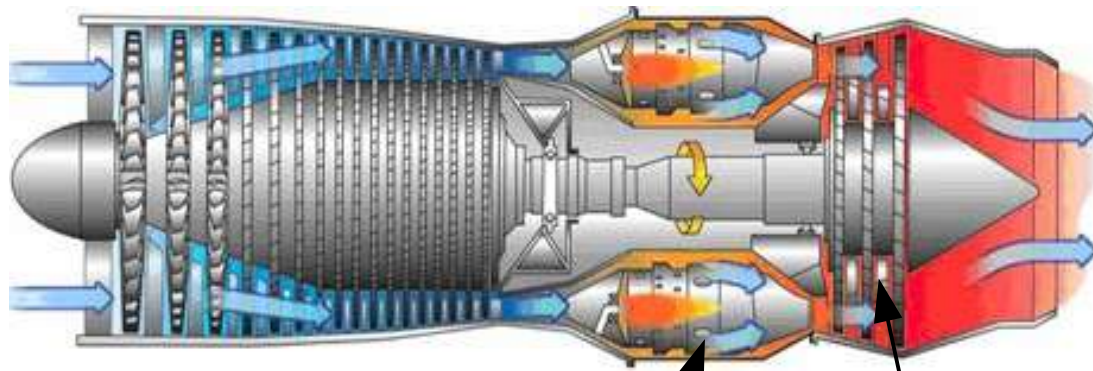




# Optimization – replica exchange sampling



# Predicted alloys



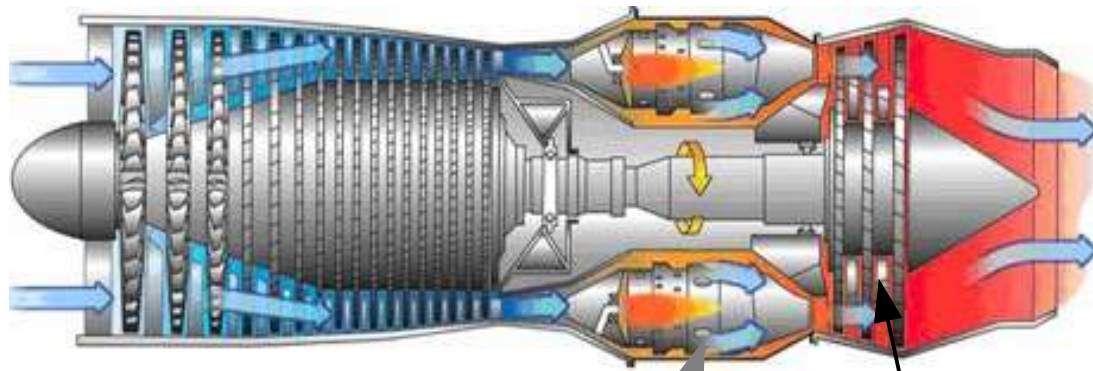
Combustor  
liner

2x disc  
alloy



2x forging  
hammer

# Predicted alloys



Combustor  
liner

**2x disc  
alloy**



2x forging  
hammer

# Case study: improved disc alloy



**Ni**  
52



**Cr**  
15



**Co**  
19



**Mo**  
5



**Ti**  
3.6



**Al**  
3



**Ta**  
2



**Hf**  
0.5



**C**  
0.1



**T**  
800



**t**  
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

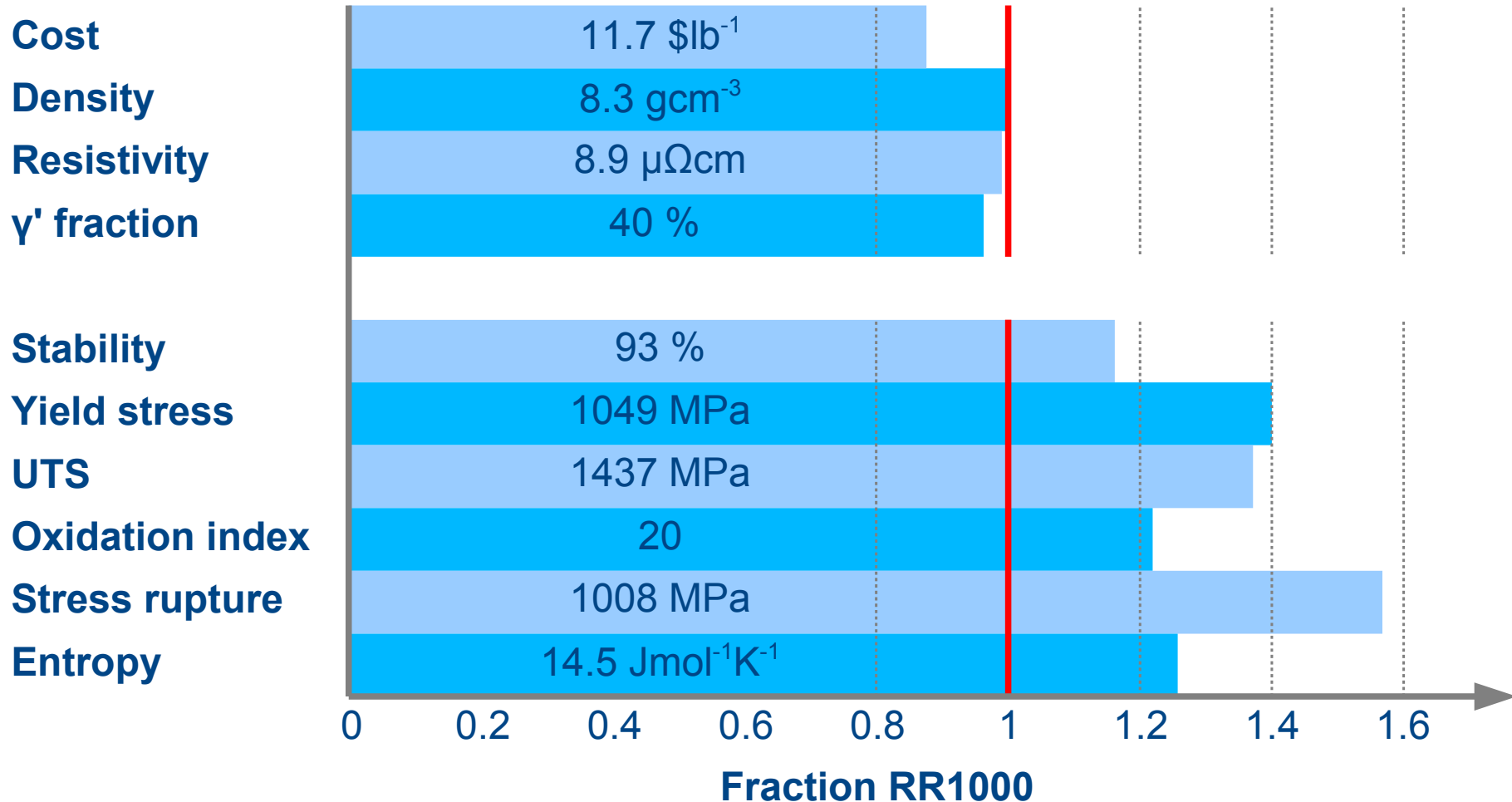


**Nb**  
5.6



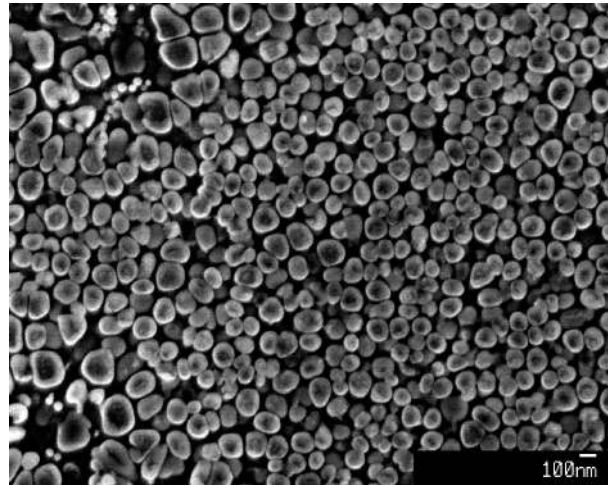
**Fe**  
3.4

# Case study: improved disc alloy



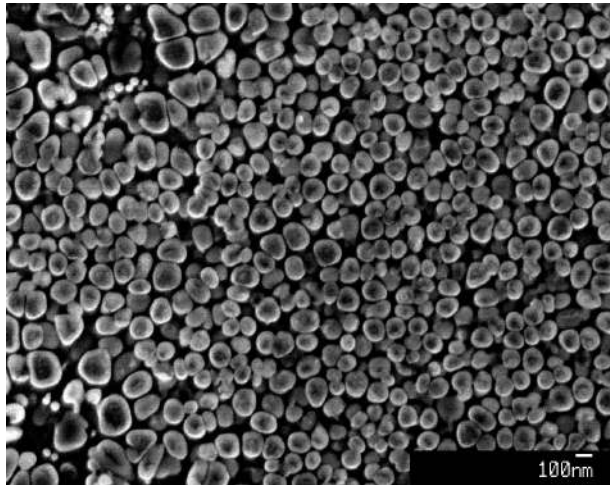
# Electron micrograph – Ni disc alloy

Ni disc alloy

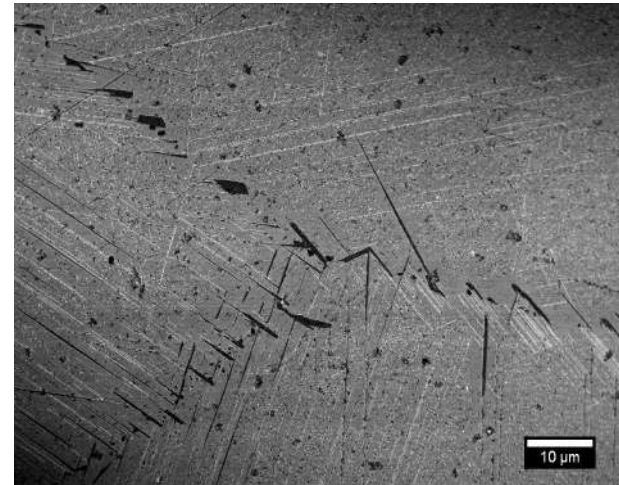


# Electron micrograph – Ni disc alloy

Ni disc alloy

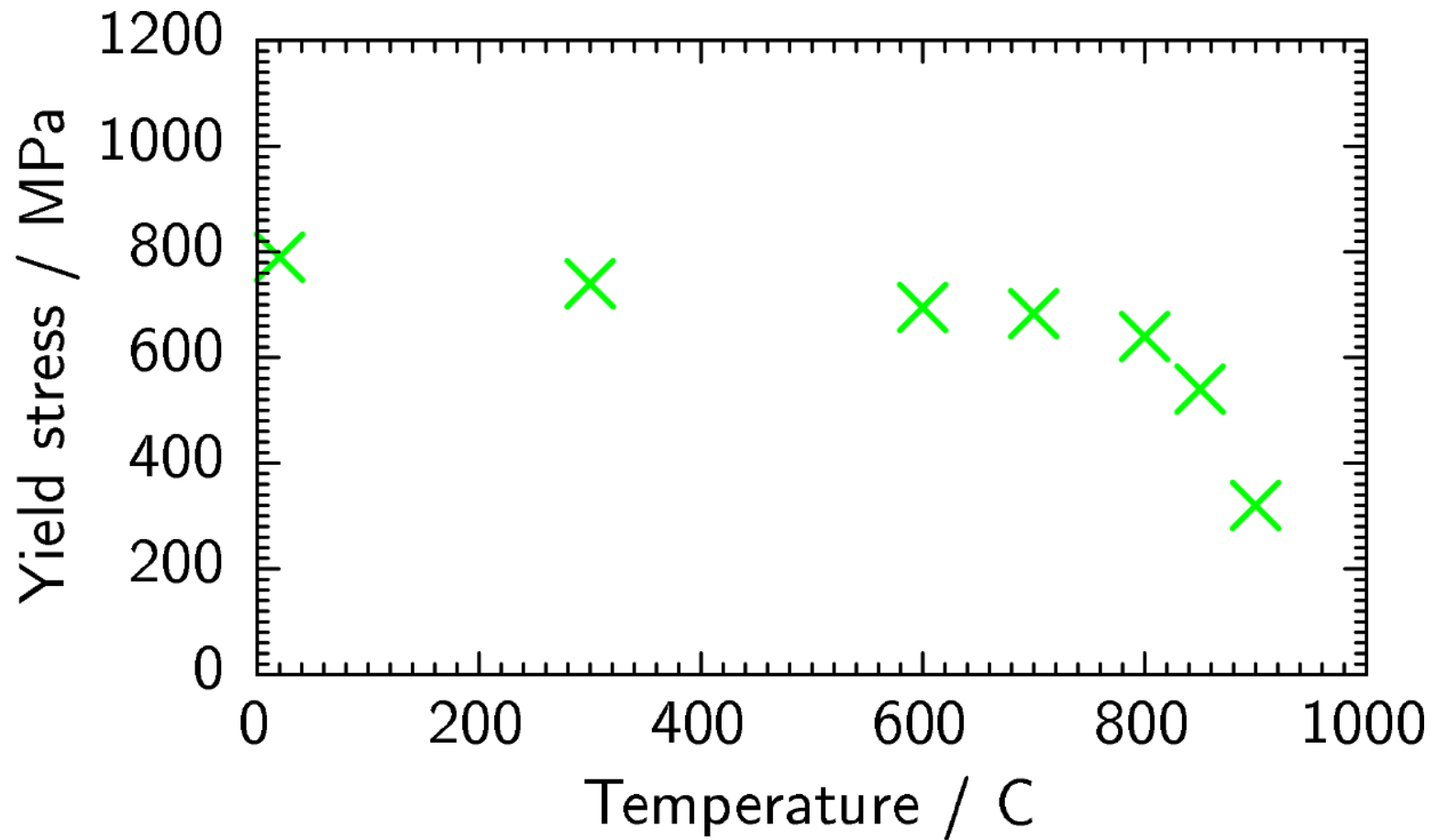


$\eta$  contaminated alloy

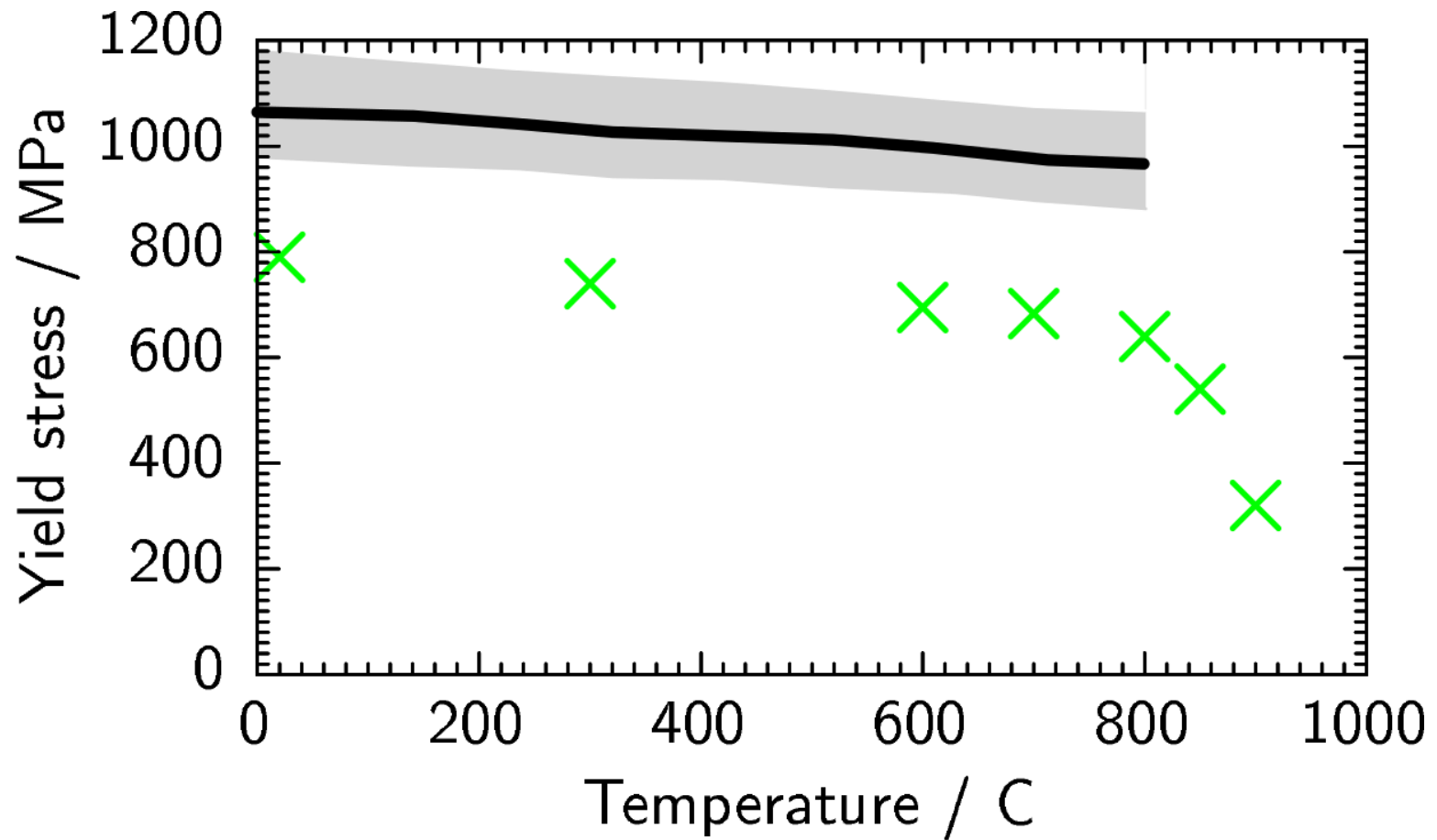




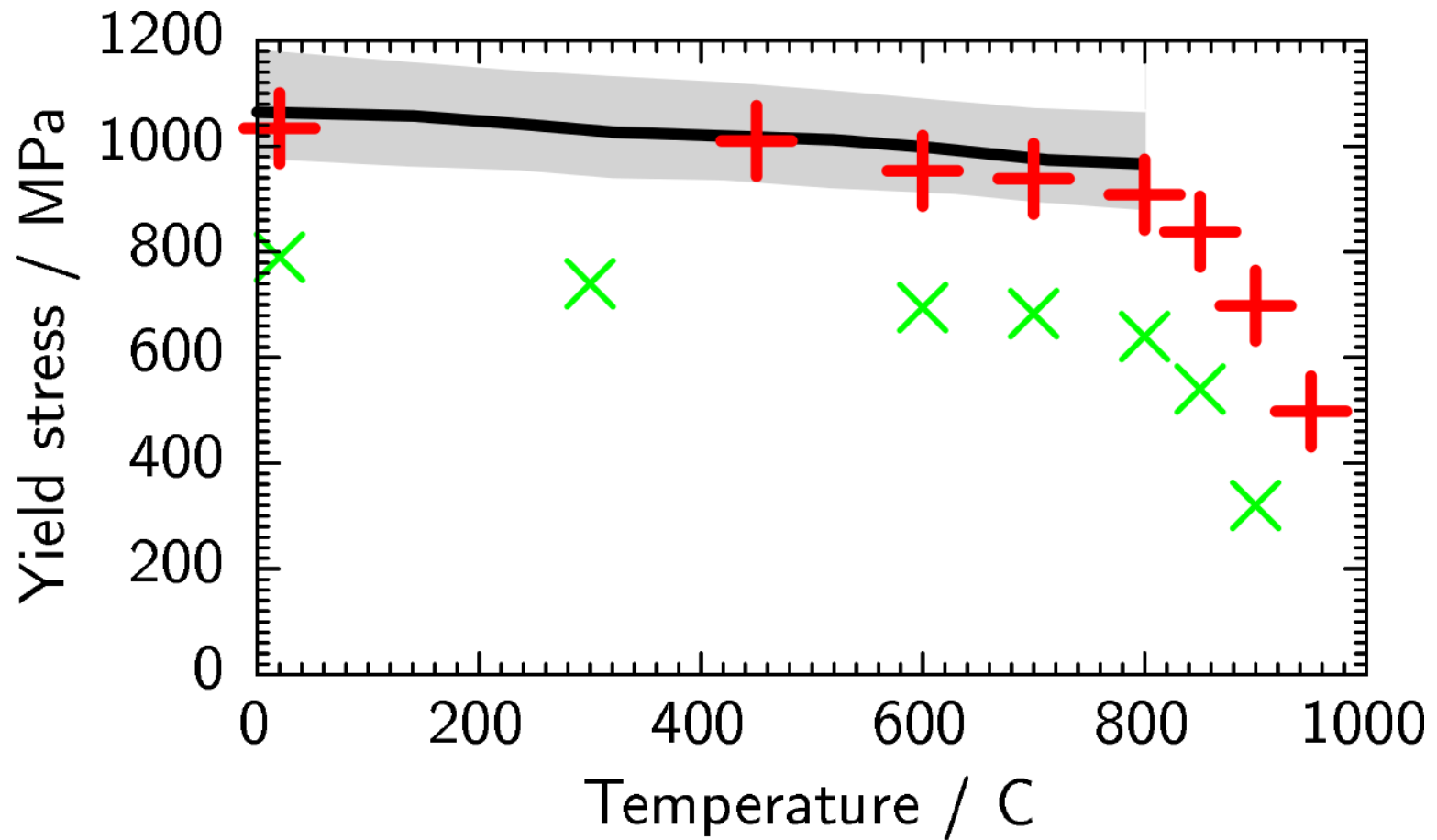
# Yield stress



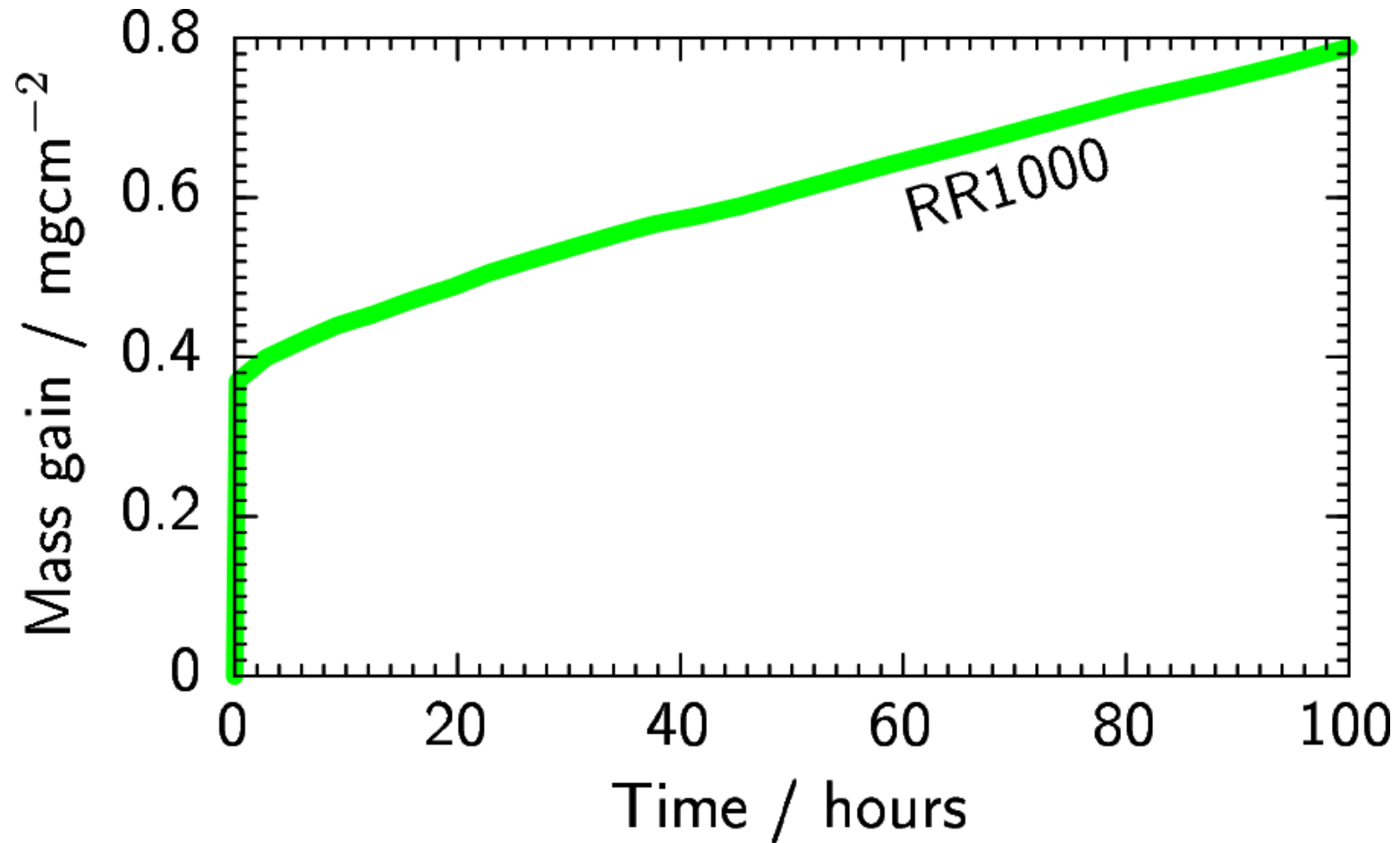
# Yield stress



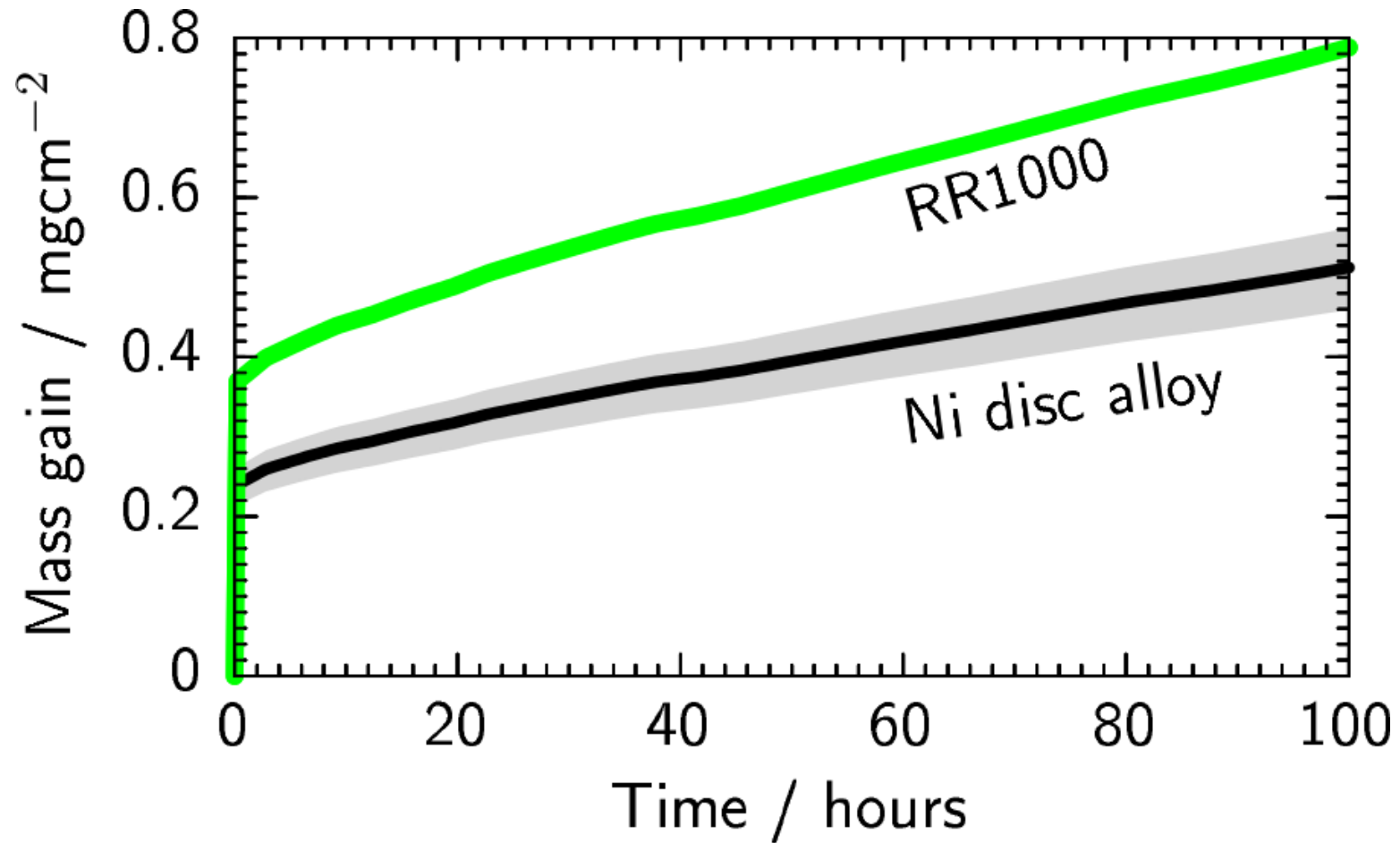
# Yield stress



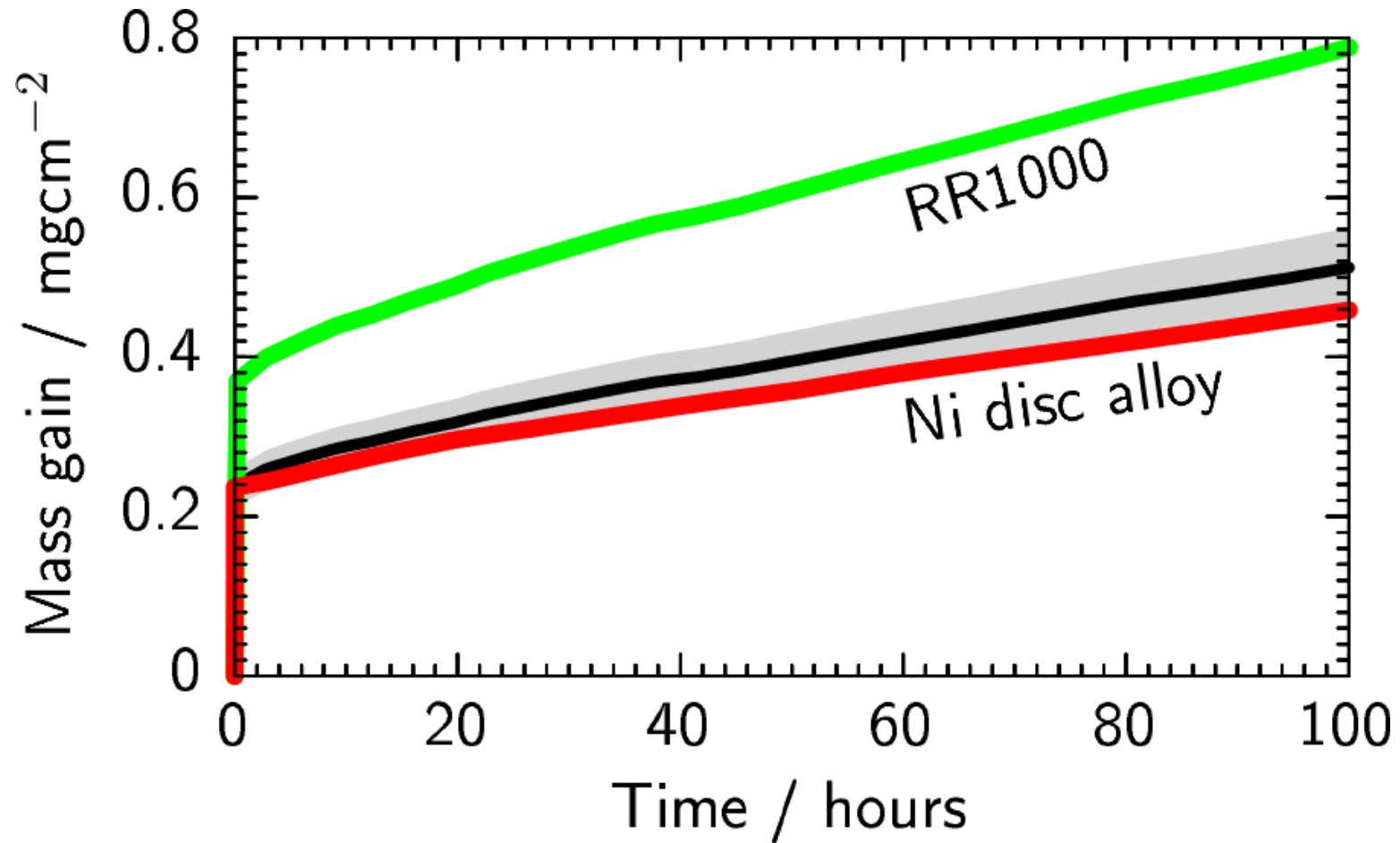
# Oxidation



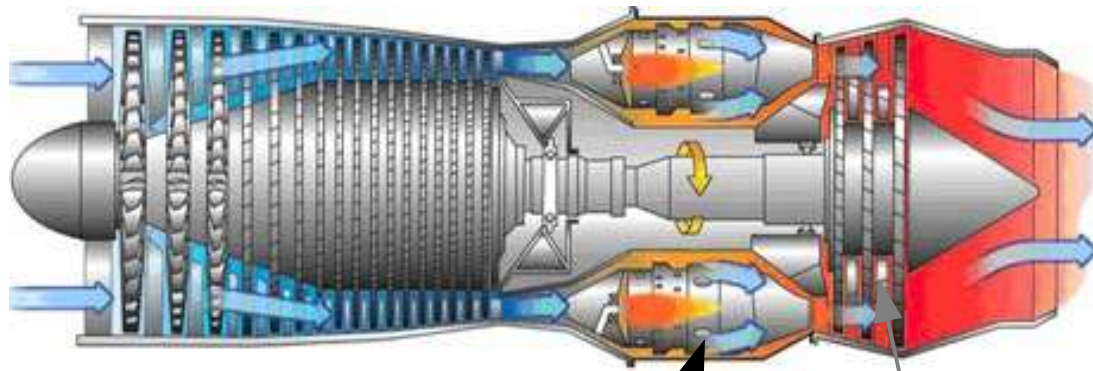
# Oxidation



# Oxidation



# Predicted alloys



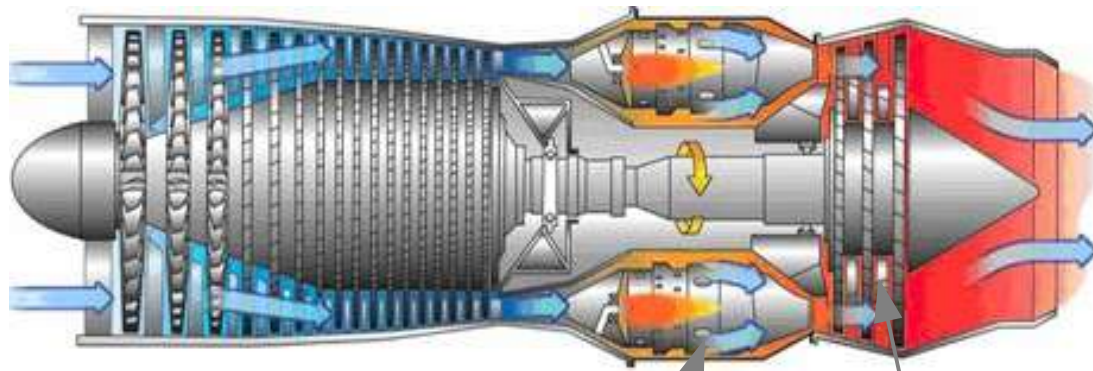
**Combustor  
liner**

2x disc  
alloy

2x forging  
hammer



# Predicted alloys



Combustor  
liner

2x disc  
alloy



2x forging  
hammer



# Case study: improved forging alloy



**Mo**

99.4



**Ti**

0.5



**C**

0.02

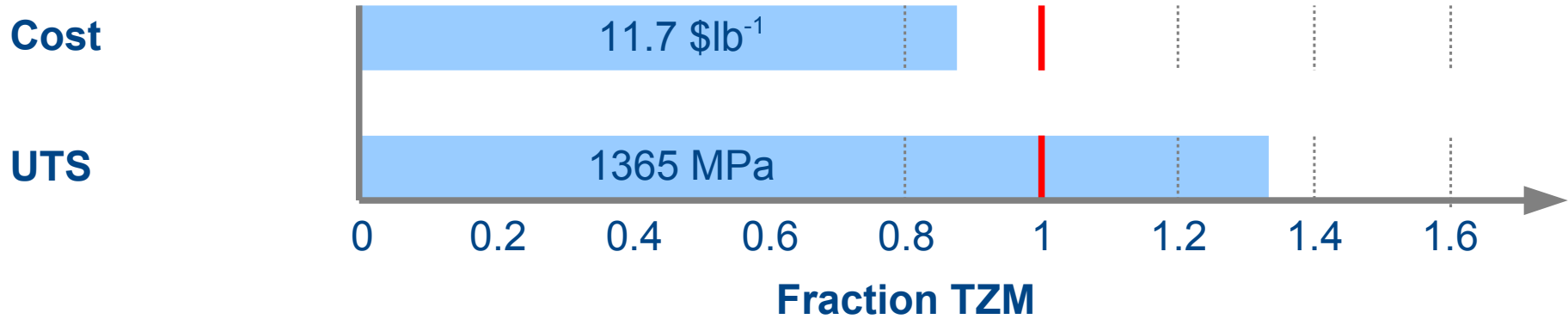


**Zr**

0.08

**TZM**

# 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

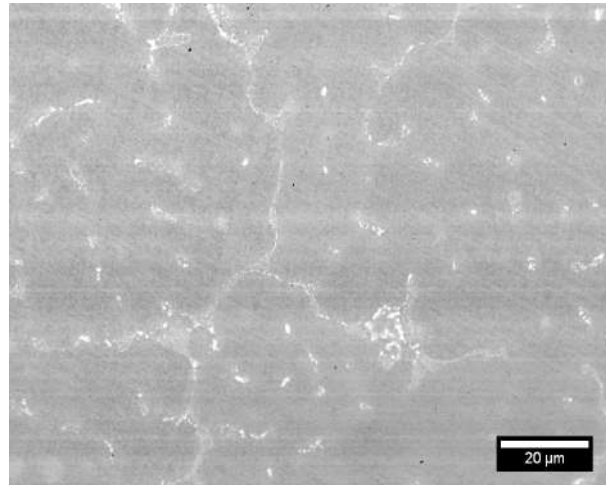
9.0

0.5

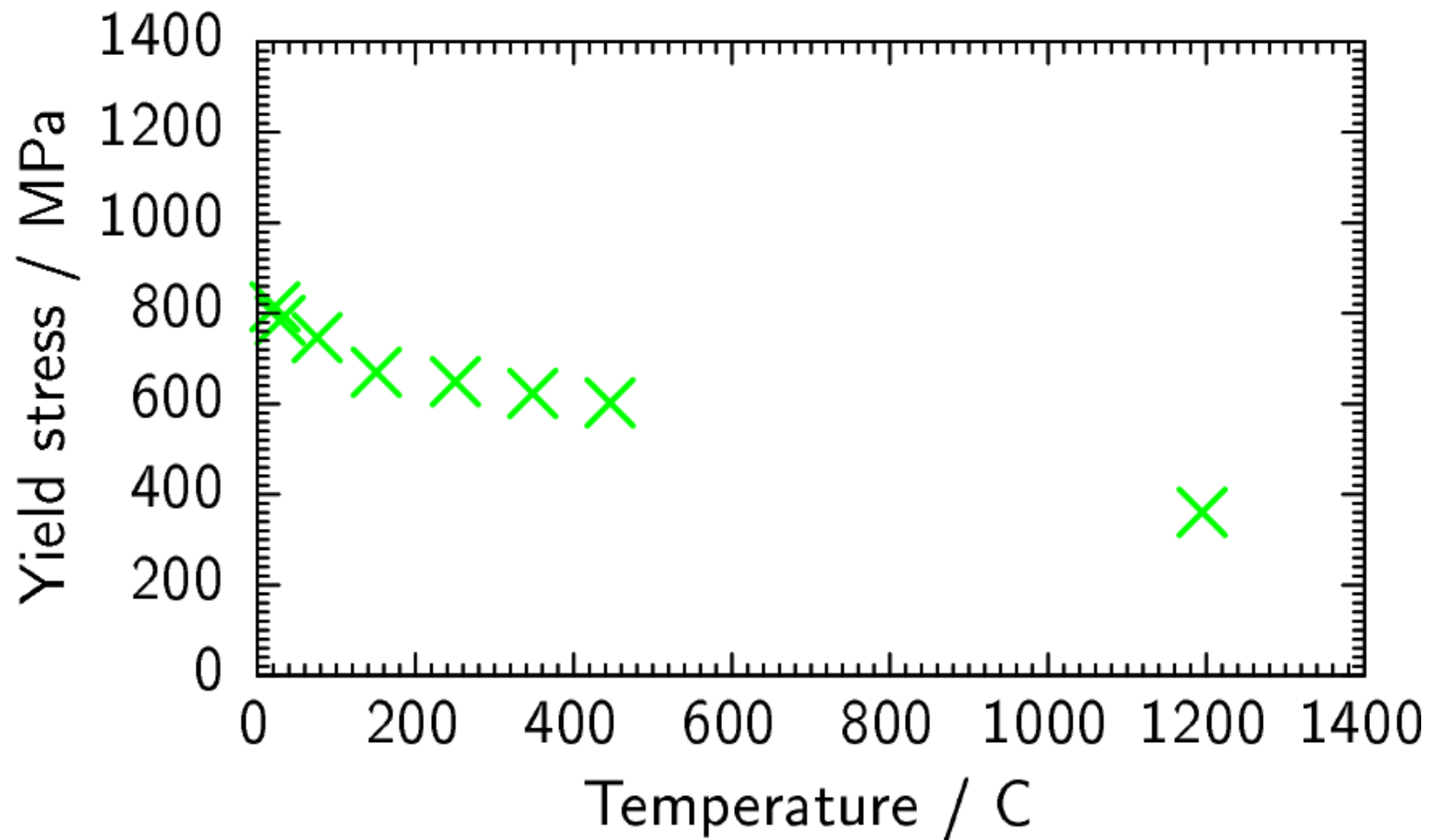
5.7

# Electron micrograph – Mo forging alloy

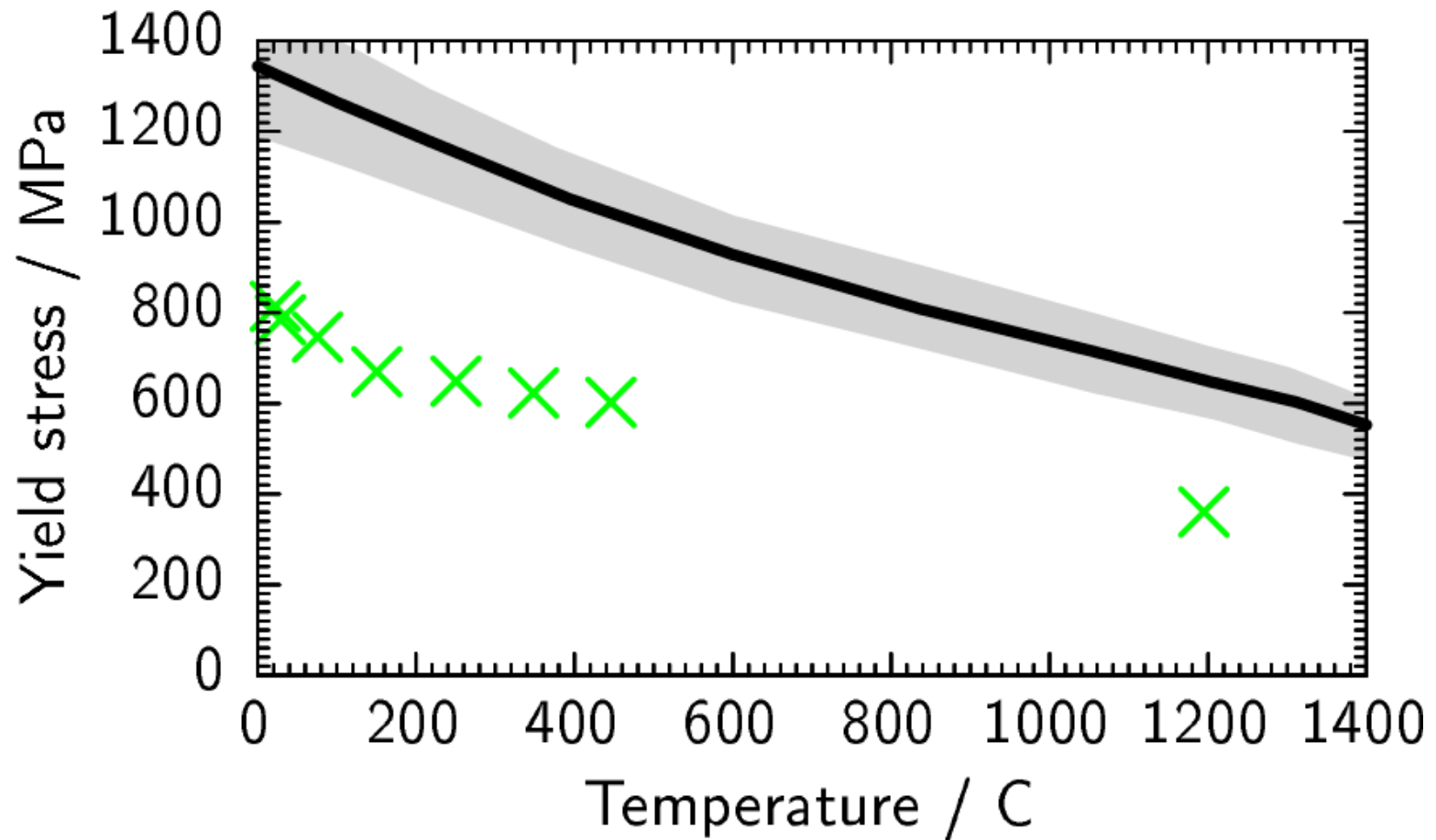
Mo forging alloy



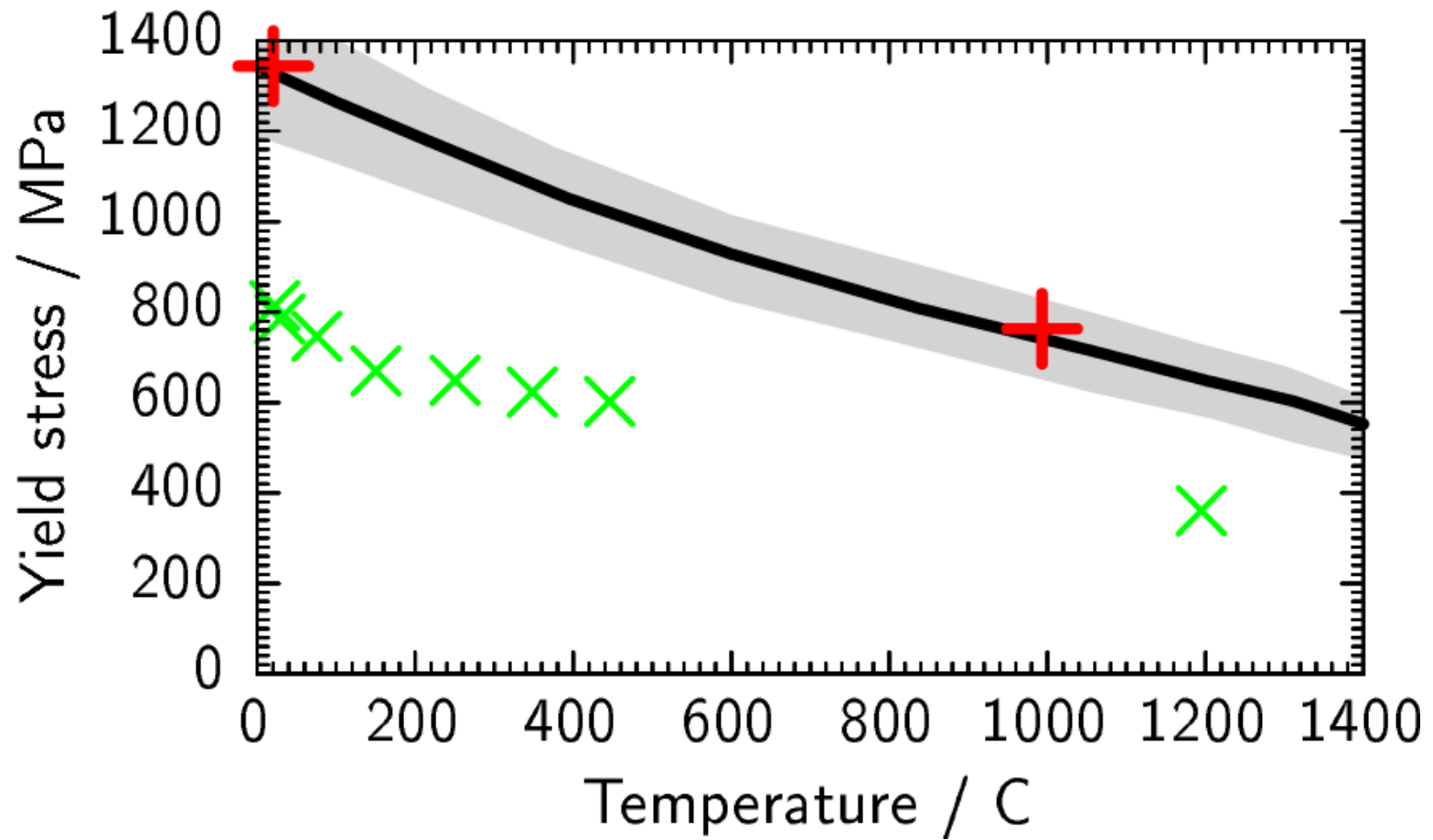
# Yield stress



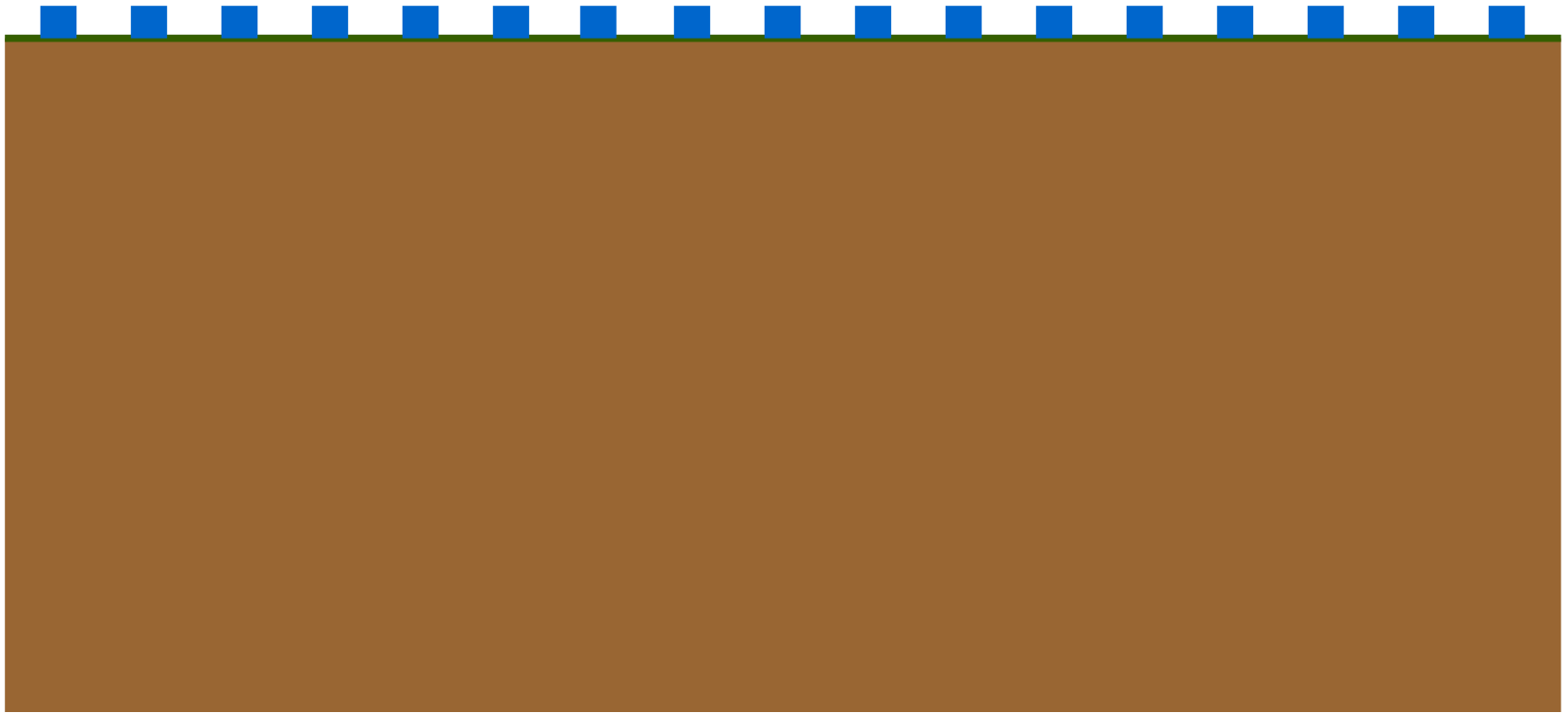
# Yield stress



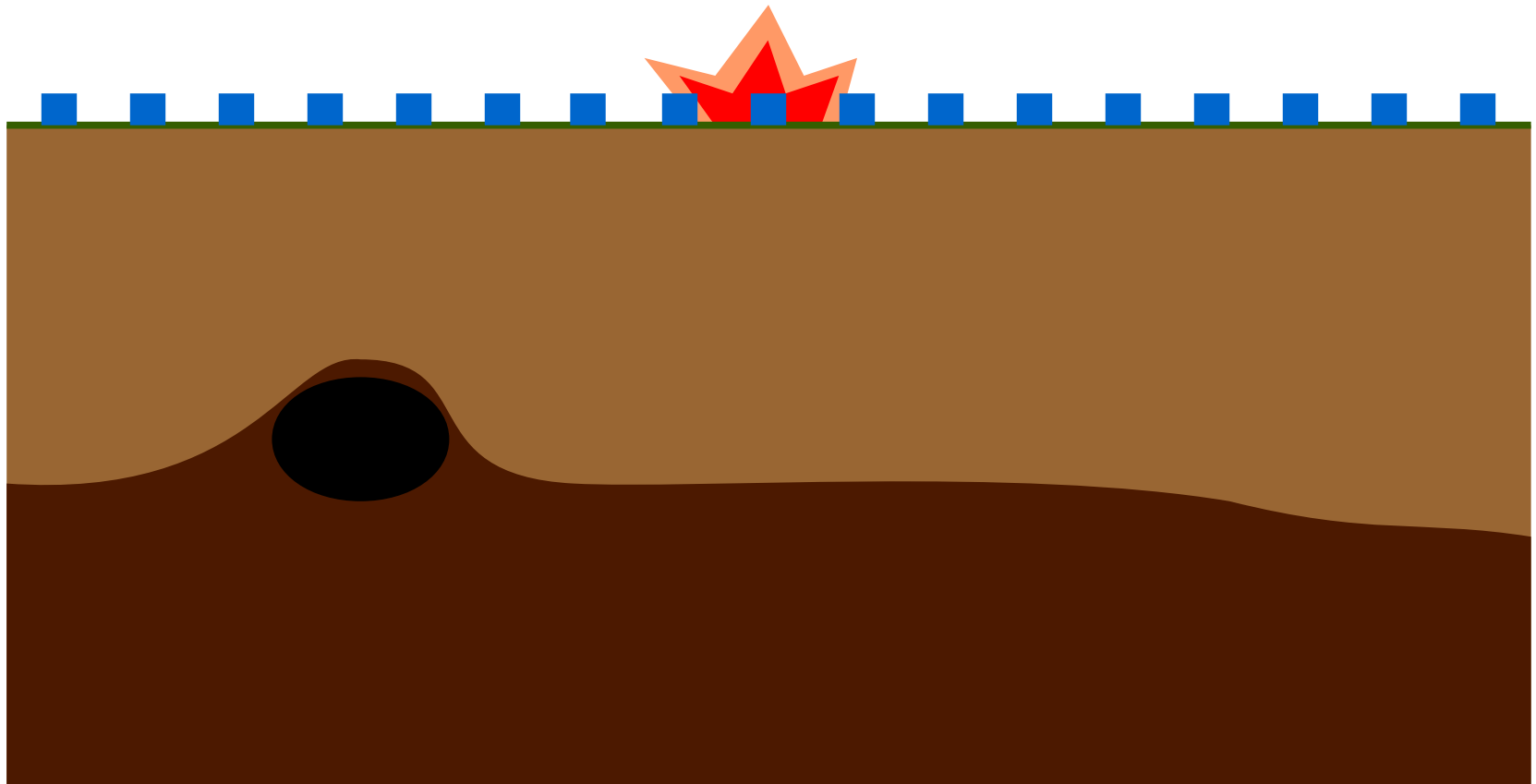
# Yield stress



# Seismic surveys

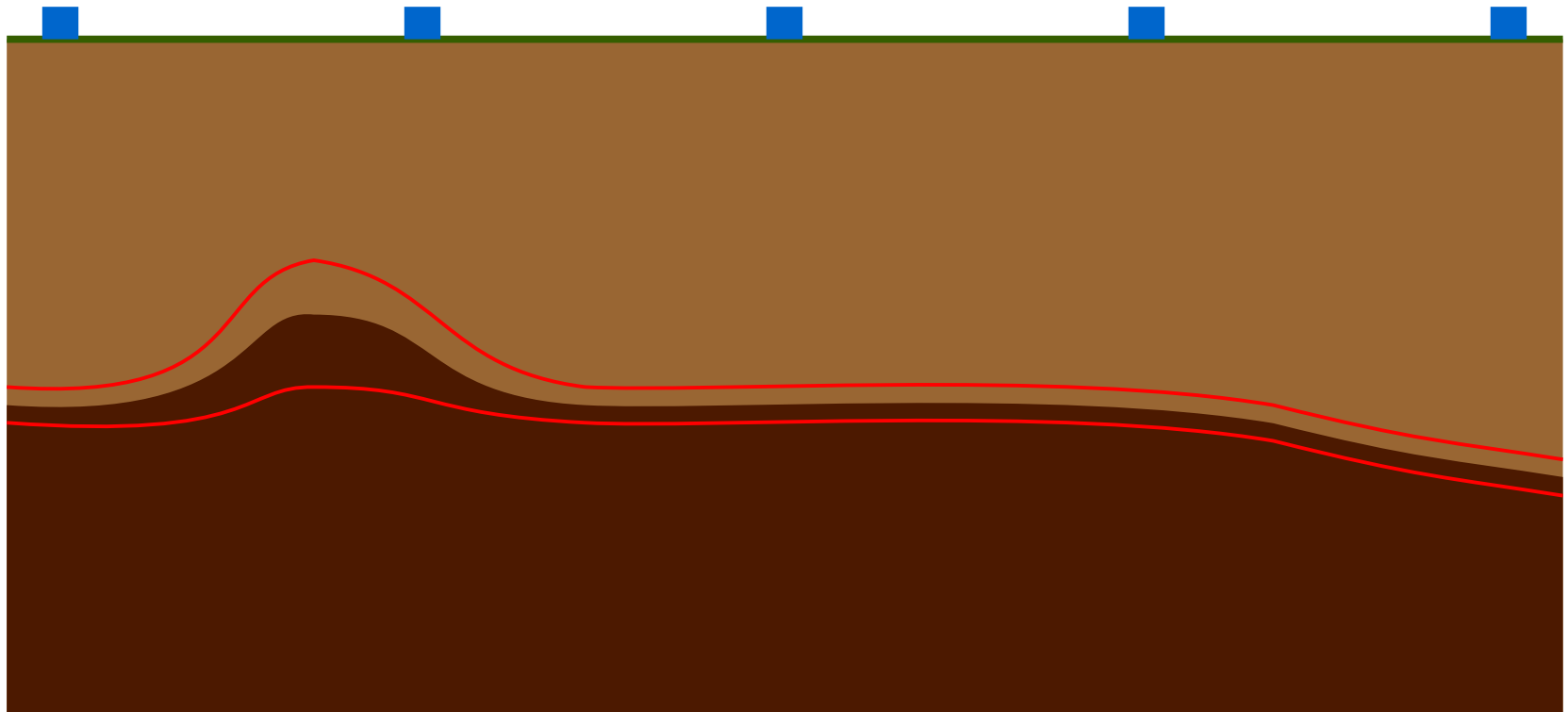


# Seismic surveys

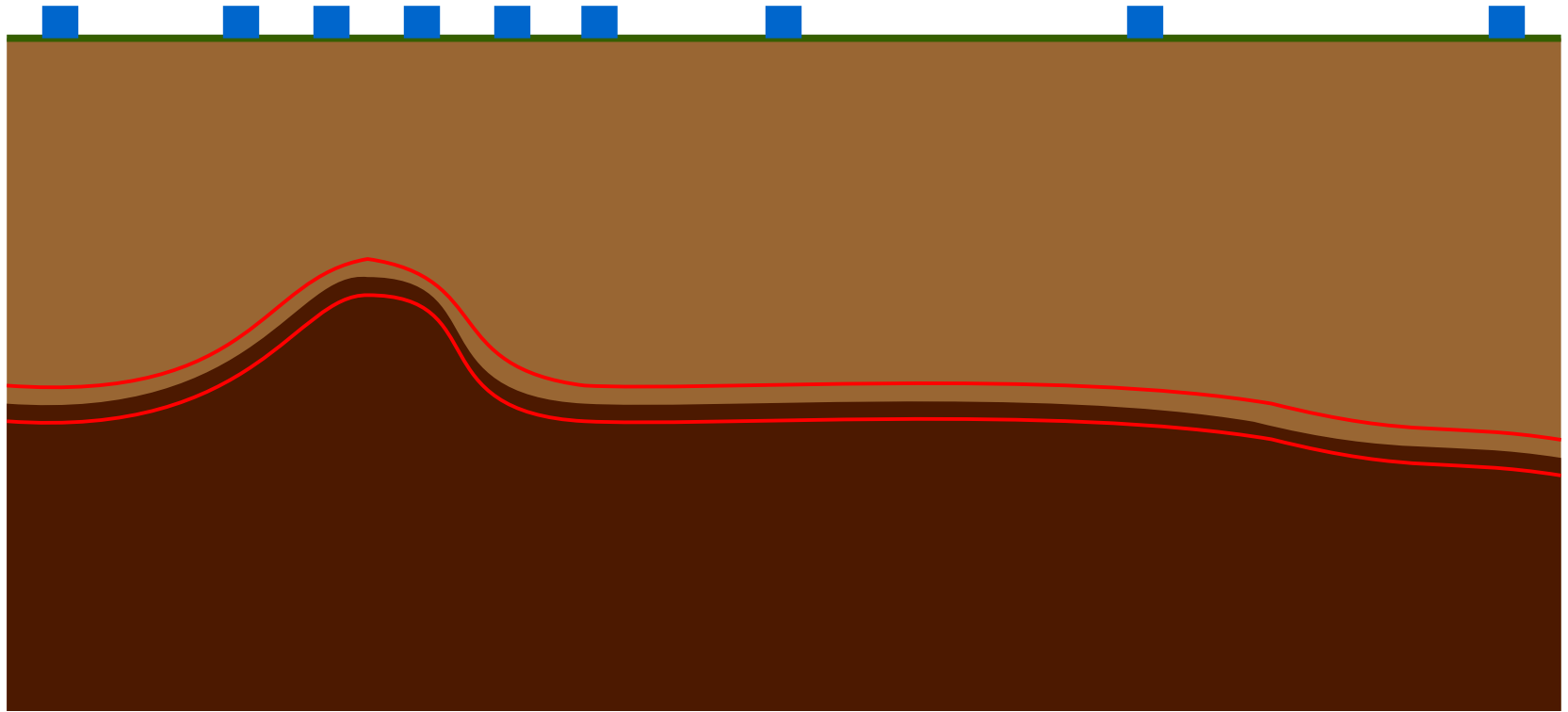




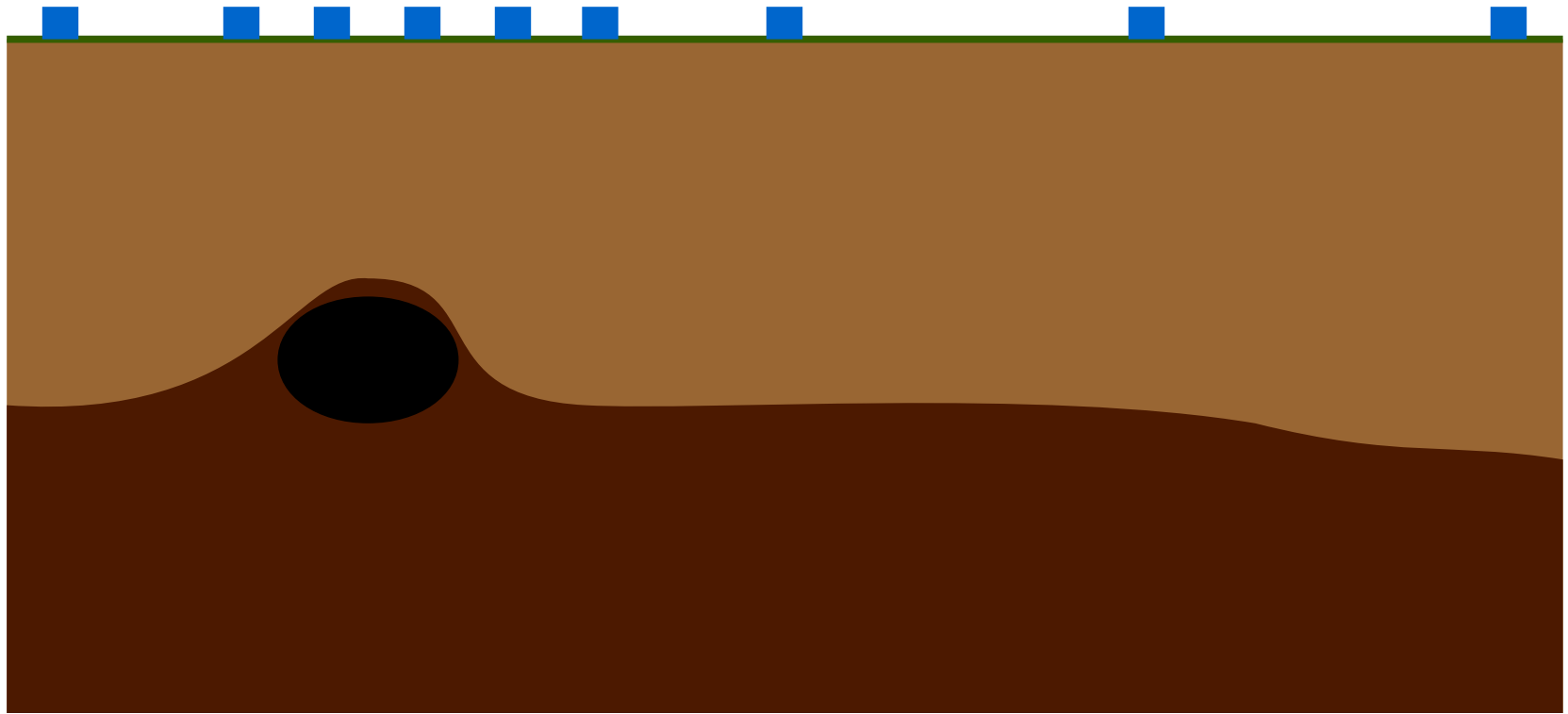
# Seismic surveys



# Seismic surveys



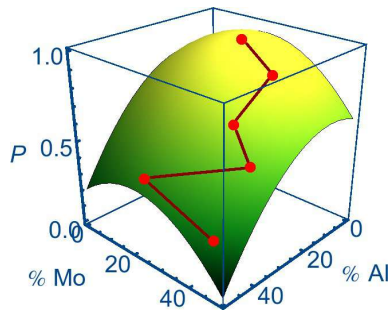
# Seismic surveys



# Concurrent materials design

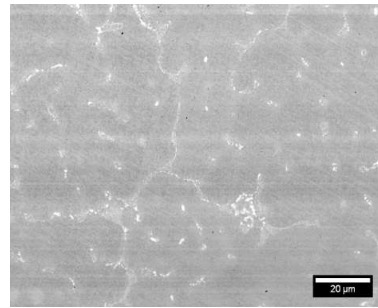
## Discovery algorithm

Patent GB1302743.8 (2013)



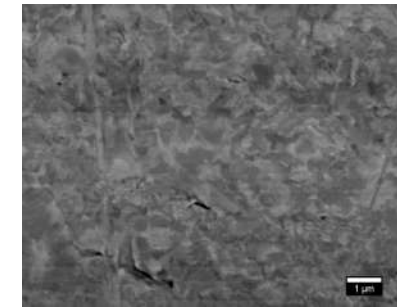
## Mo-Hf forging alloy

Patent GB1307533.8 (2013)



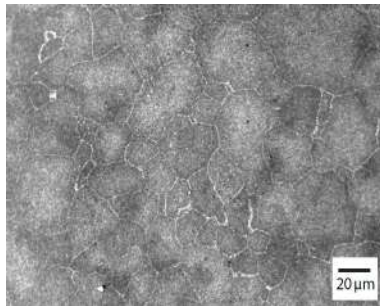
## Mo-Nb forging alloy

Patent GB1307535.3 (2013)



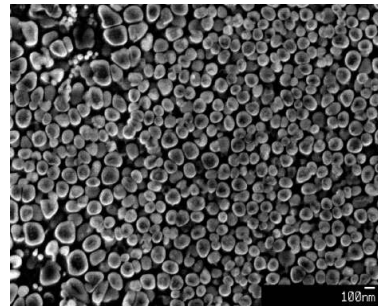
## RR1000 grain growth

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



## Ni disc alloy

Rolls-Royce invention  
NC12261 (2012)



## Ni combustor liner

Rolls-Royce invention  
NC13006 (2013)

