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Top Trumps: materials and alloys

Gareth Conduit

Patent GB1302743.8 (2013)

Patent GB1307533.8 (2013)

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

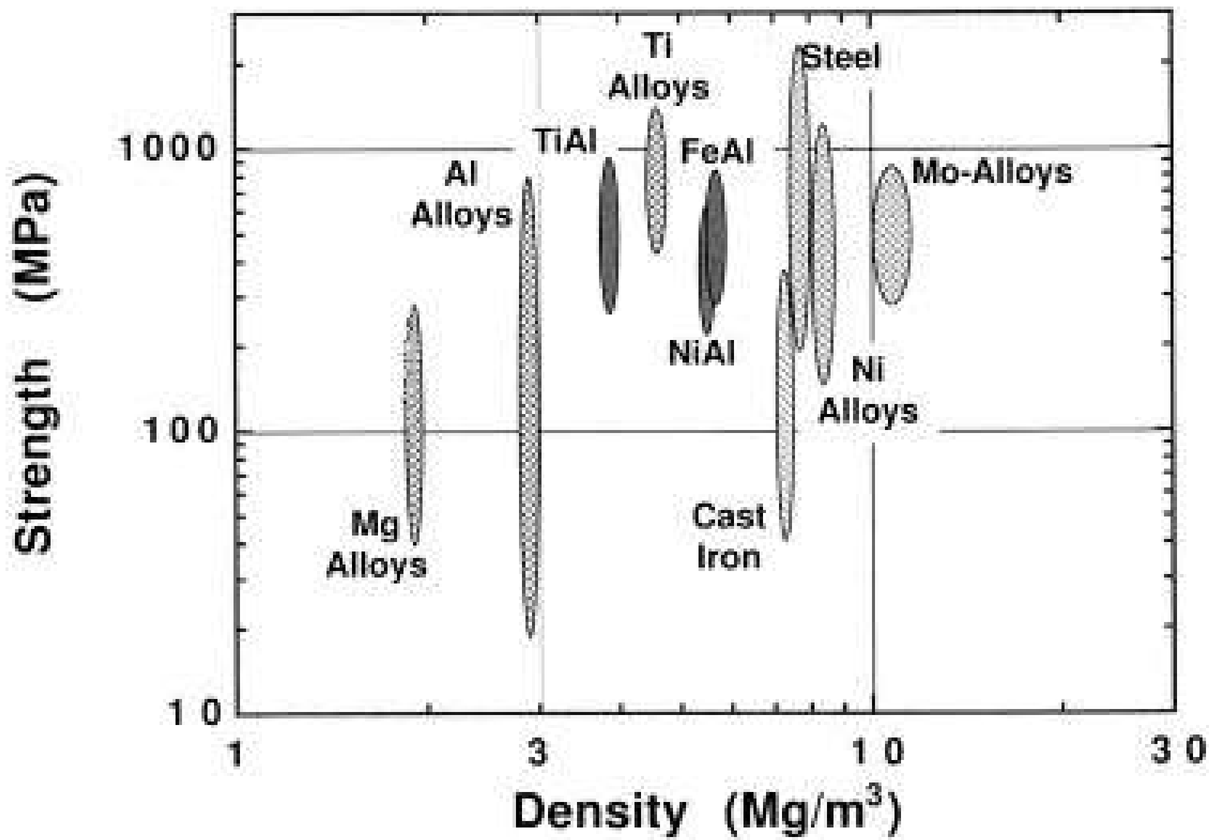
Rolls-Royce Group plc invention submission NC12261 (2012)

Rolls-Royce Group plc invention submission NC13006 (2013)

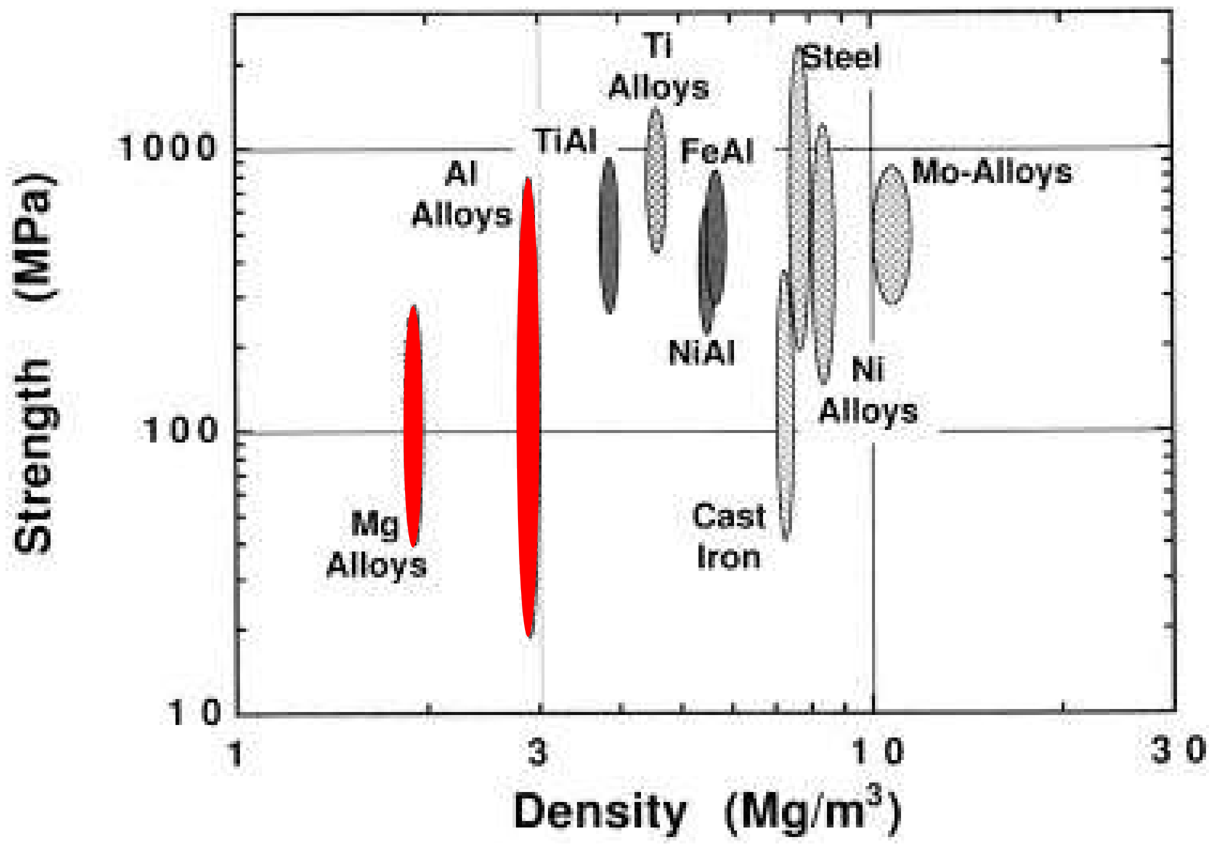
Rolls-Royce Group plc invention submission NC13024 (2013)

TCM Group, Department of Physics

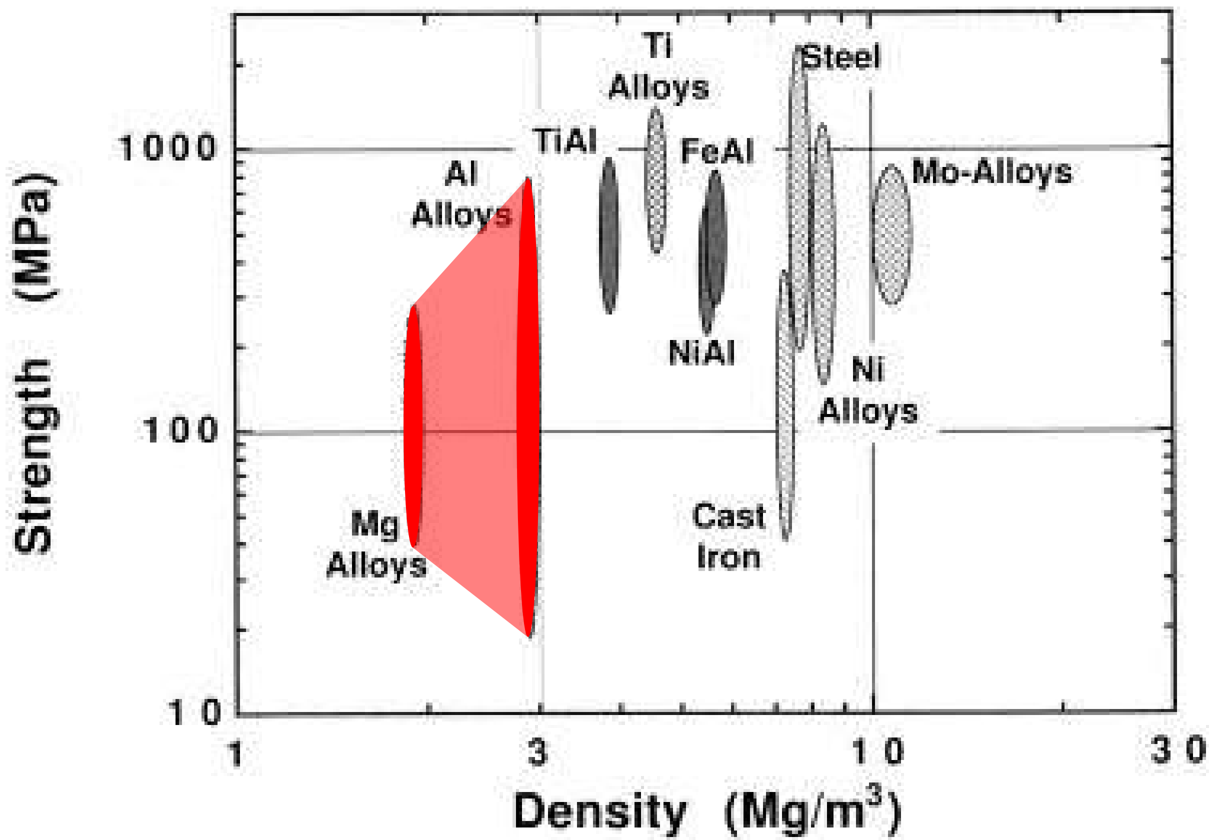
Materials selection



Materials selection

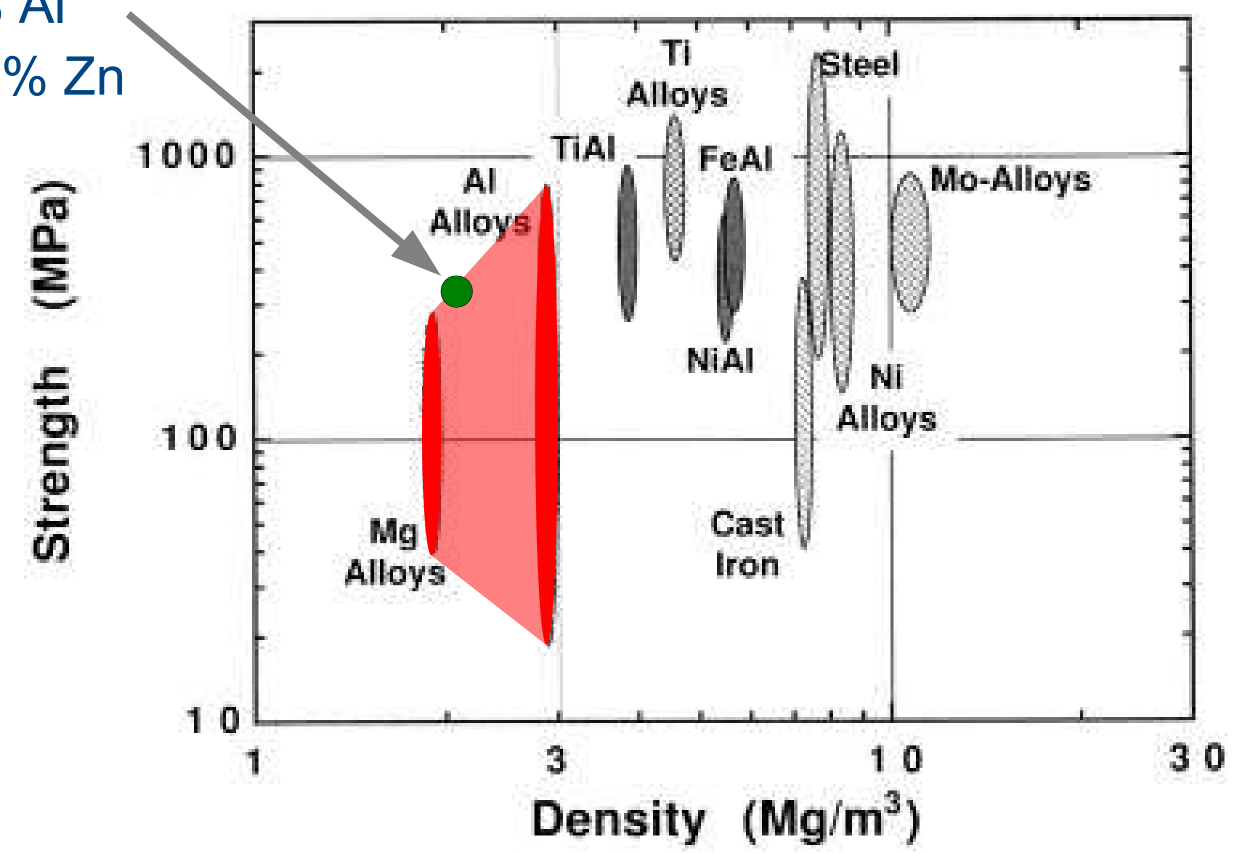


Materials selection

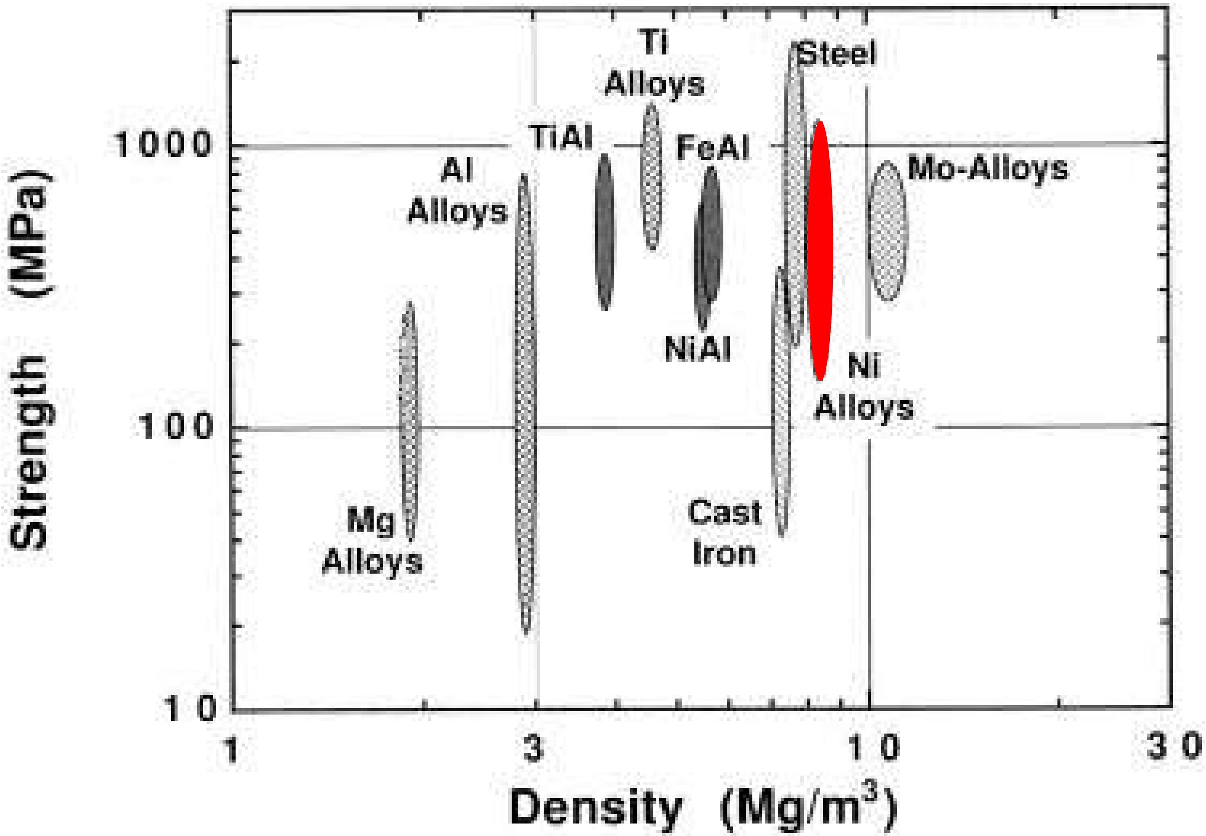


Materials selection

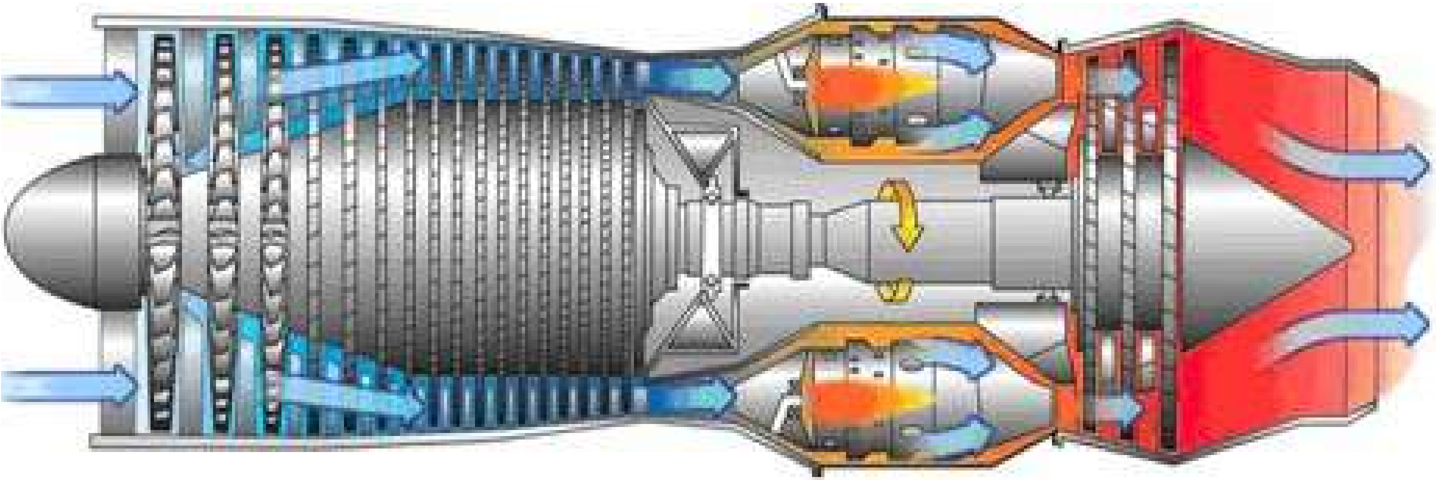
91.5% Mg
8% Al
0.5% Zn



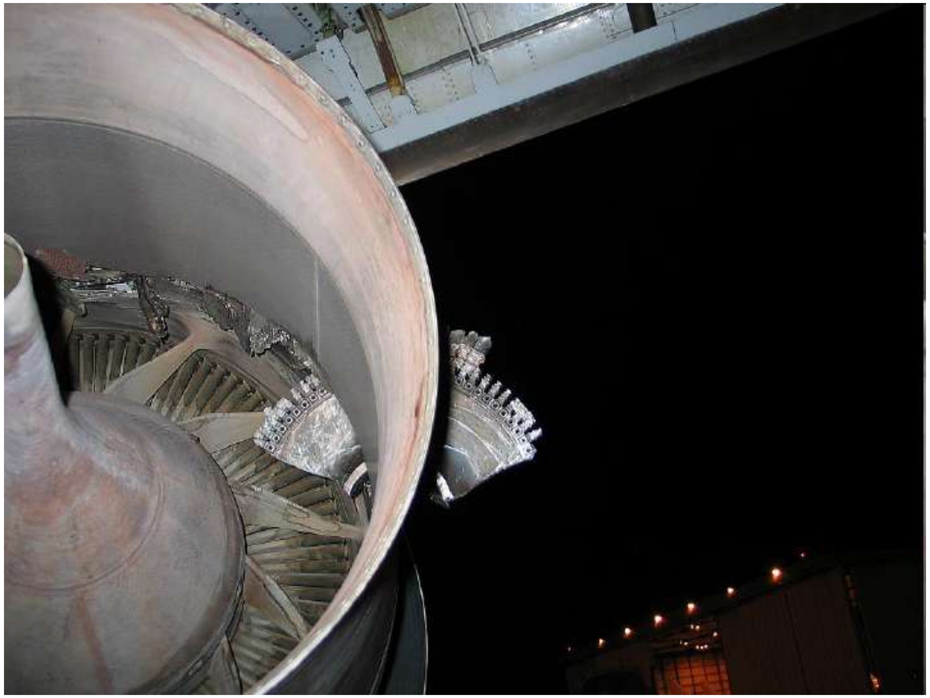
Materials selection



Jet engine



Jet engine: turbine discs



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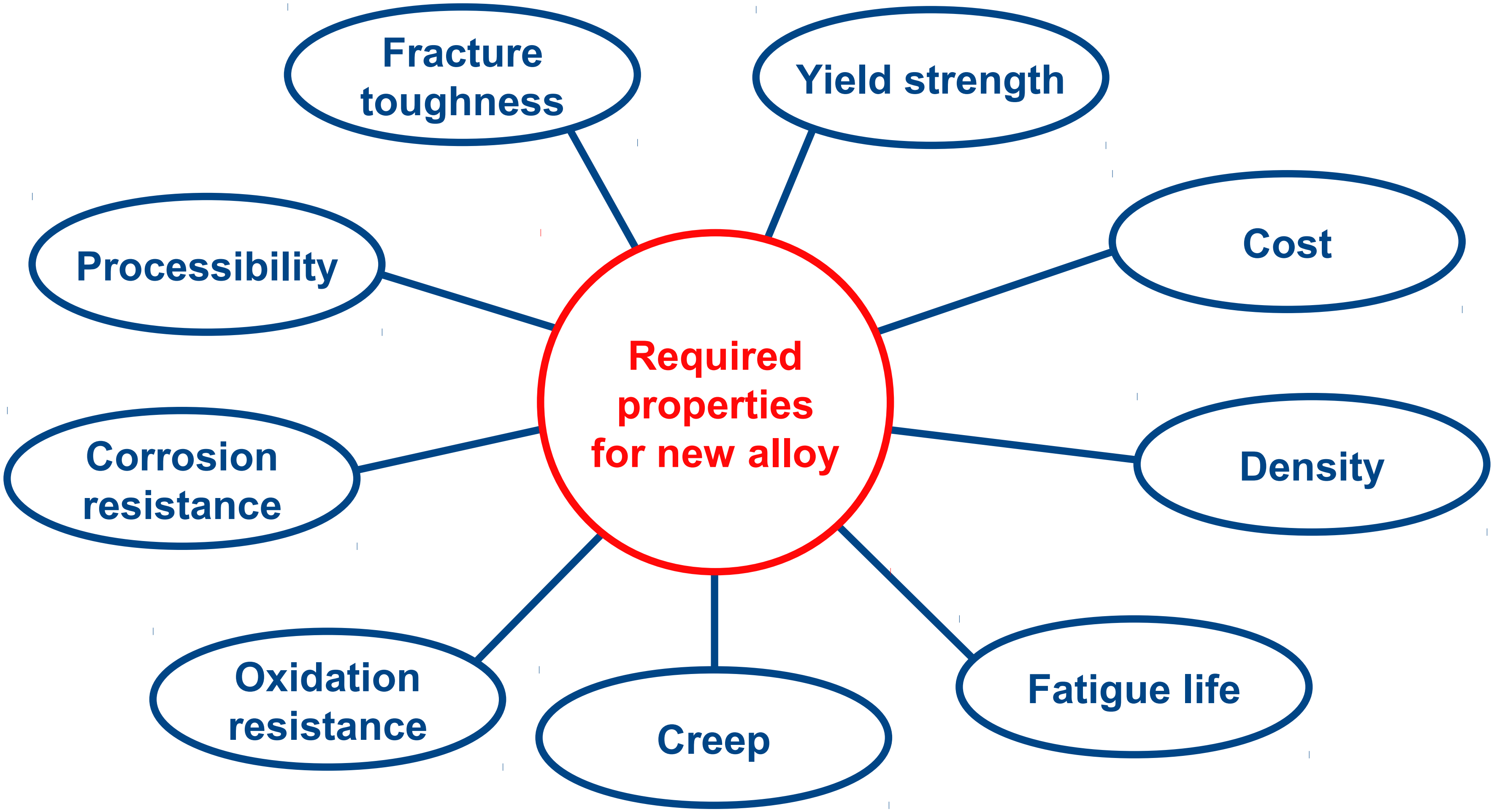
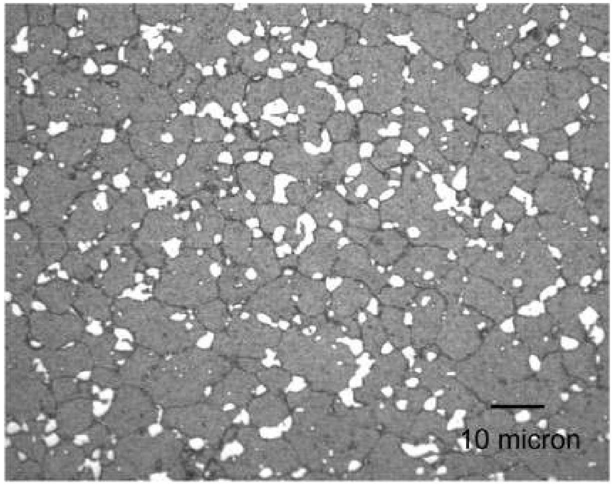
Designing a new alloy – what is required ?

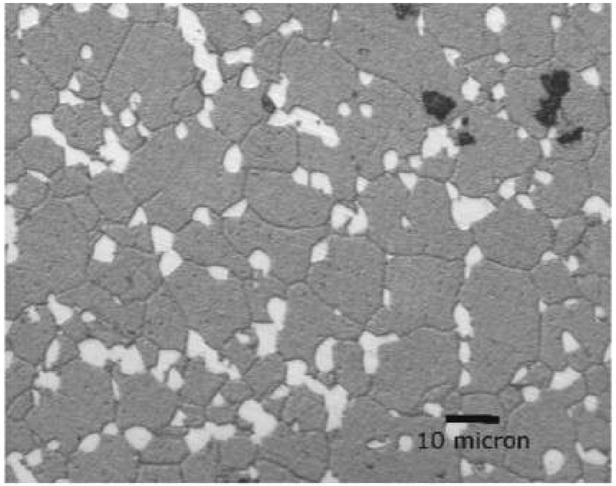


Contemporary alloys

RR1000

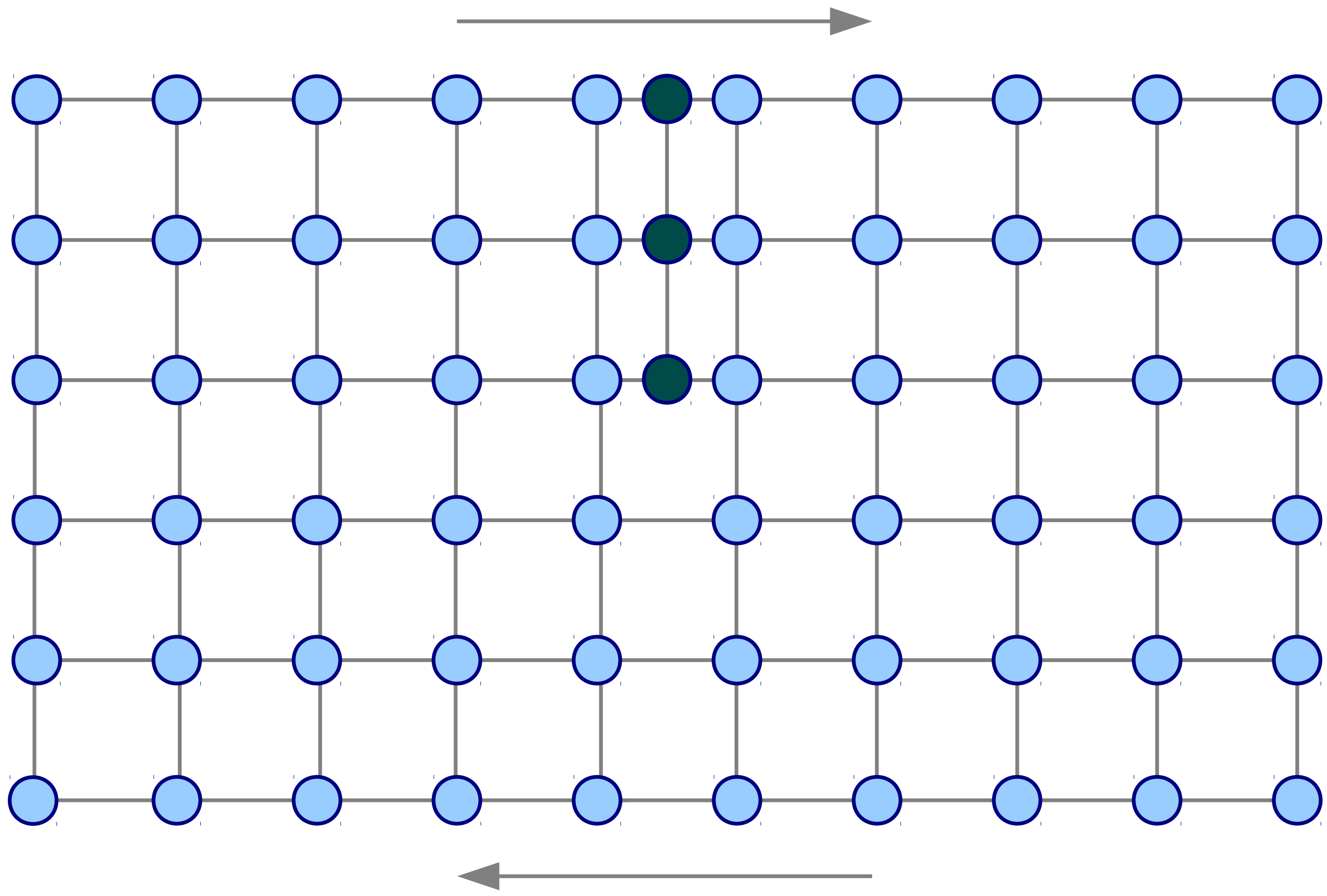


N18

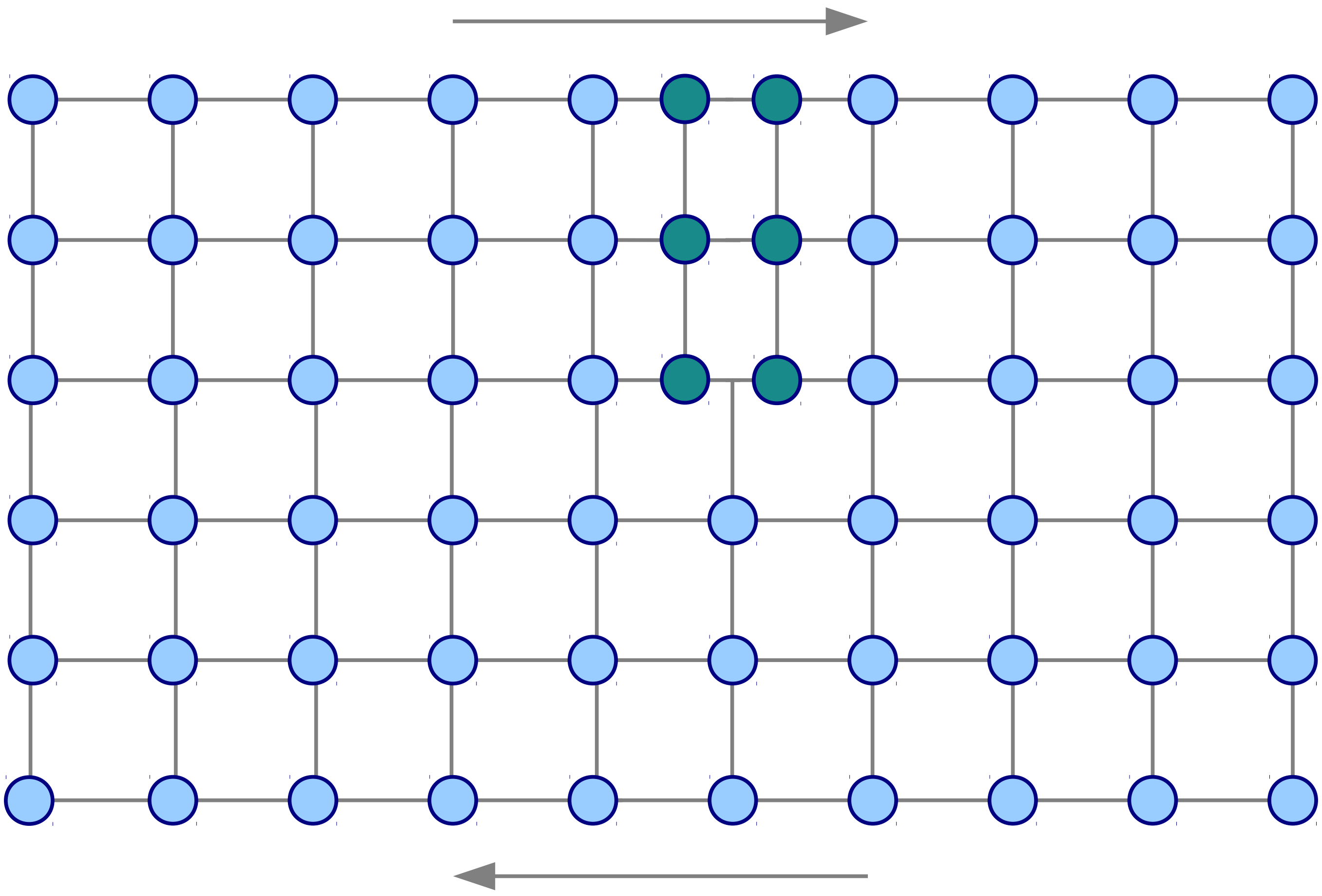


Alloy	Firm	Ni	Cr	Co	Mo	Ti	Al	Ta	Hf	C	W	Nb
RR1000	Rolls Royce	52.4	15	18.5	5	3.6	3	2	0.5	0.03		
N18	SNECMA	58	11.1	15.4	6.4	4.3	4.3		0.5	0.02		
Rene 88	General Elec.	56.5	16	13	4	3.7	2.1			0.03	4	0.7
Waspaloy	UTC	58	19	13	4	3	1.4					

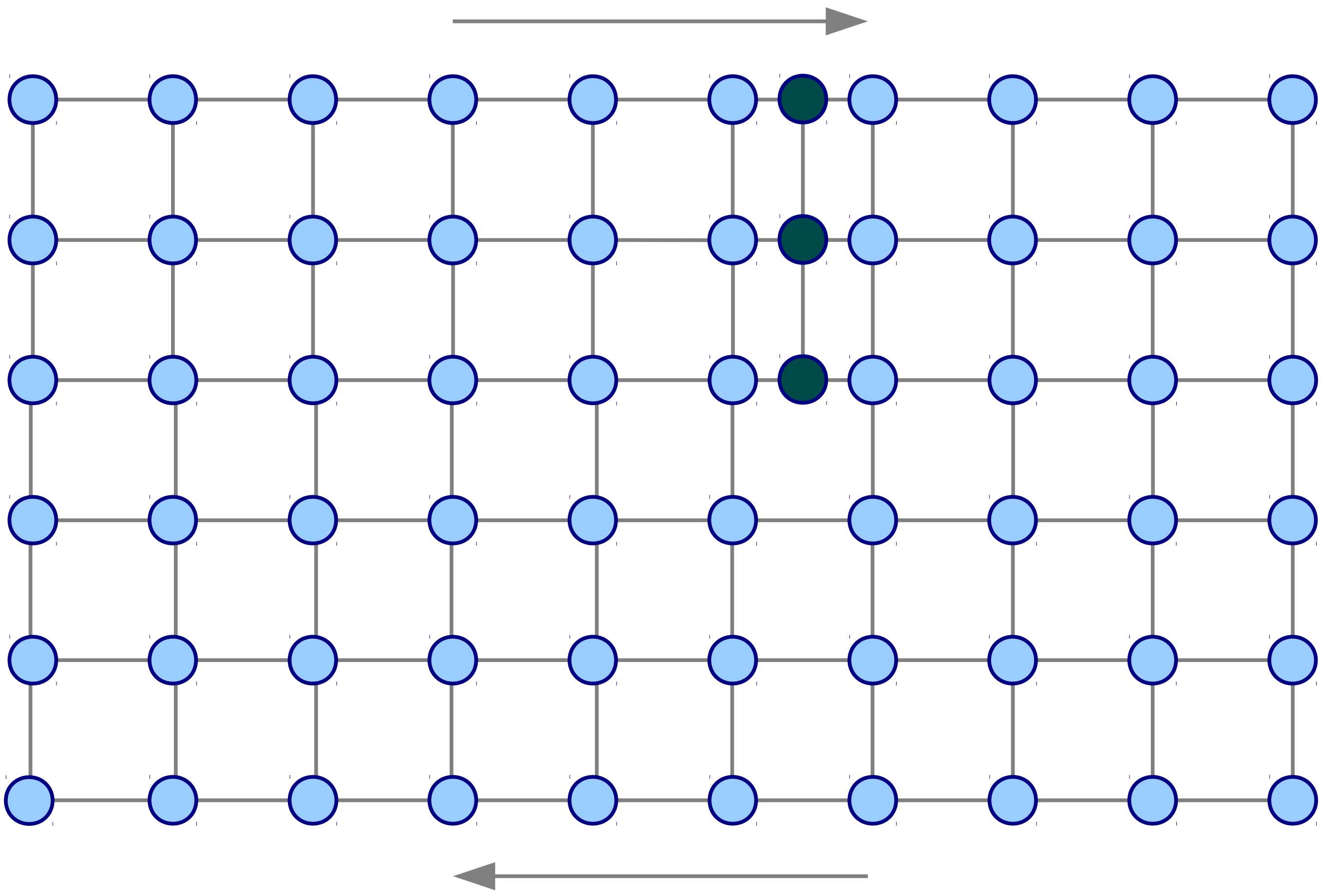
Creep



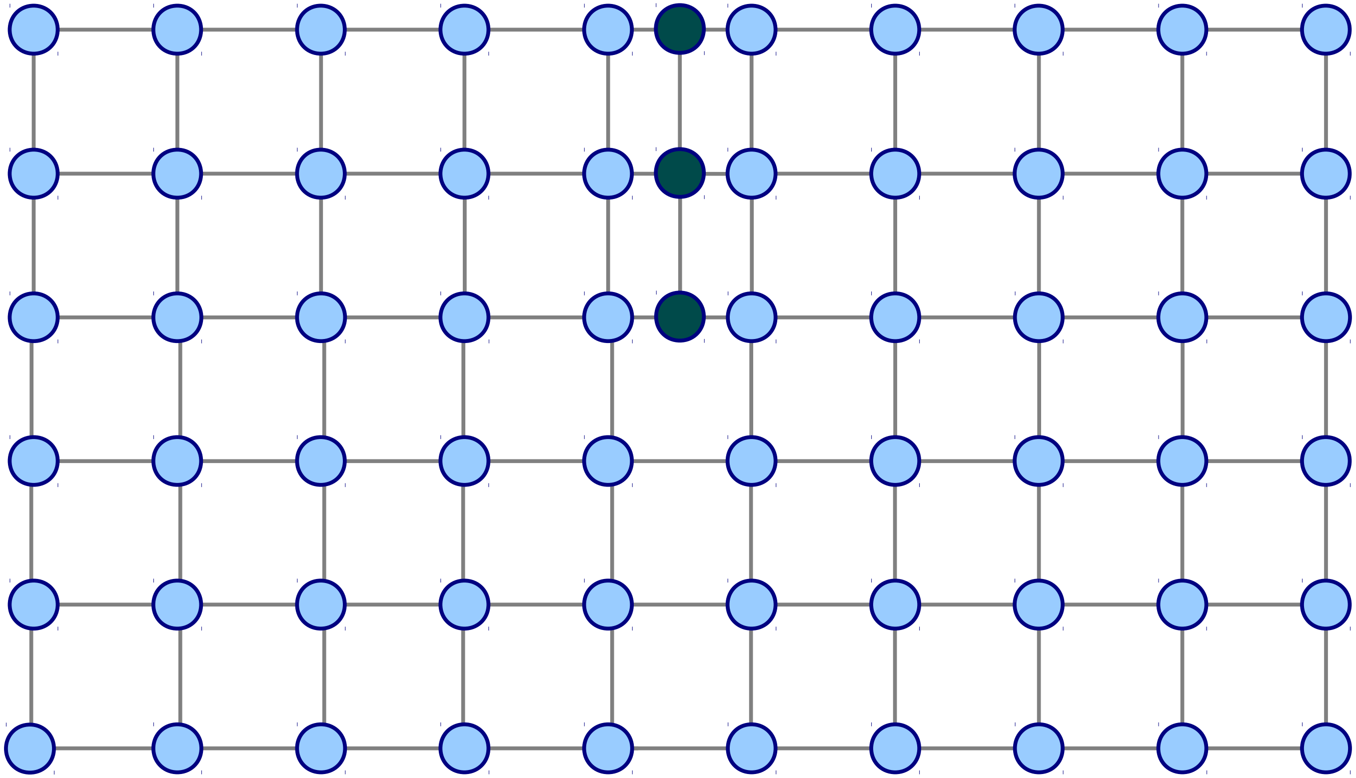
Creep



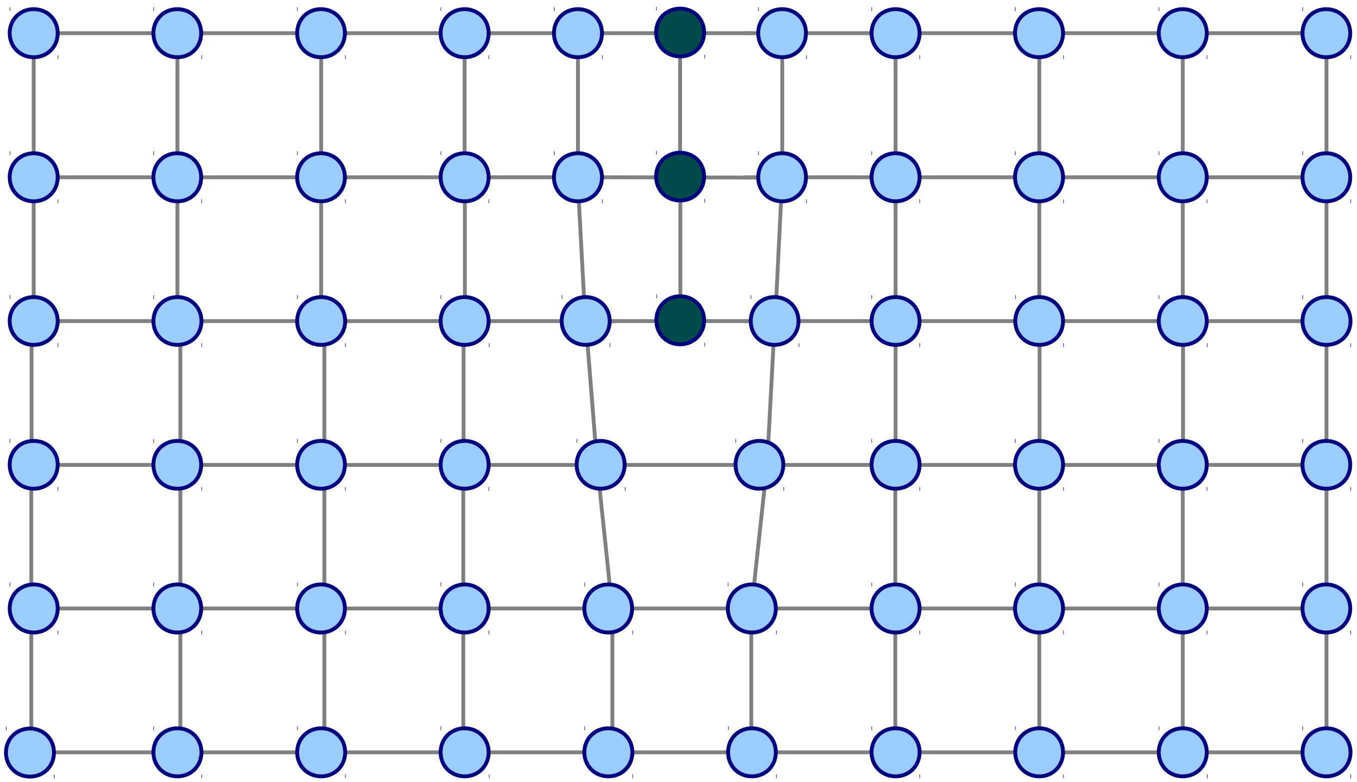
Creep



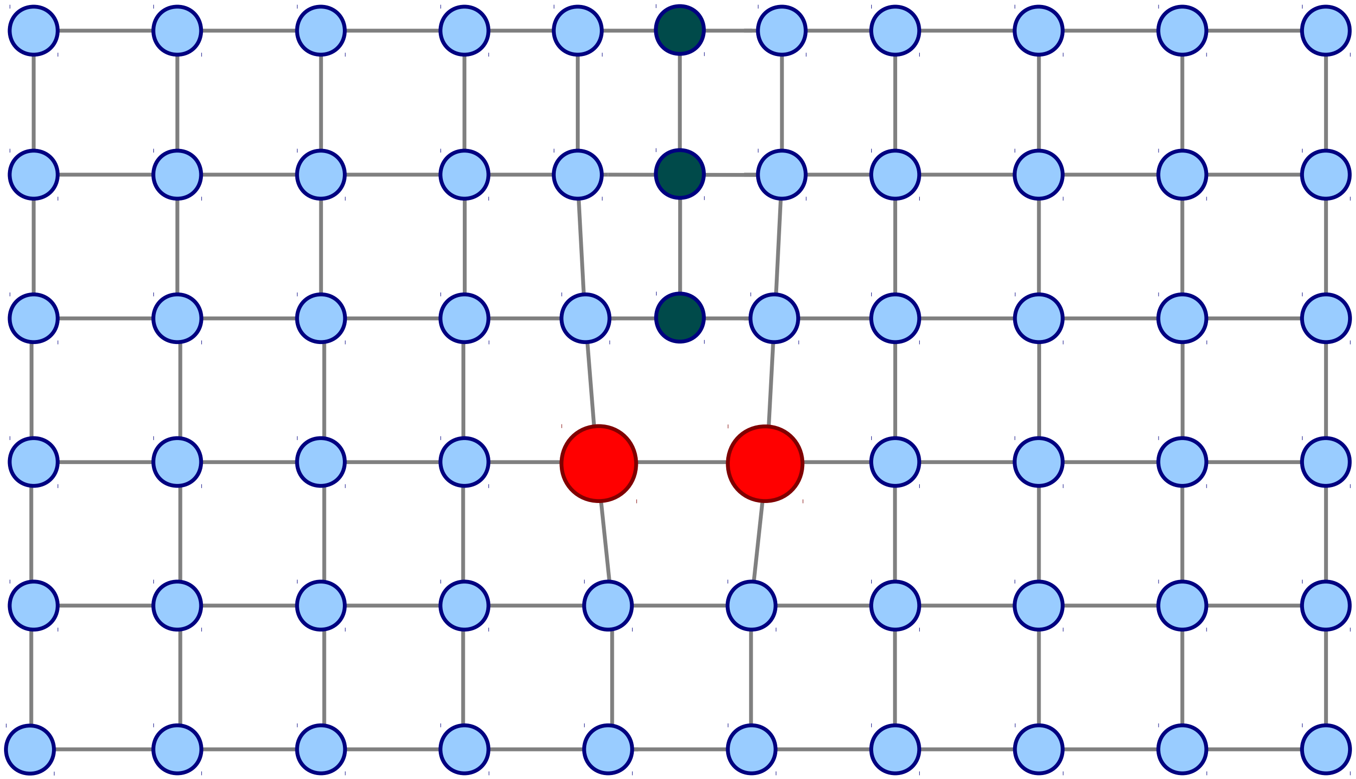
Solution hardening



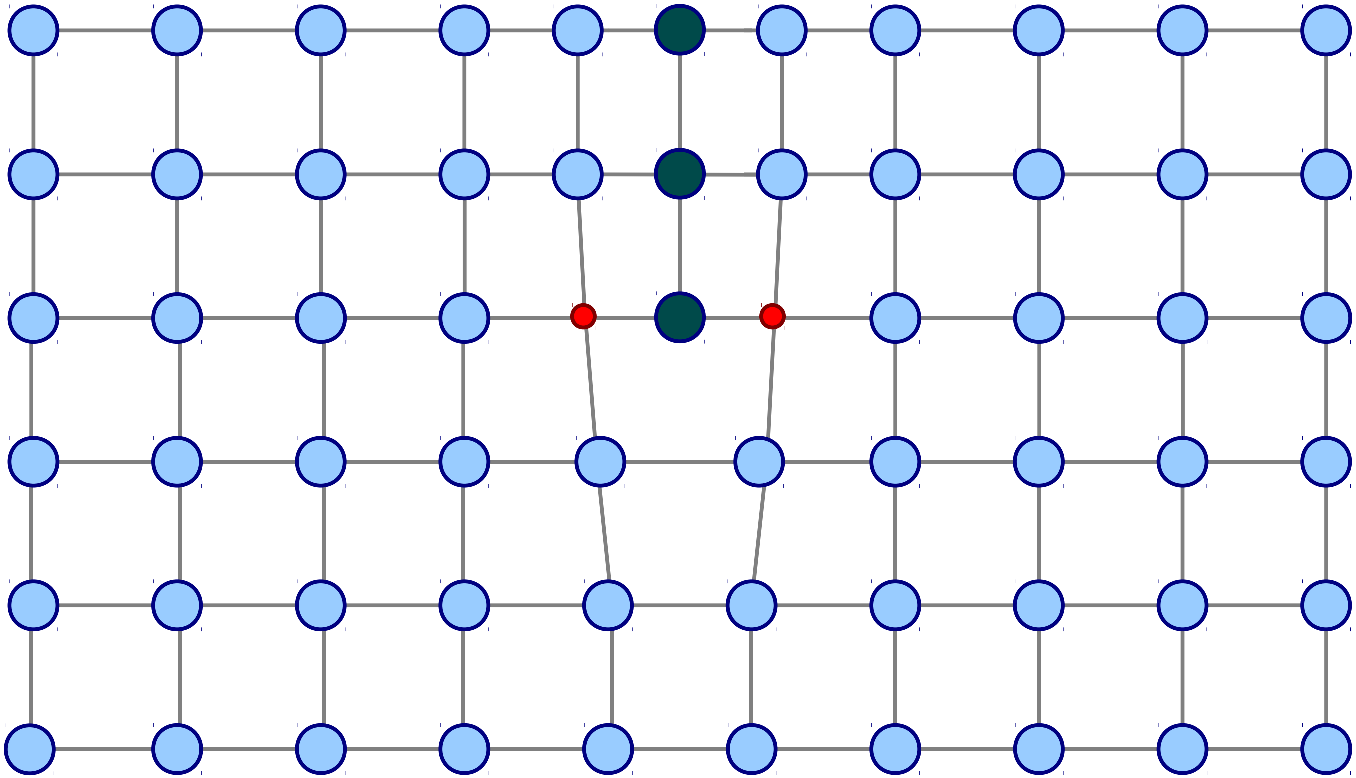
Solution hardening



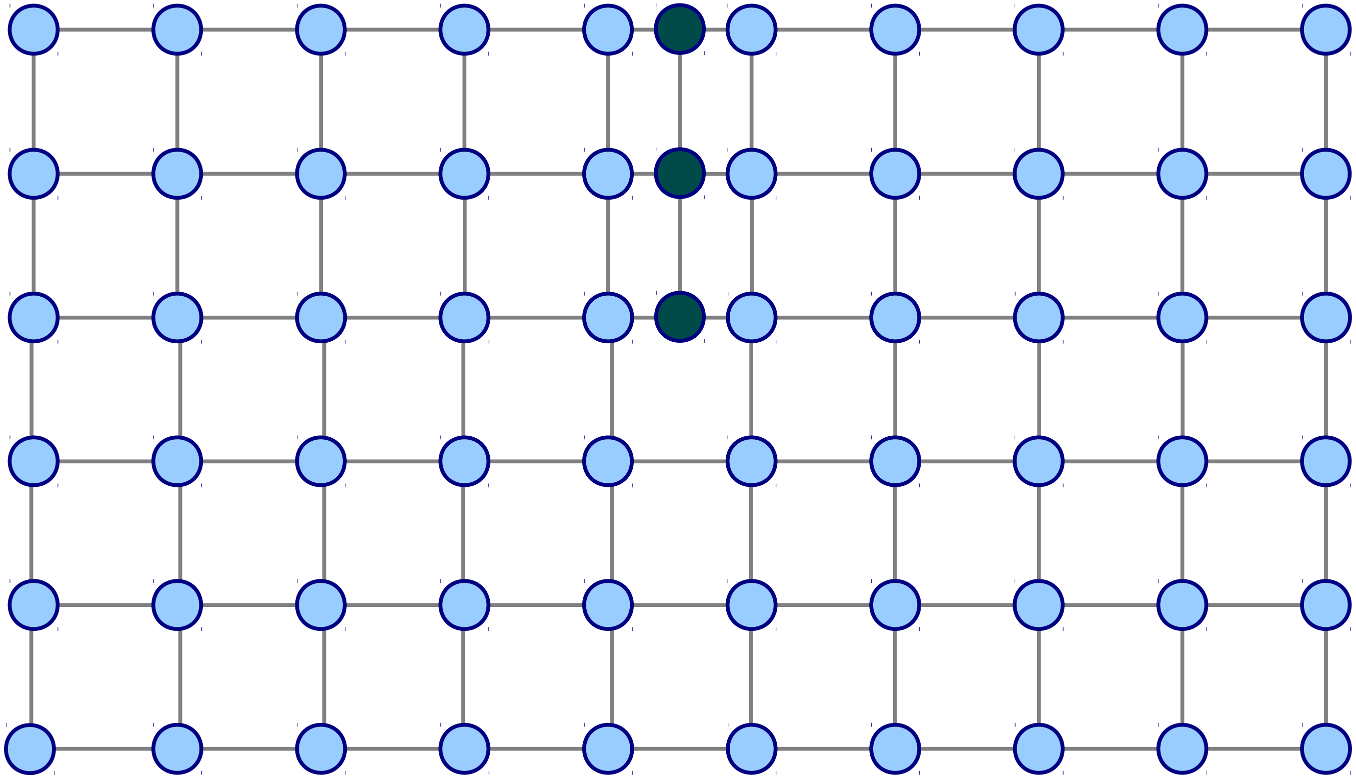
Solution hardening



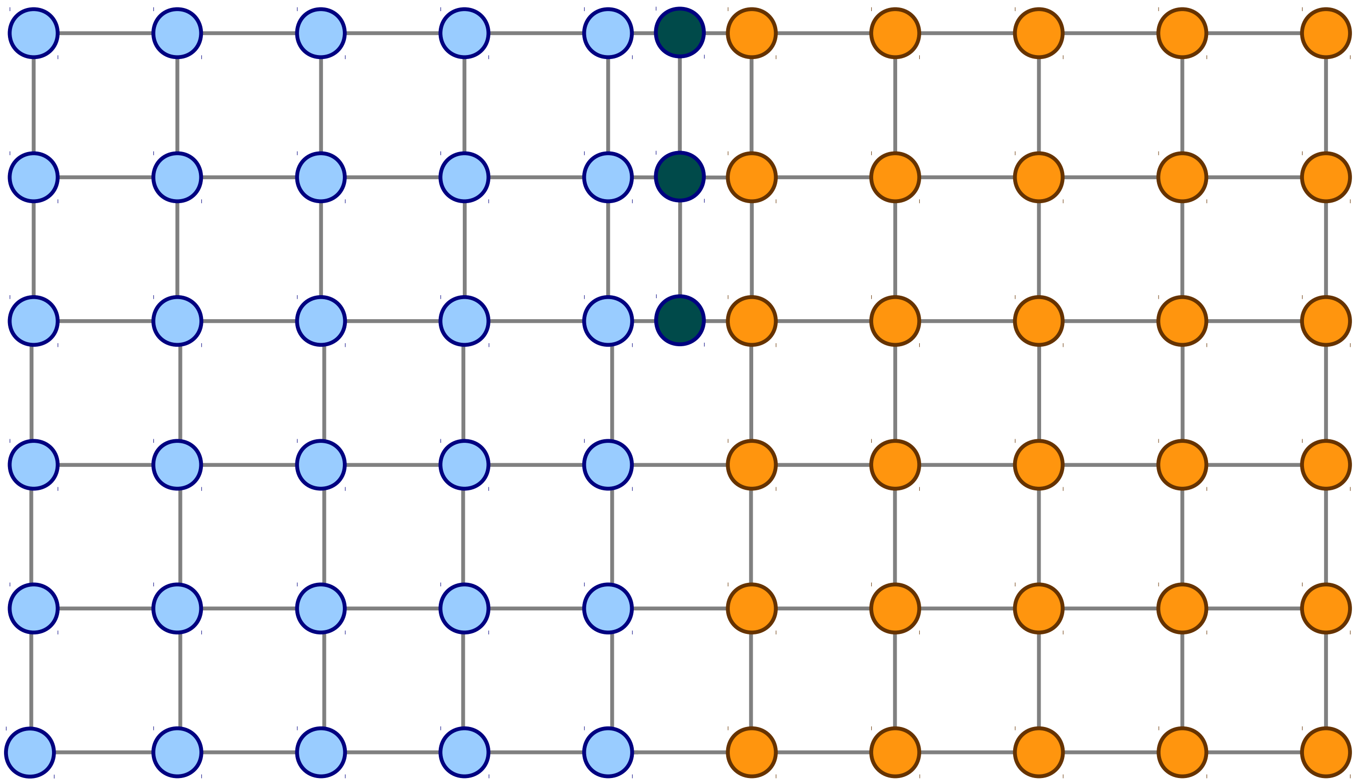
Solution hardening



Precipitate hardening

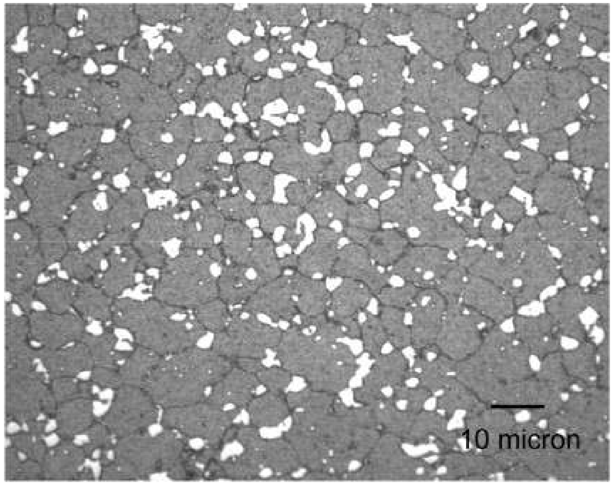


Precipitate hardening

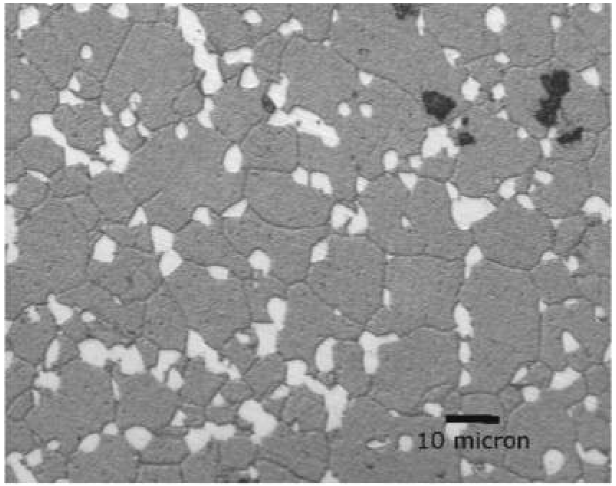


Contemporary alloys

RR1000



N18



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RR1000	Rolls Royce	52.4	15	18.5	5	3.6	3	2	0.5	0.03		
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Rene 88	General Elec.	56.5	16	13	4	3.7	2.1			0.03	4	0.7
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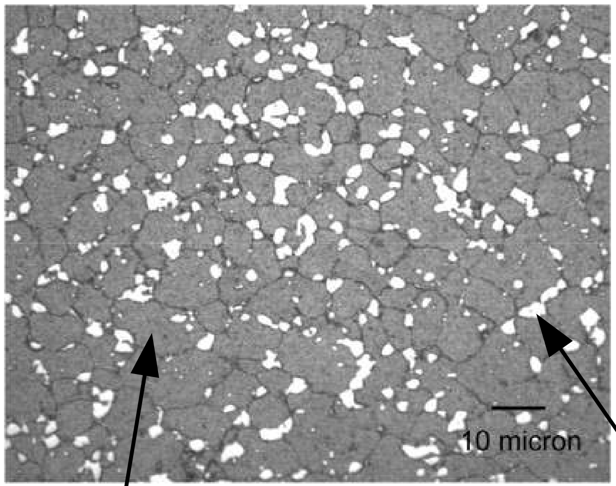
Contemporary alloys

RR1000



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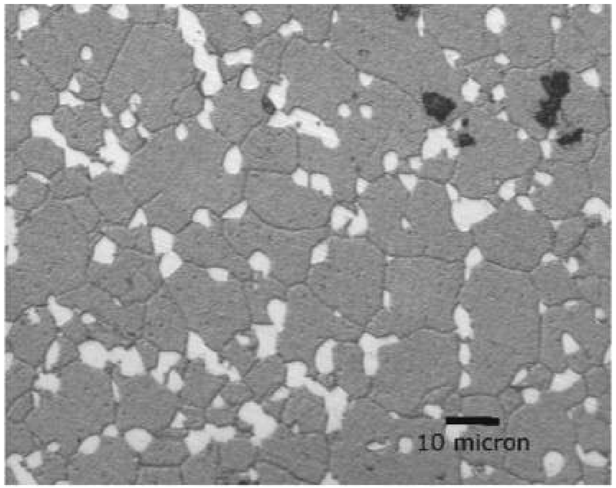
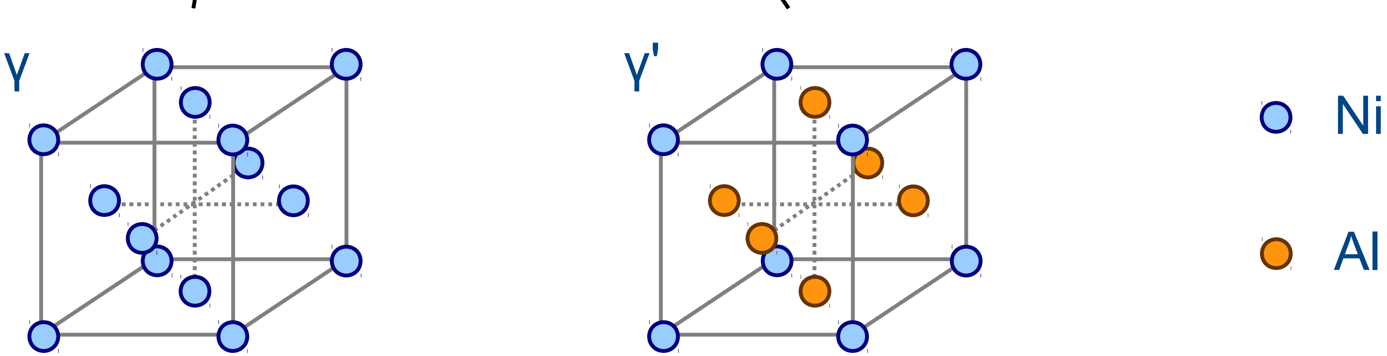
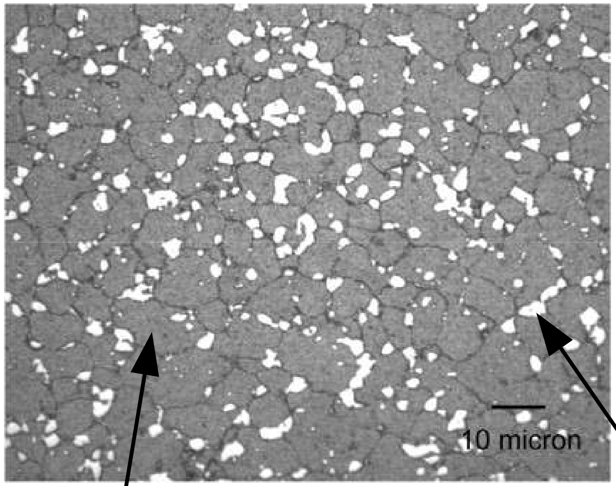


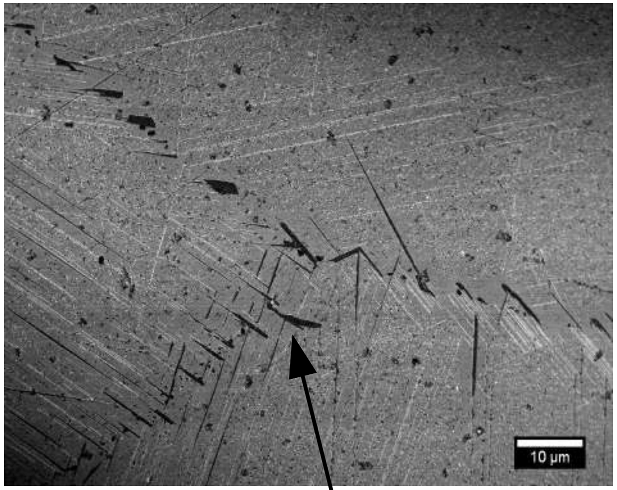


High entropy alloy

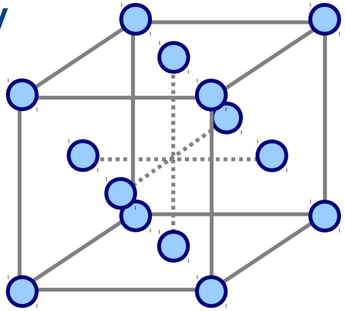
RR1000



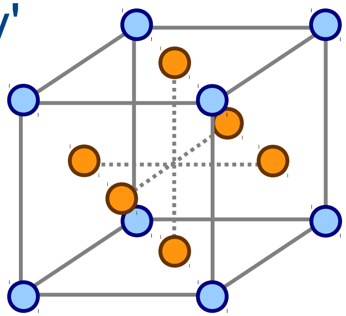
Attempted alloy



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 $Jmol^{-1}K^{-1}$

Properties

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

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

Properties

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

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}

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

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

Collect data for yield stress from 2248 alloys

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

Calculate uncertainty in neural network model

Properties

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

Collect data for yield stress from 2248 alloys

↓

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

Properties

Cost $\$lb^{-1}$
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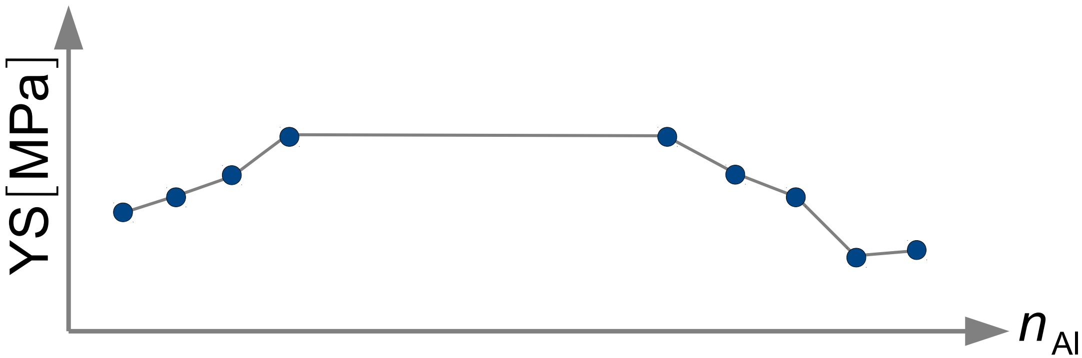

Properties

Cost $lb^{-1}
γ' fraction
Stability
Density gcm^{-3}
Yield stress MPa
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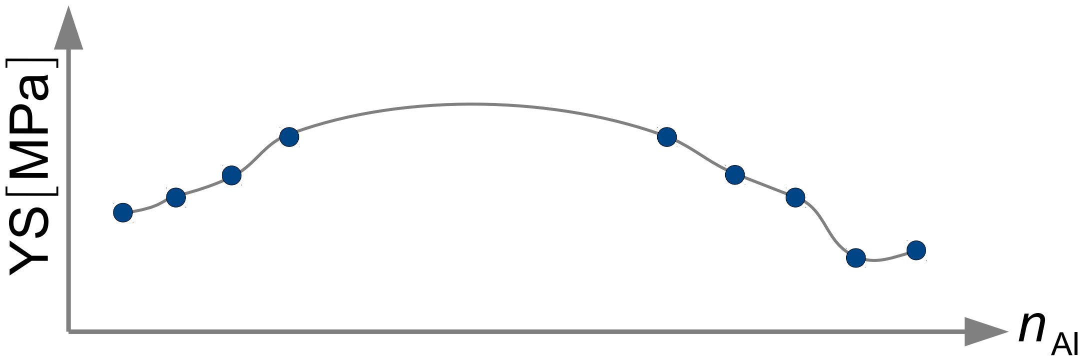

Properties

Cost $lb^{-1}
γ' fraction
Stability
Density gcm^{-3}
Yield stress MPa
UTS MPa
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Stress rupture MPa
Resistivity μΩcm
Entropy Jmol^{-1}K^{-1}

Collect data for yield stress from 2248 alloys

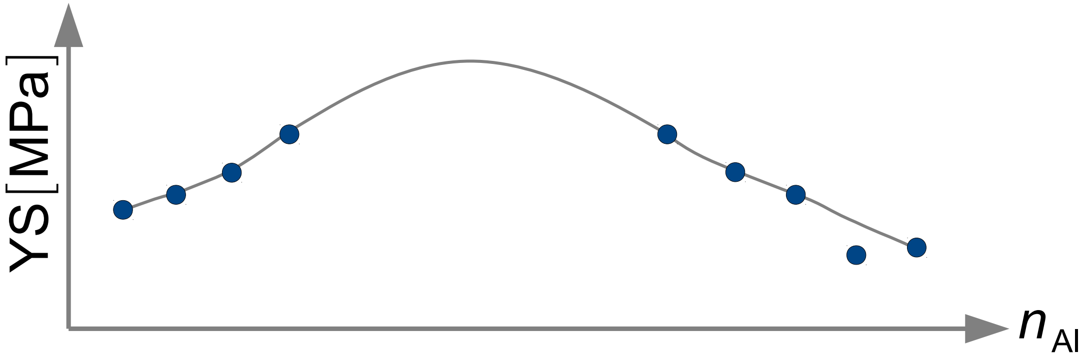
↓

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



Properties

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γ' fraction
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Density gcm^{-3}
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Collect data for yield stress from 2248 alloys

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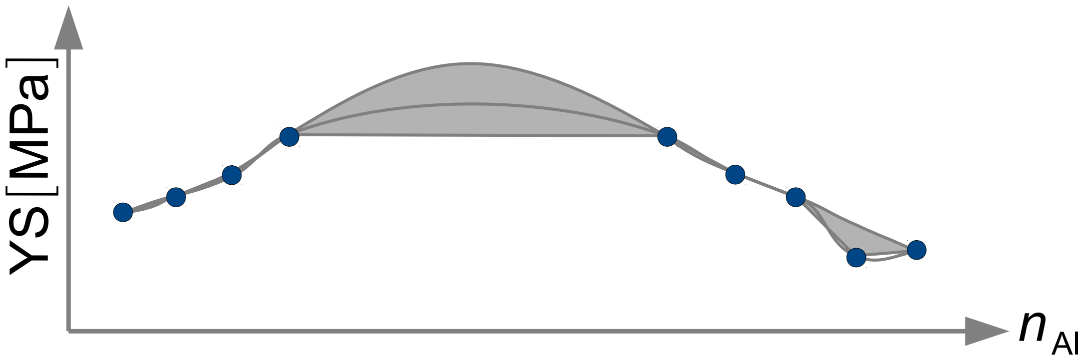
Generate neural network model

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

↓

Calculate uncertainty in neural network model



Properties

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

Calculate grid of

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

Properties

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

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 $Jmol^{-1}K^{-1}$

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 $Jmol^{-1}K^{-1}$

Calculate grid of

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

Generate neural network models

Calculate phase equilibrium and uncertainty

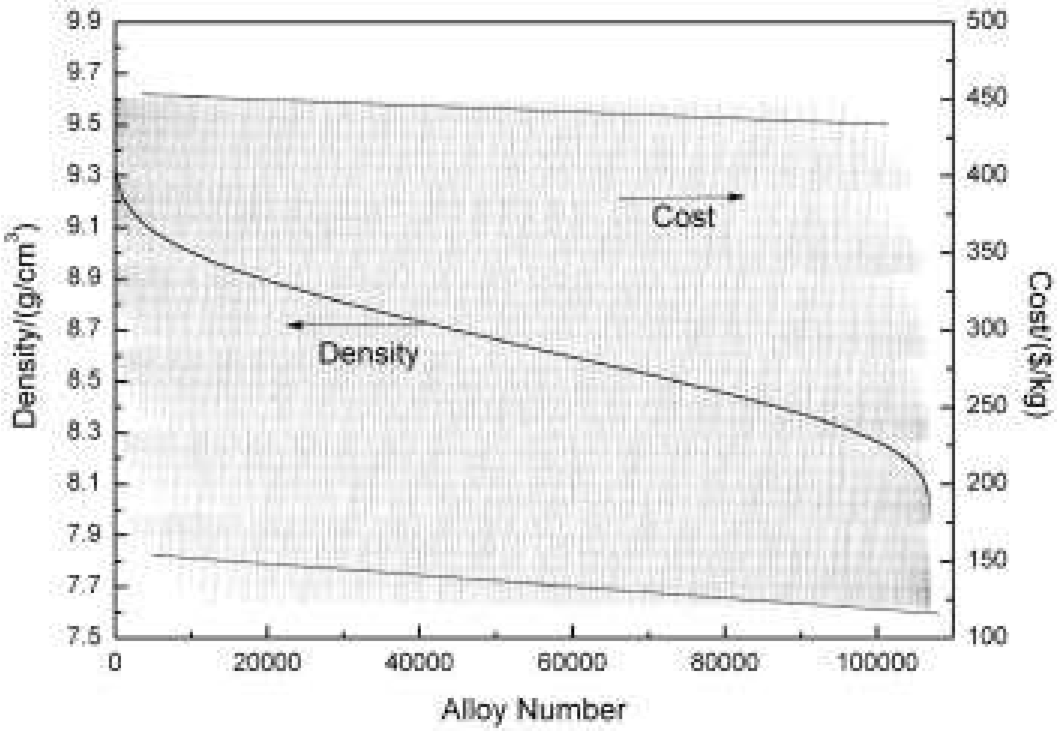
Large uncertainty

Merit factor

Cost $lb^{-1}	S_{cost}	$P_{cost}(\mathbf{C})$
γ' fraction	$S_{\gamma'}$	$P_{\gamma'}(\mathbf{C})$
Stability	S_{stable}	$P_{stable}(\mathbf{C})$
Density gcm^{-3}	$S_{density}$	$P_{density}(\mathbf{C})$
Yield stress MPa	S_{YS}	$P_{YS}(\mathbf{C})$
UTS MPa	S_{UTS}	$P_{UTS}(\mathbf{C})$
Oxidation index	$S_{oxidize}$	$P_{oxidize}(\mathbf{C})$
Stress rupture MPa	S_{SR}	$P_{SR}(\mathbf{C})$
Resistivity μΩcm	S_{resis}	$P_{resis}(\mathbf{C})$
Entropy Jmol^{-1}K^{-1}	$S_{entropy}$	$P_{entropy}(\mathbf{C})$

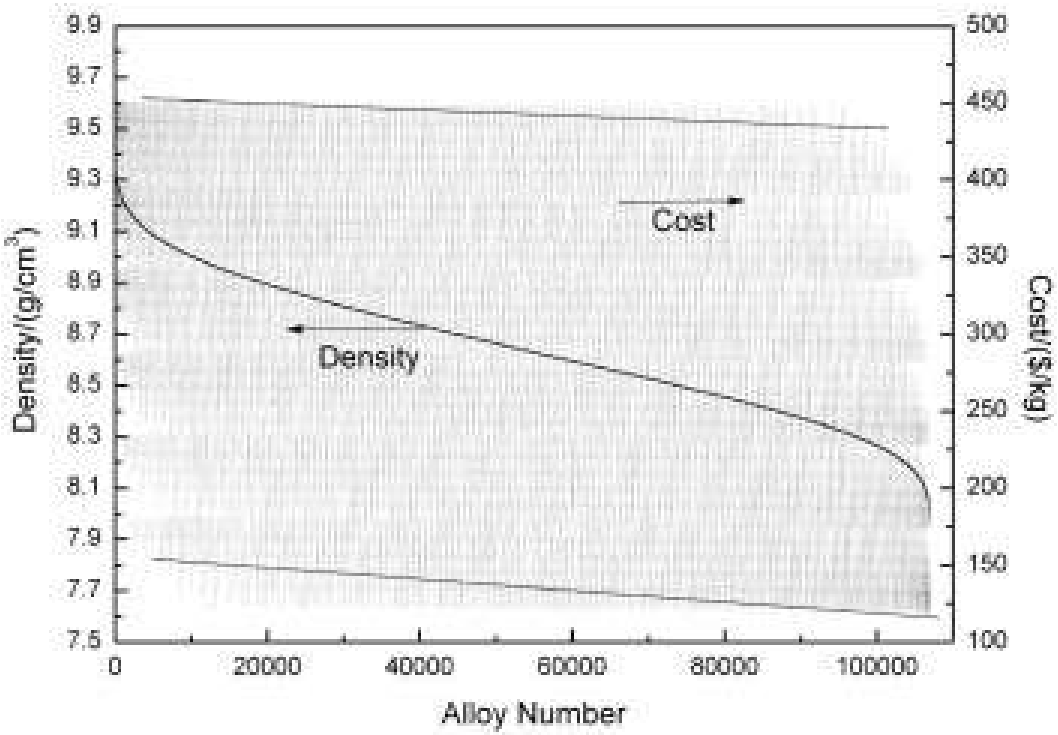
→ $P_{spec}(\mathbf{C})$

Optimization – tradeoff diagrams



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

Optimization – tradeoff diagrams

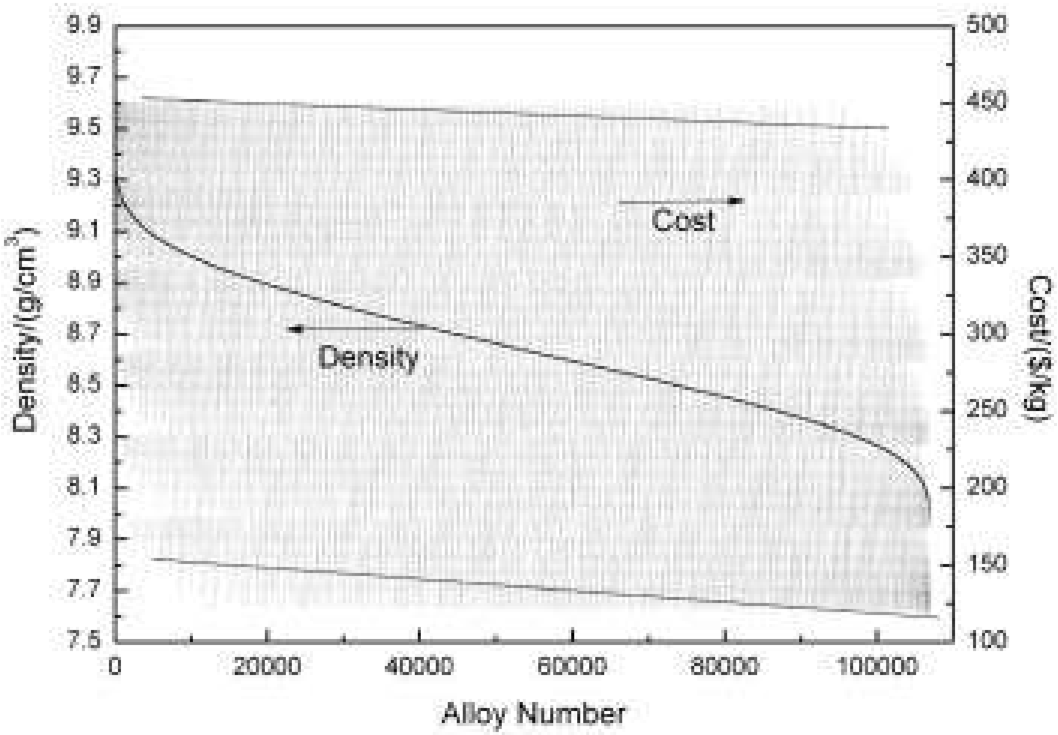


Probability of success

$0.5^5 \sim 0.03$

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

Optimization – tradeoff diagrams



Probability of success

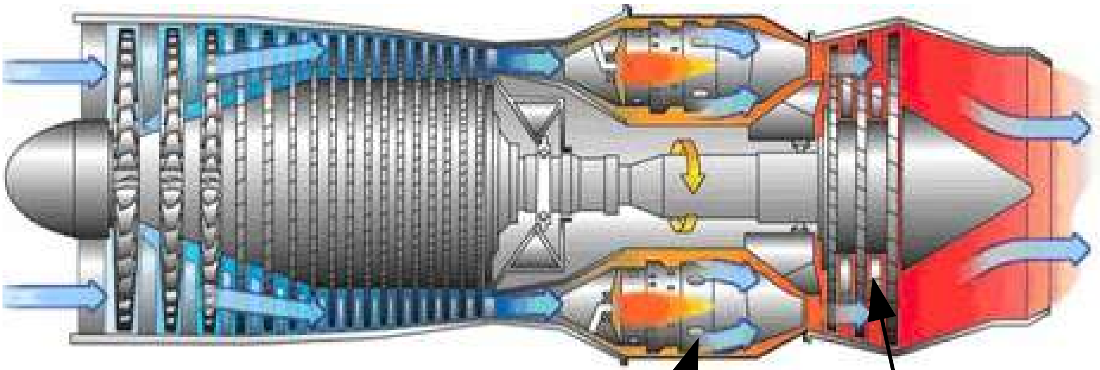
$0.5^5 \sim 0.03$

Composition resolution

$100000^{1/6} \sim 7$

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

Predicted alloys

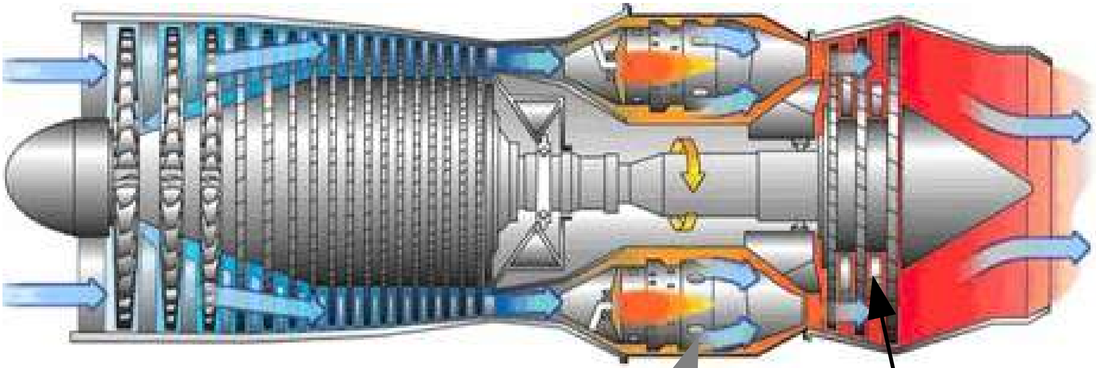


Combustor liner

2x disc alloy

2x forging hammer

Predicted alloys



Combustor liner

2x disc alloy

2x forging hammer

Case study: RR1000

At 725ºC	RR1000
Cost $\$lb^{-1}$	13.46 ± 0.01
γ' fraction	42.2 ± 0.9
Stability	89.1 ± 1.6
Density gcm^{-3}	8.32 ± 0.01
Yield stress MPa	753.4 ± 30.7
UTS MPa	1054.5 ± 24.1
Oxidation index	16.50 ± 0.01
Stress rupture MPa	599.4 ± 18.8
Resistivity μΩcm	9.02 ± 0.01
Entropy $Jmol^{-1}K^{-1}$	11.60 ± 0.01

	Ni	Cr	Co	Mo	Ti	Al	Ta	Hf	C	W	Mn	B	Ta	Si	Zr	Nb	Fe	T	t
RR1000	52	15	19	5	3.6	3	2	0.5	0.1									800	8

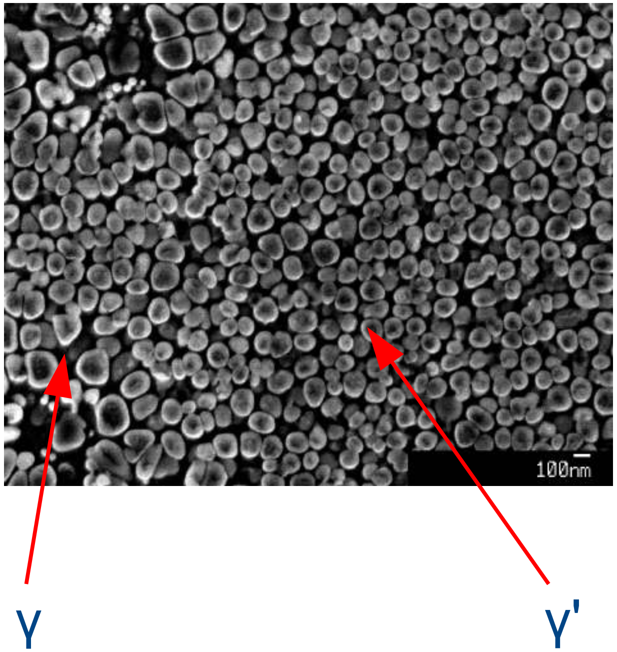
Case study: improved

At 725ºC	RR1000	Optimal
Cost $\$lb^{-1}$	13.46 ± 0.01	11.67 ± 0.01
γ' fraction	42.2 ± 0.9	39.7 ± 3.1
Stability	89.1 ± 1.6	93.0 ± 0.7
Density gcm^{-3}	8.32 ± 0.01	8.26 ± 0.01
Yield stress MPa	753.4 ± 30.7	1048.8 ± 50.9
UTS MPa	1054.5 ± 24.1	1436.9 ± 46.9
Oxidation index	16.50 ± 0.01	19.2 ± 0.01
Stress rupture MPa	599.4 ± 18.8	1137.5 ± 208.3
Resistivity μΩcm	9.02 ± 0.01	8.93 ± 0.01
Entropy $Jmol^{-1}K^{-1}$	11.60 ± 0.01	14.50 ± 0.01

	Ni	Cr	Co	Mo	Ti	Al	Ta	Hf	C	W	Mn	B	Ta	Si	Zr	Nb	Fe	T	t
RR1000	52	15	19	5	3.6	3	2	0.5	0.1									800	8
Optimal	56	17	1.0	4.0	1.5	4.3	0.2	0.1	0.2	6.0	0.1	0.1	0.2	0.1	0.2	5.6	3.4	980	61

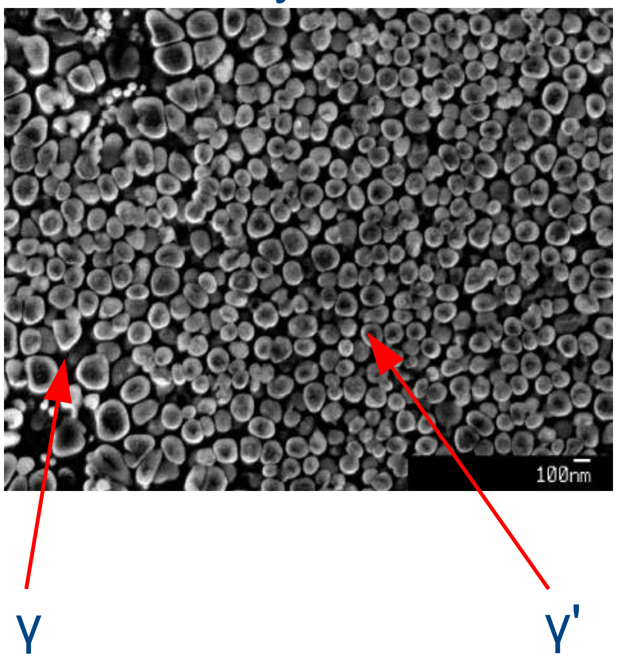
Optical micrograph – Ni disc alloy

Ni disc alloy

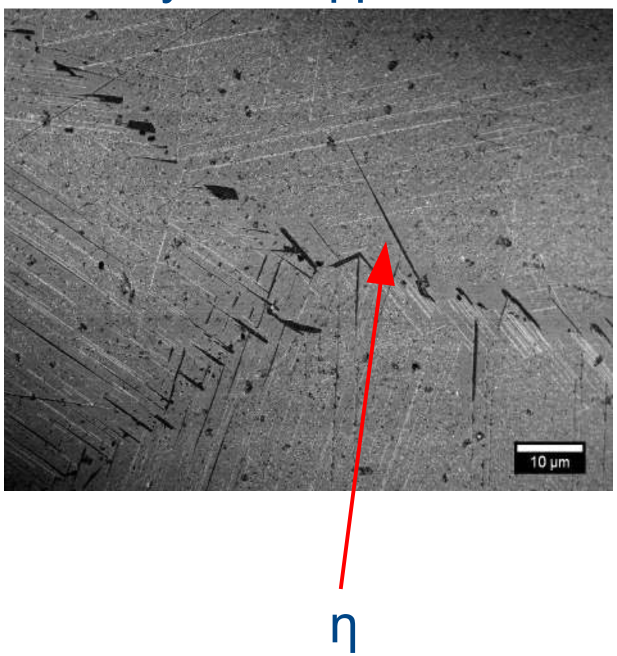


Optical micrograph – Ni disc alloy

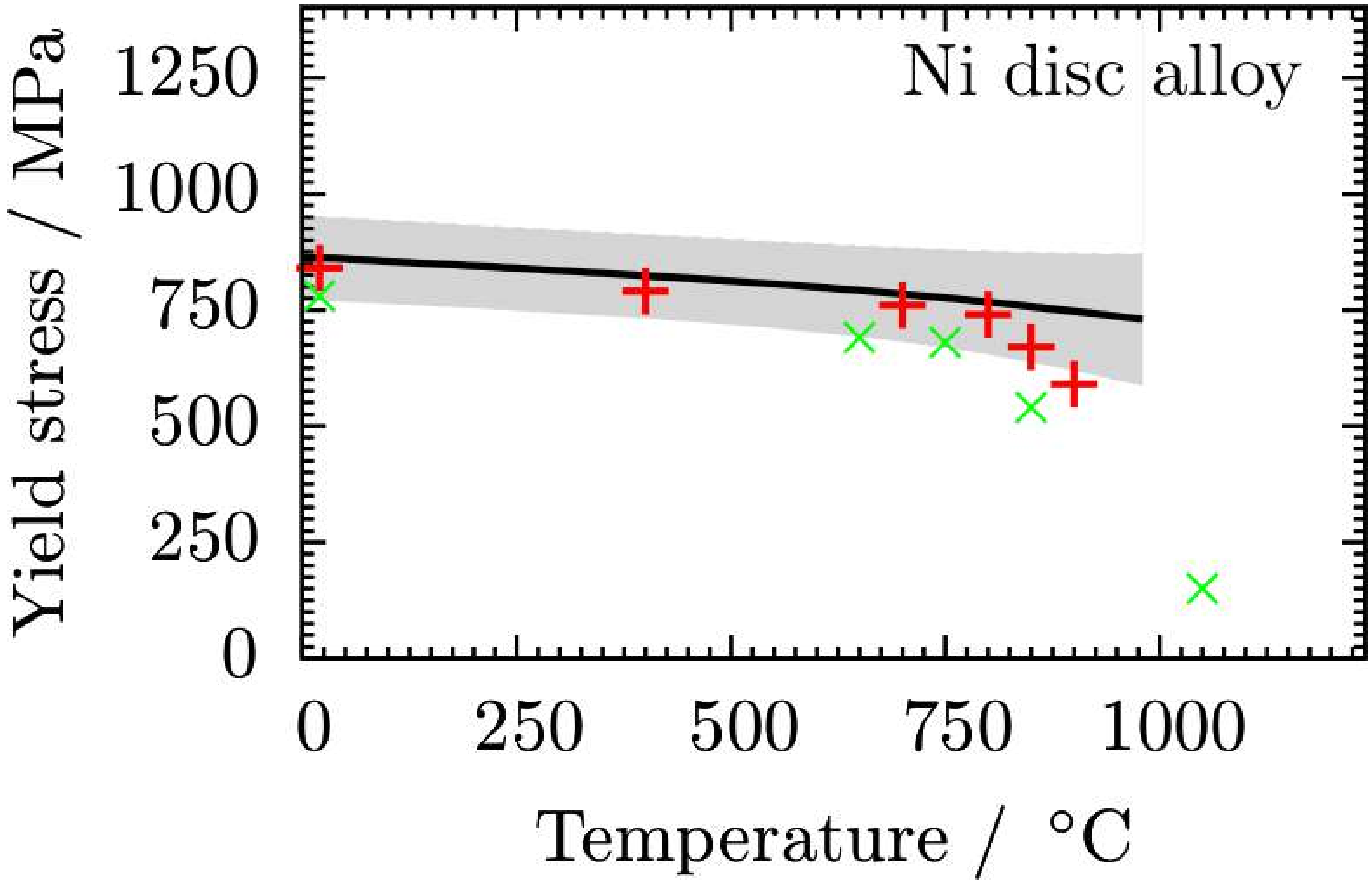
Ni disc alloy



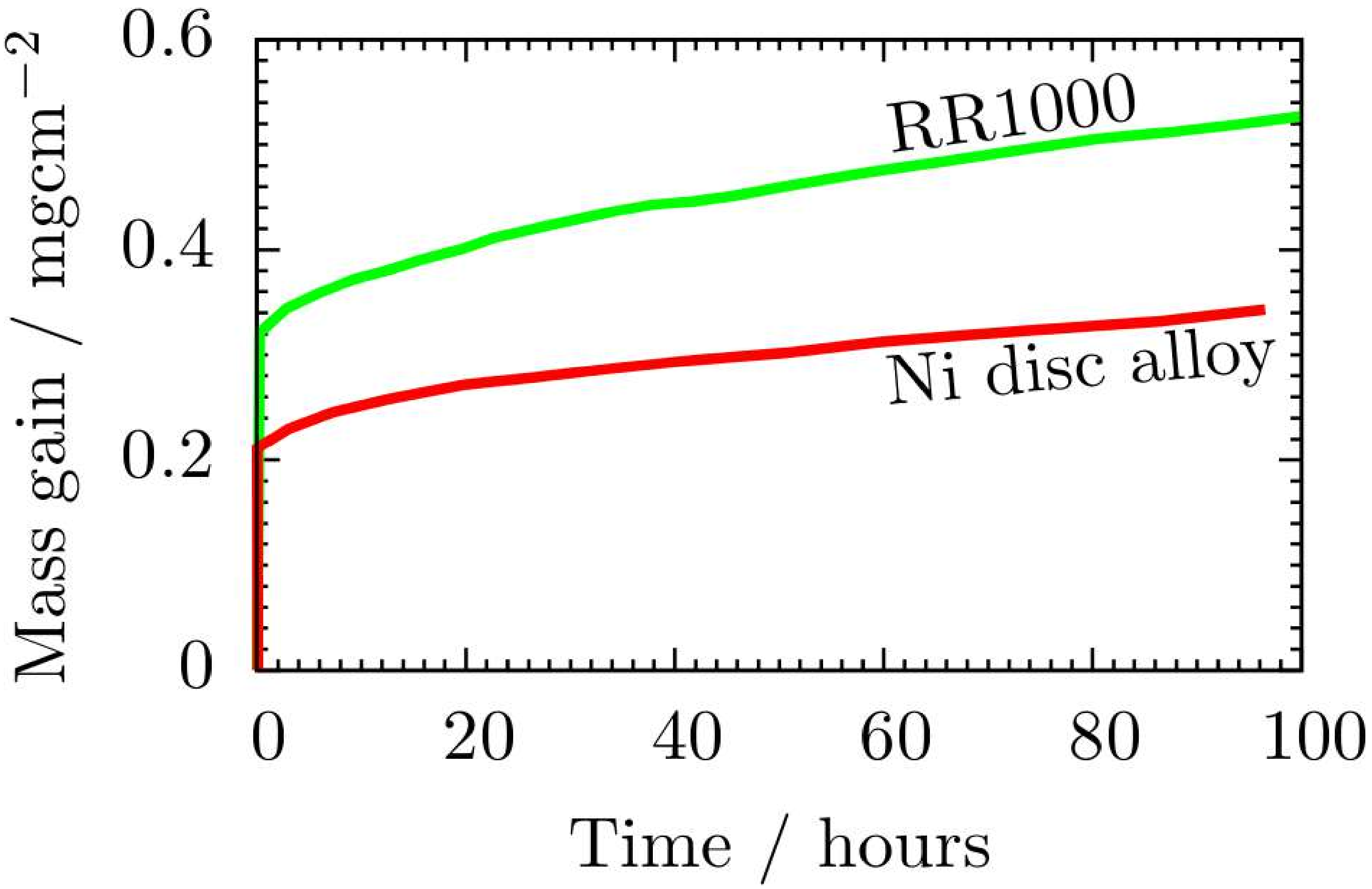
Ni alloy with η phase



Yield stress

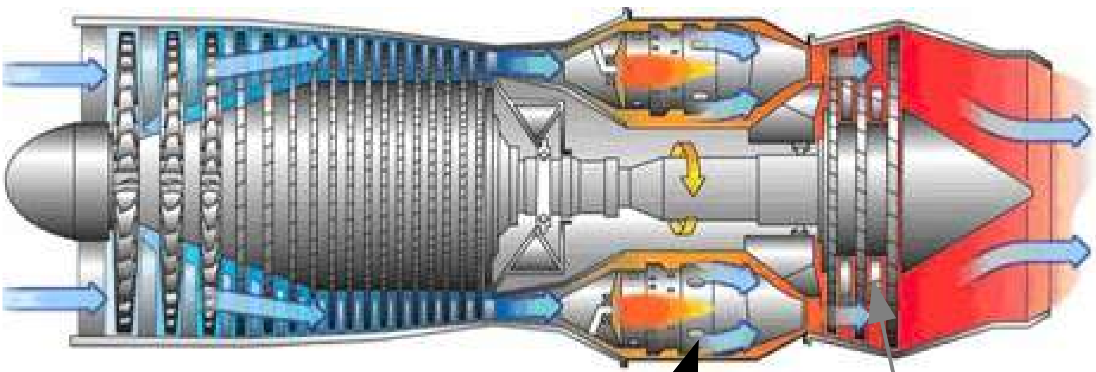


Oxidation



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

Predicted alloys



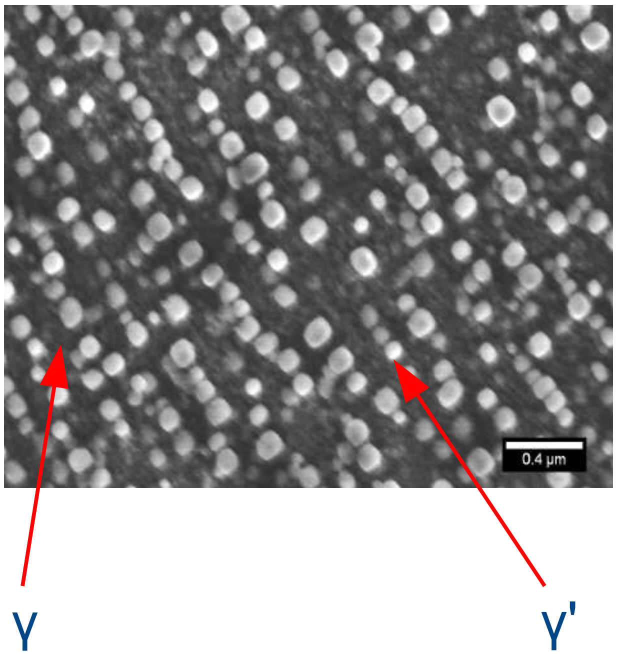
Combustor liner

2x disc alloy

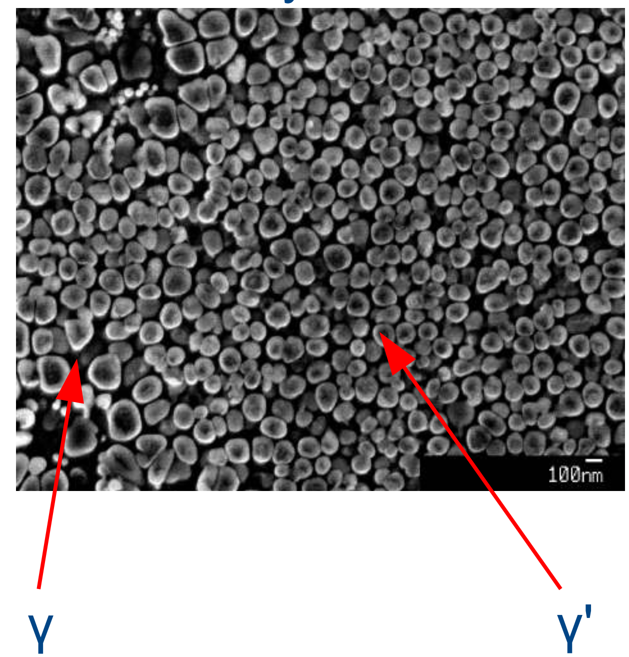
2x forging hammer

Optical micrograph – Ni combustor liner

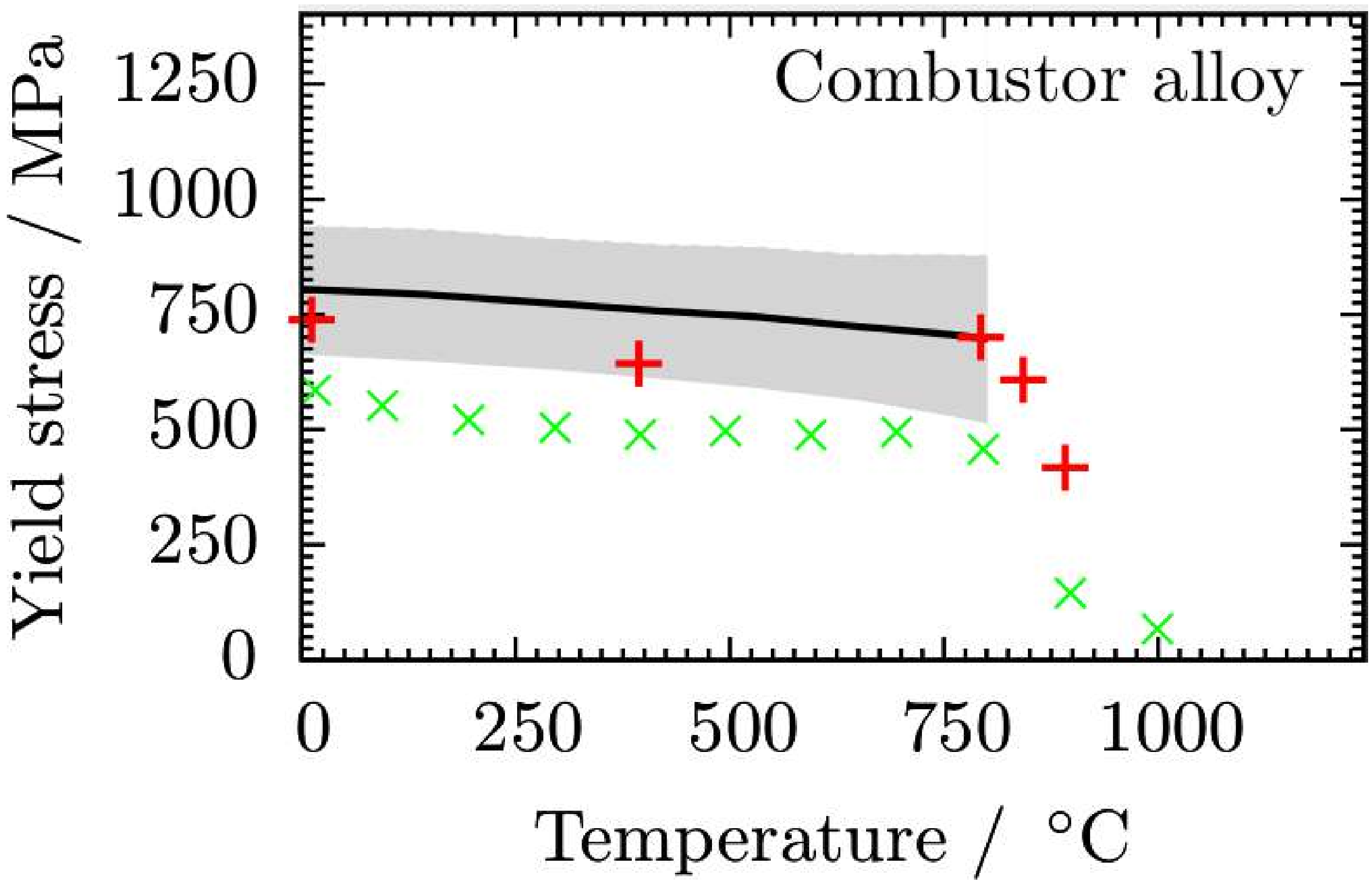
Ni combustor liner



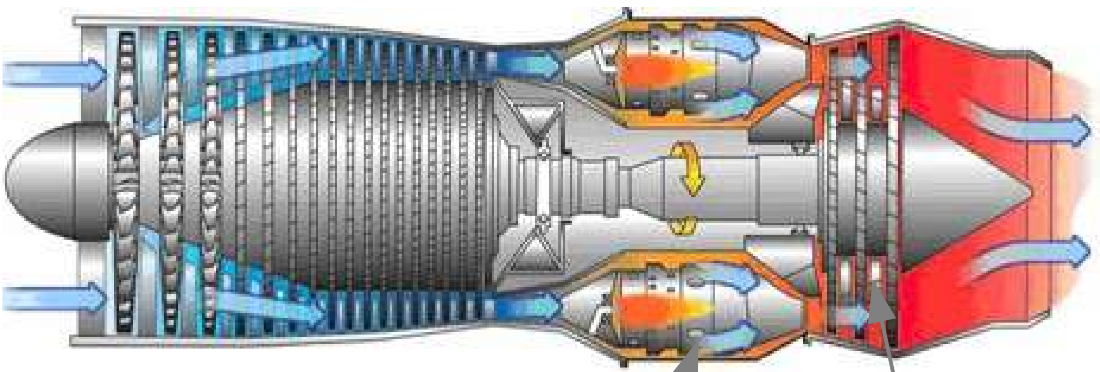
Ni disc alloy



Yield stress



Predicted alloys



Combustor liner

2x disc alloy

2x forging hammer

Case study: TZM

At 1000ºC	TZM
Cost $lb^{-1}	13.46 ± 0.01
UTS MPa	1054.5 ± 24.1

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

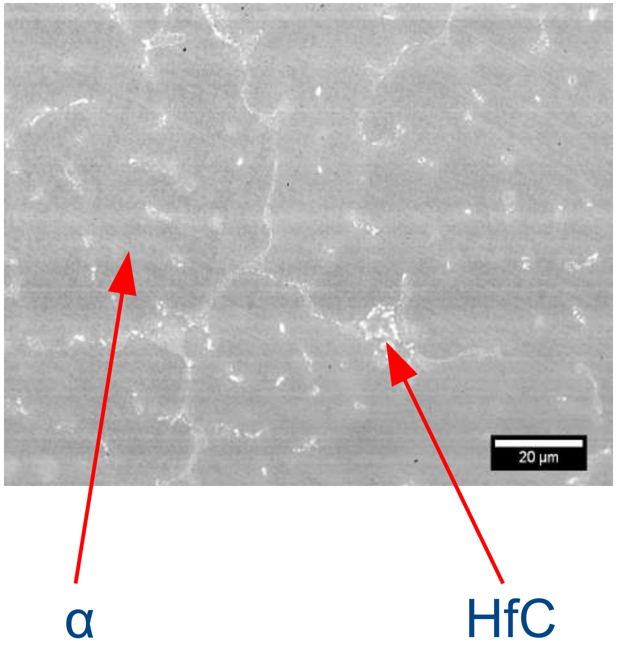
Case study: improved

At 1000ºC	TZM	Optimal
Cost $lb^{-1}	13.46 ± 0.01	11.67 ± 0.01
UTS MPa	42.2 ± 0.9	39.7 ± 3.1

	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

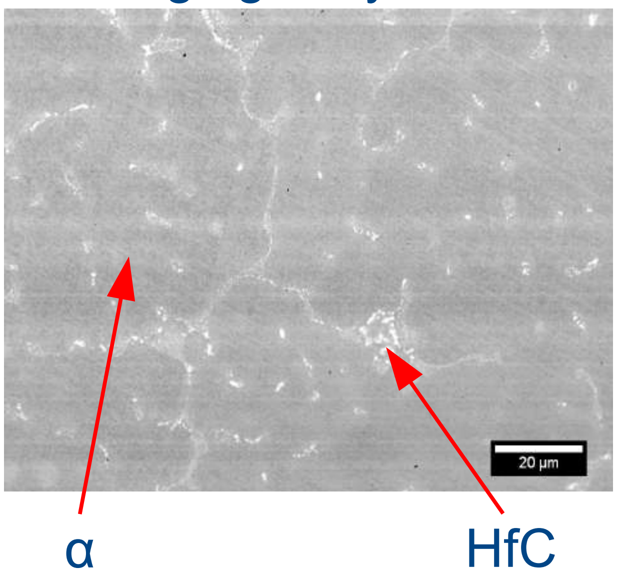
Optical micrograph – Mo forging alloy

Mo forging alloy

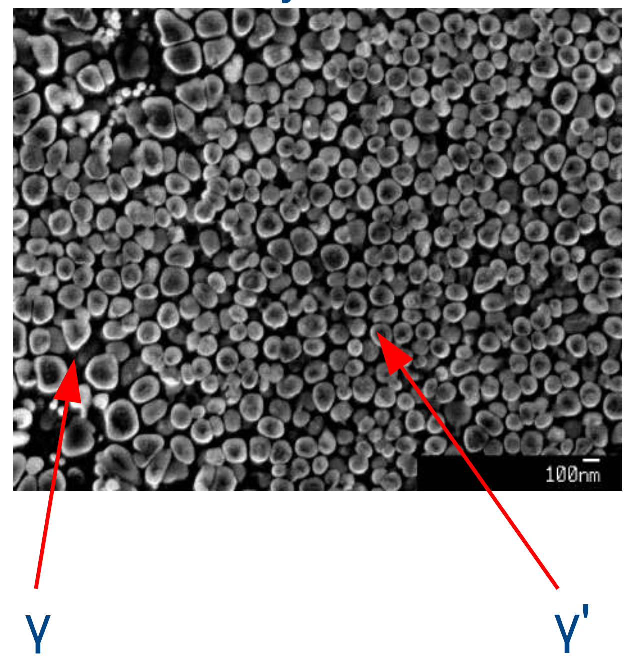


Optical micrograph – Mo forging alloy

Mo forging alloy

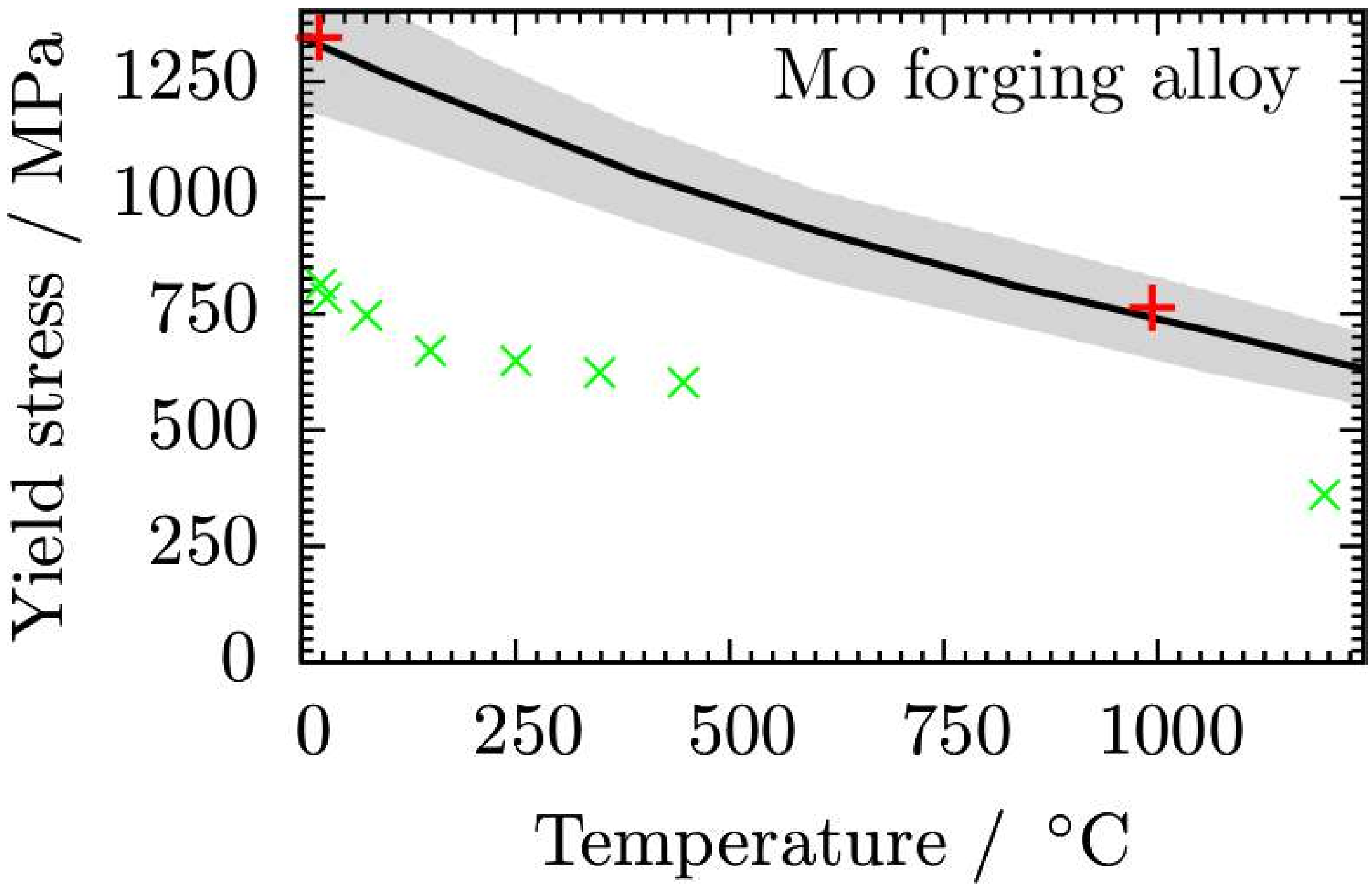


Ni disc alloy



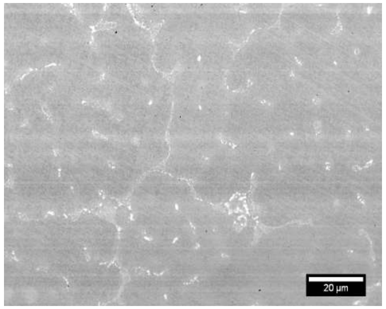
	Mo	Ti	C	Zr	Hf	W	Nb
TZM	99.4	0.5	0.02	0.08			
Optimal	82.7	1.0	0.2	0.9	9.0	0.5	5.7

Yield stress

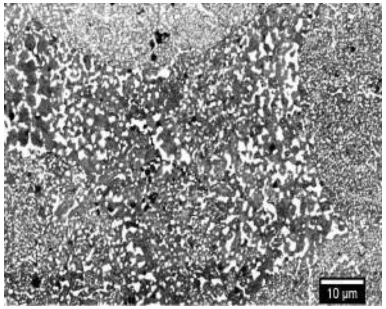


Alloys designed

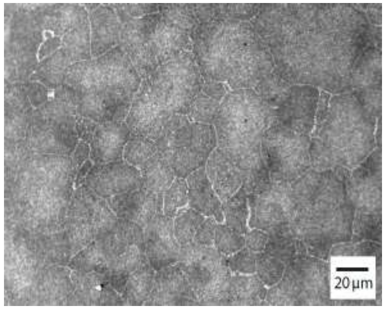
Mo-Hf forging alloy
Patent GB1307533.8 (2013)



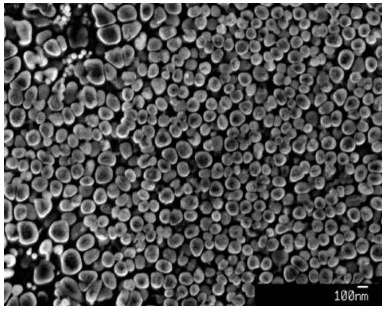
Mo-Nb forging alloy
Rolls-Royce invention
NC13024 (2013)



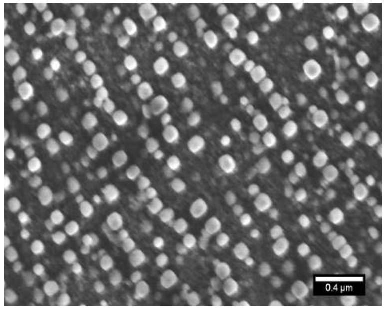
RR1000 grain growth
Acta Materialia, **61**,
3378 (2013)



Ni disc alloy
Rolls-Royce invention
NC12261 (2012)



Ni combustor liner
Rolls-Royce invention
NC13006 (2013)



High entropy alloy