Concurrent materials design

Gareth Conduit

TCM Group, Department of Physics

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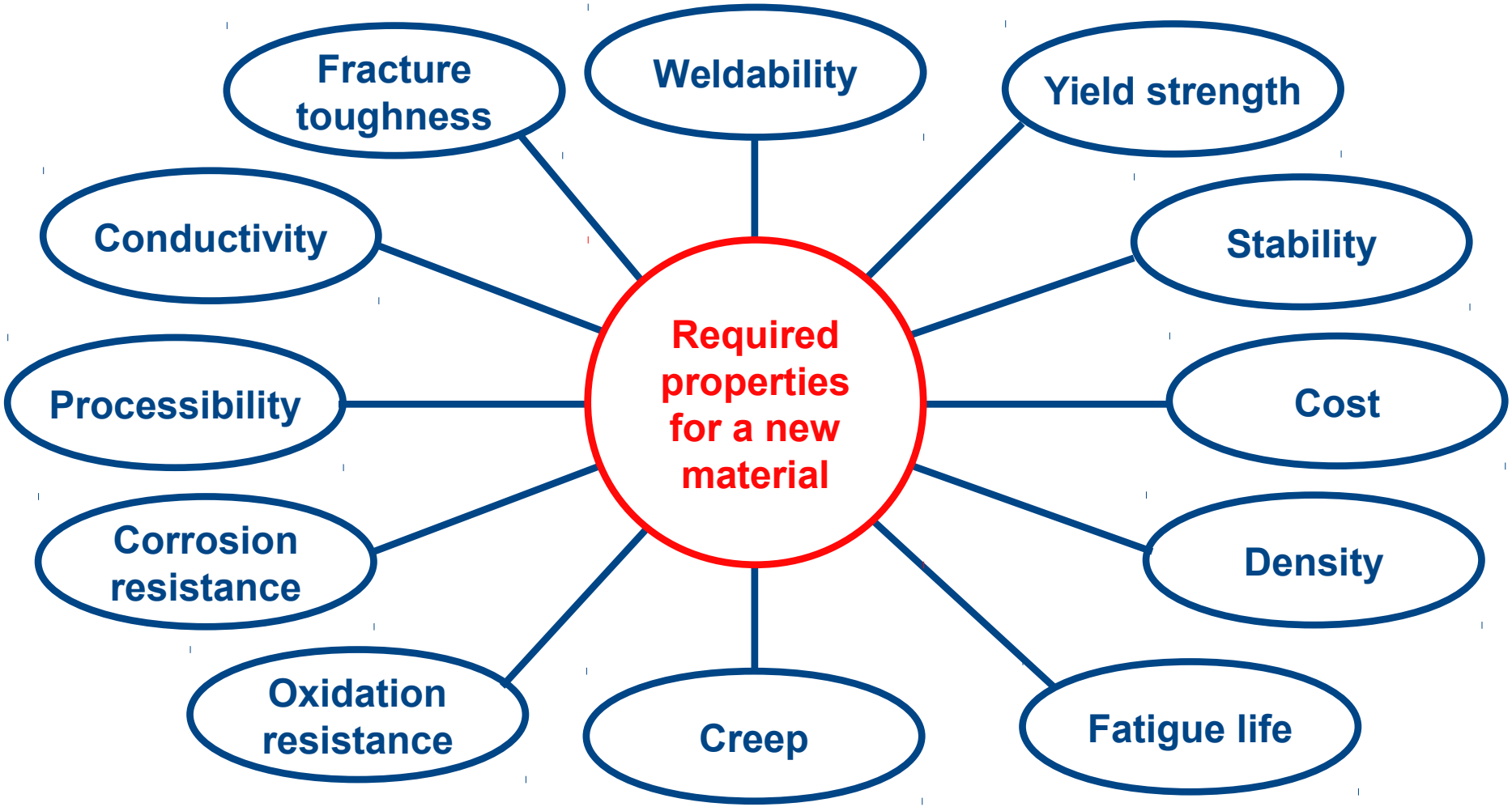
Designing a new material – what is required ?



Properties: Yield stress

Collect data for yield stress from 2248 alloys

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Generate neural network model

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

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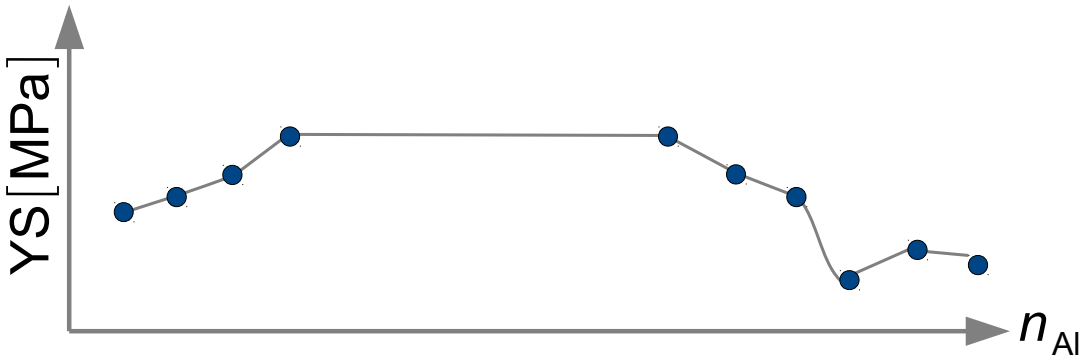

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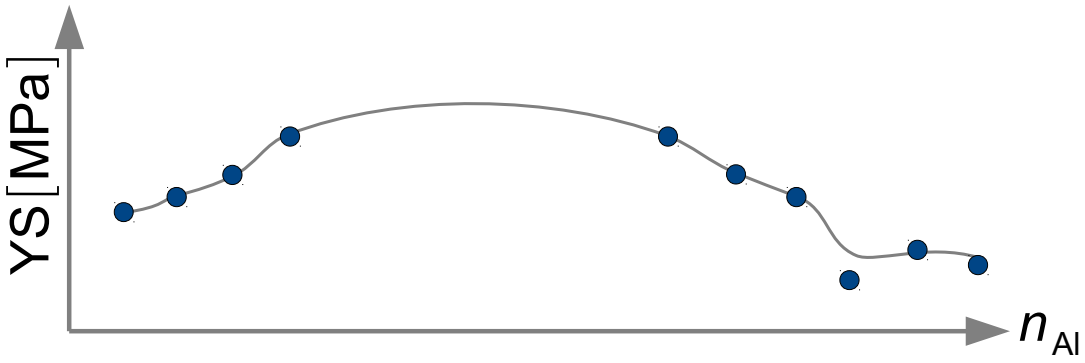

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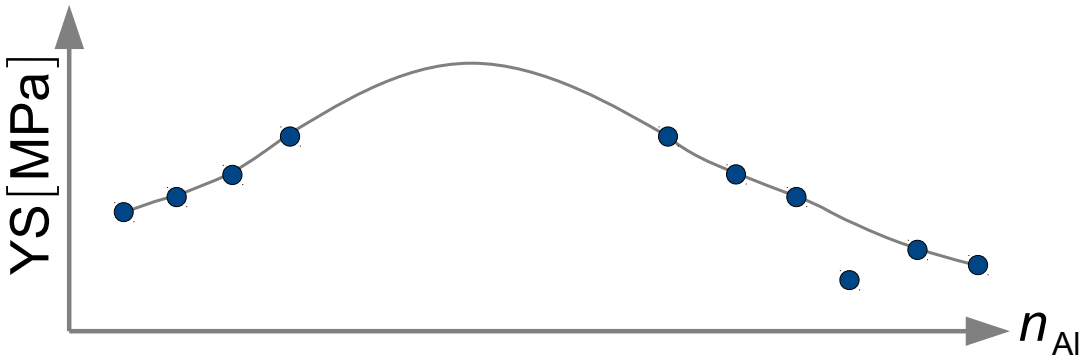

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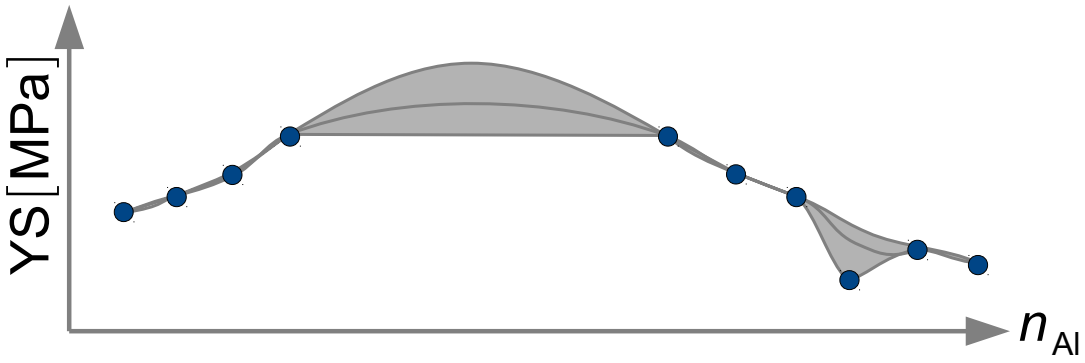
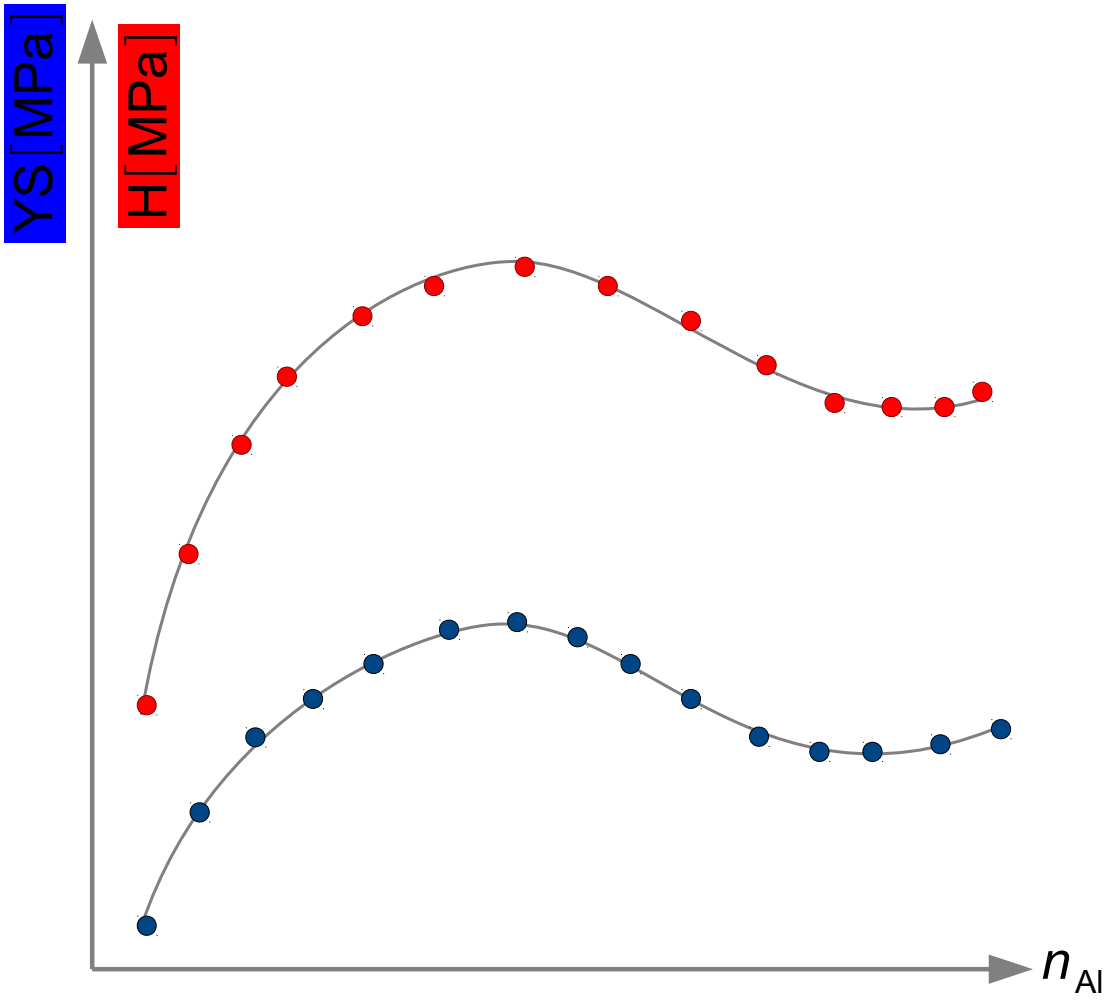


Properties: Yield stress and hardness



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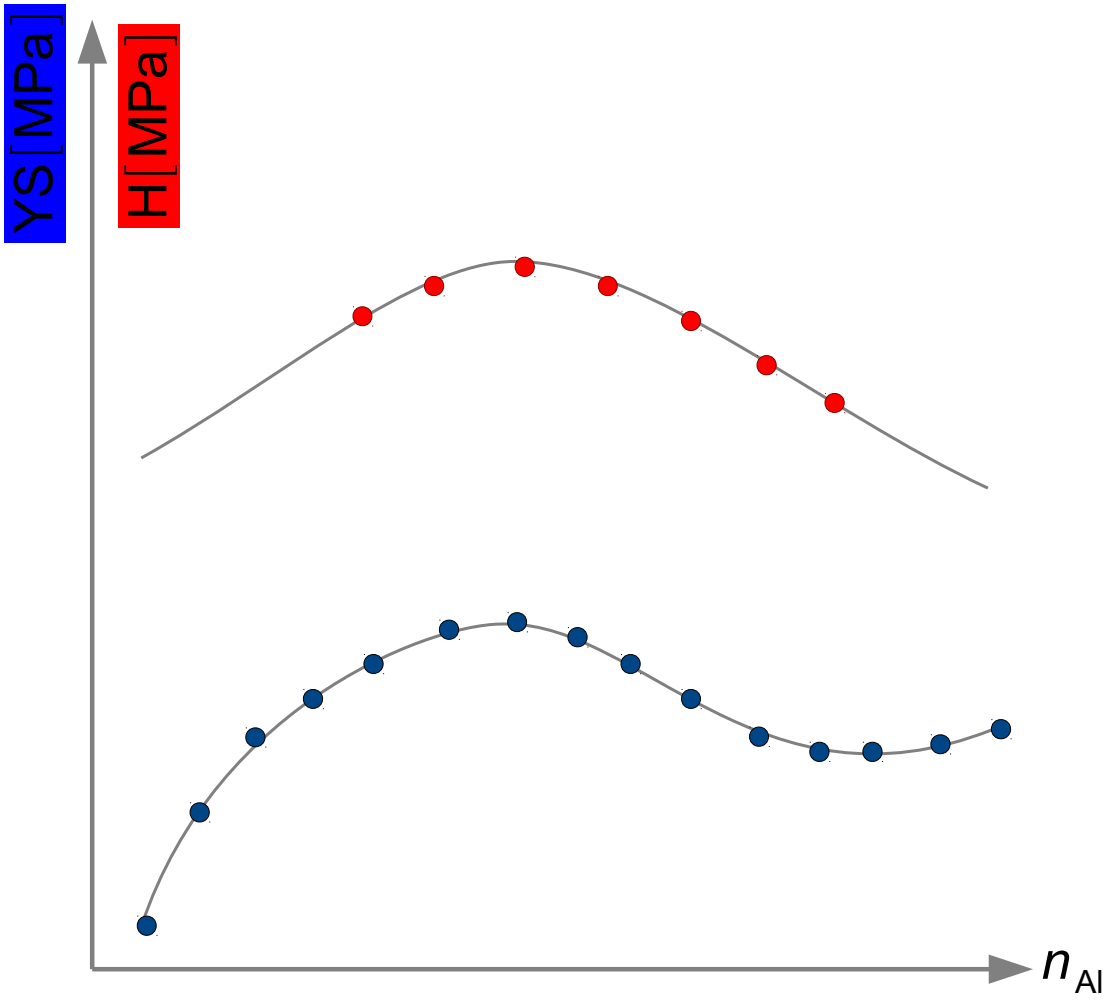

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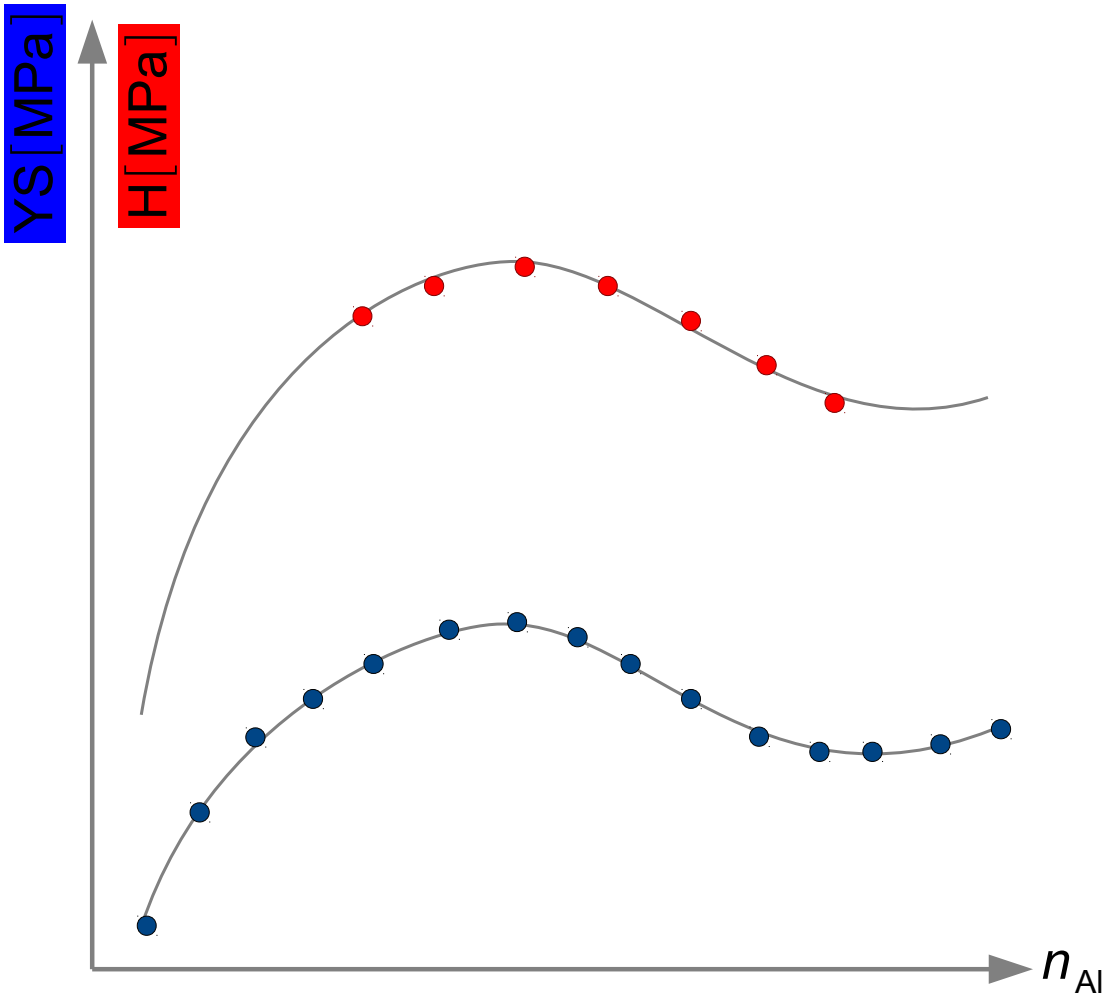
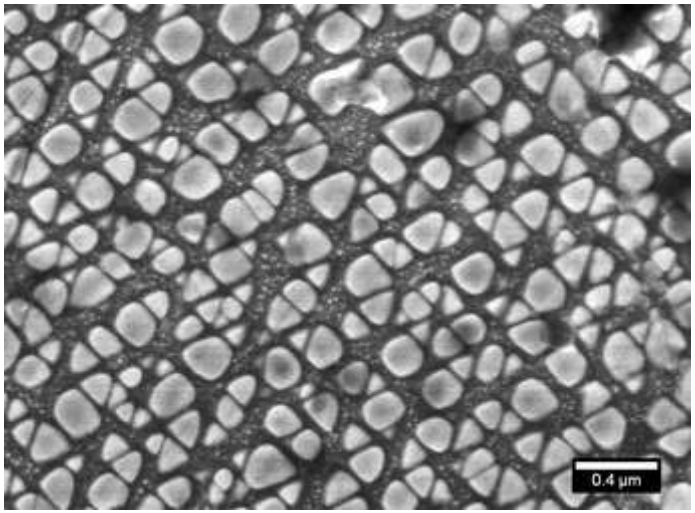


Phase equilibrium



Properties: γ' fraction

Calculate grid of

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

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Generate neural network model and uncertainty

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Calculate phase equilibrium and uncertainty

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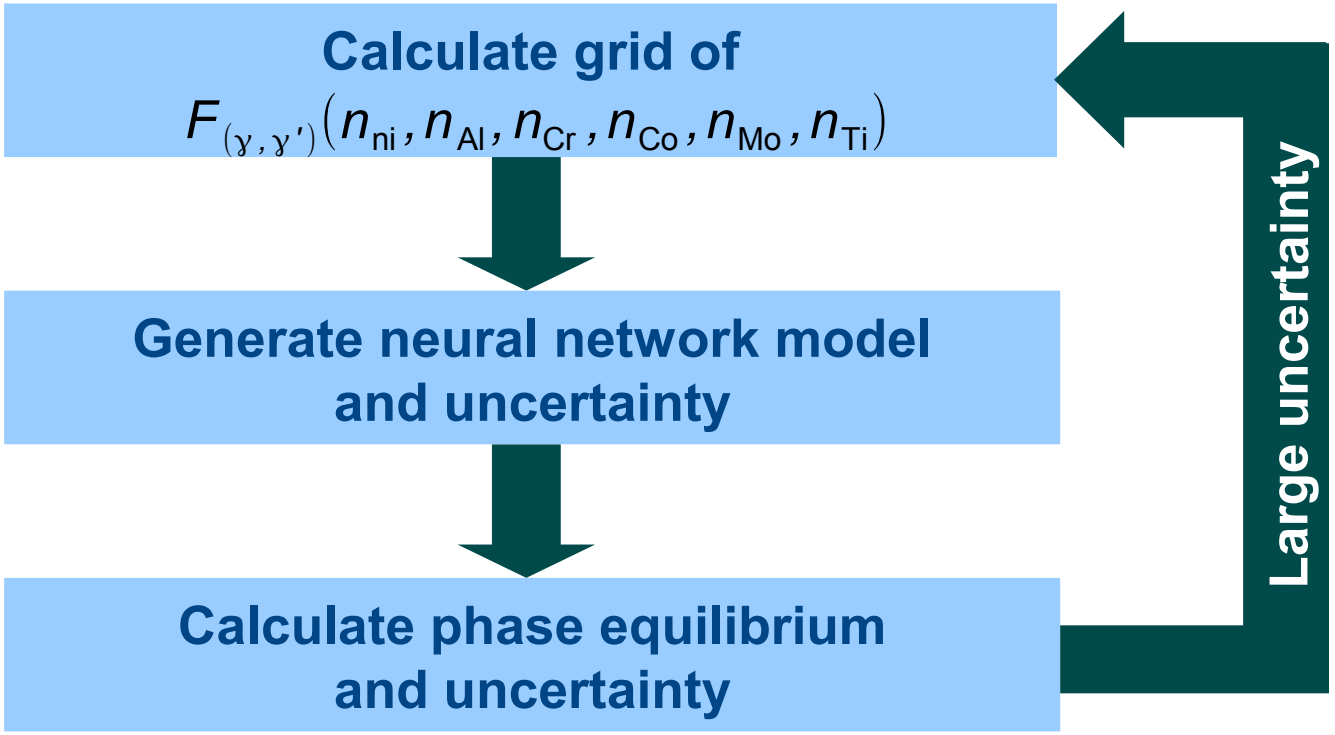

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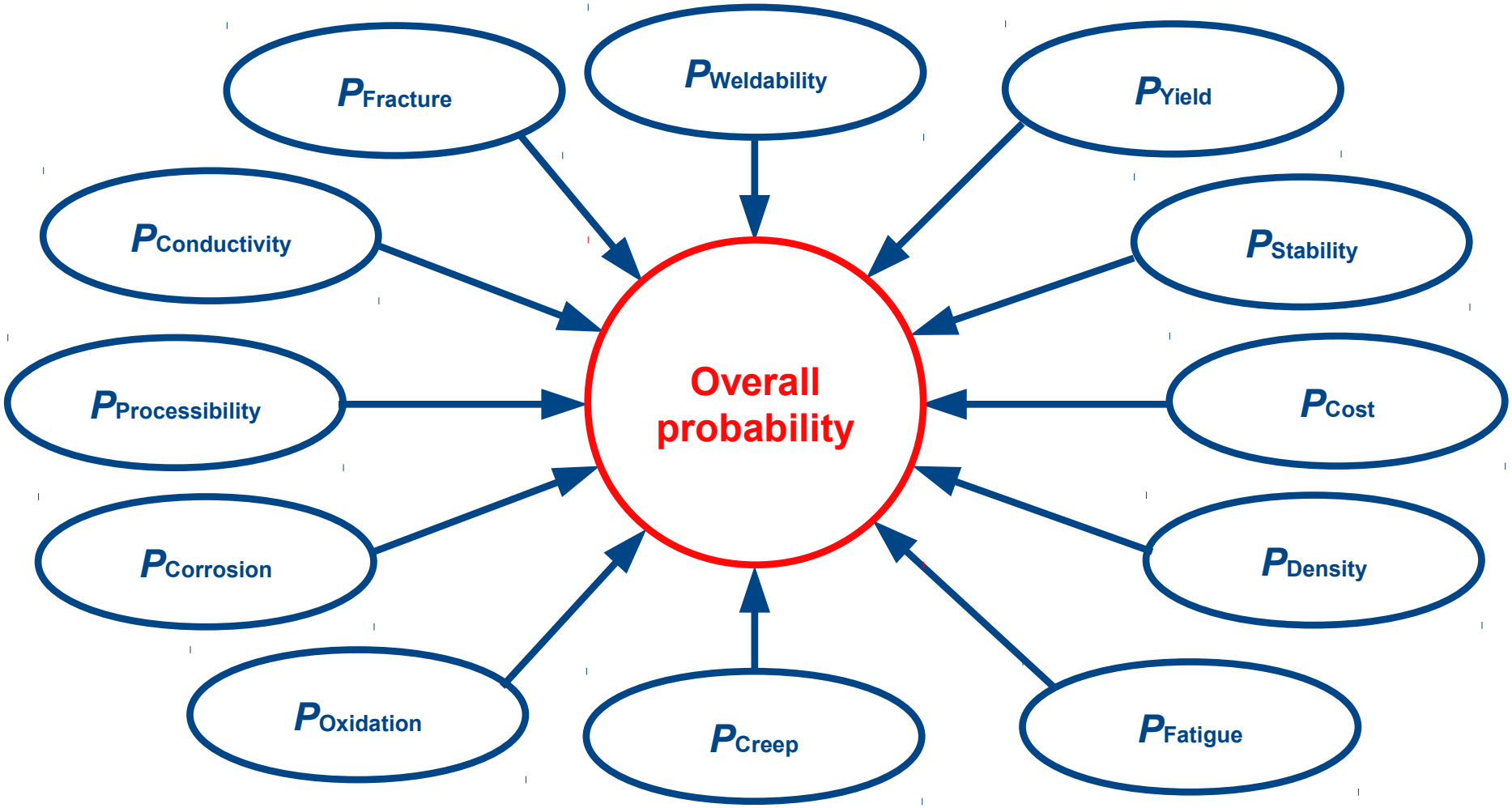

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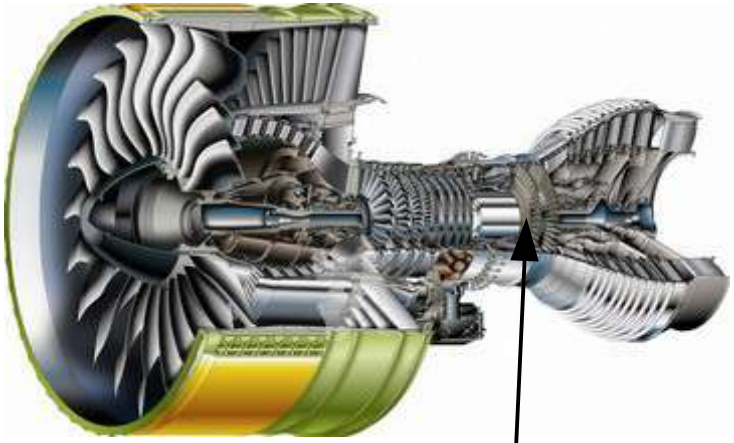


Disc
alloy

Case study: RR1000











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

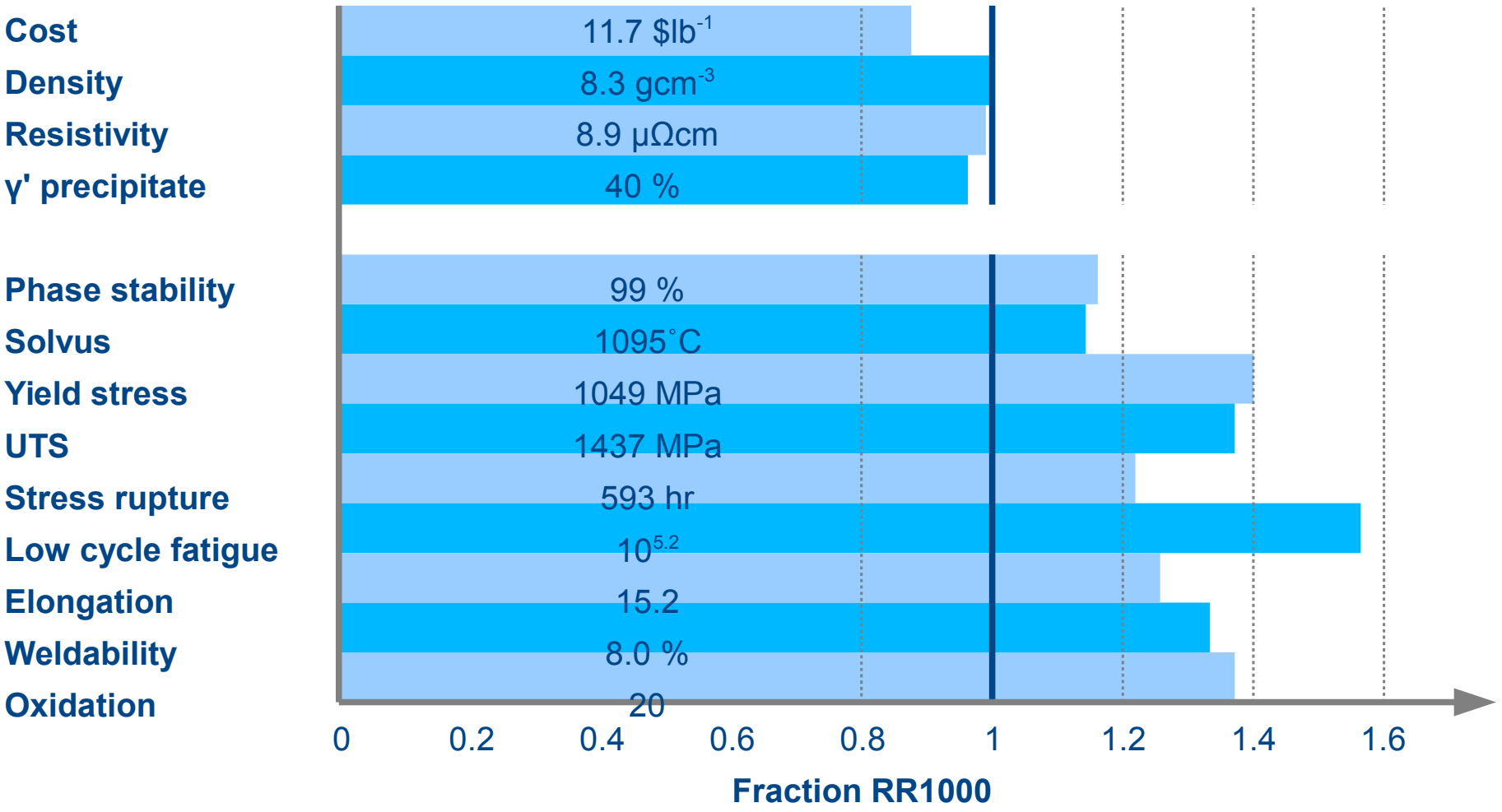
Nb

5.6

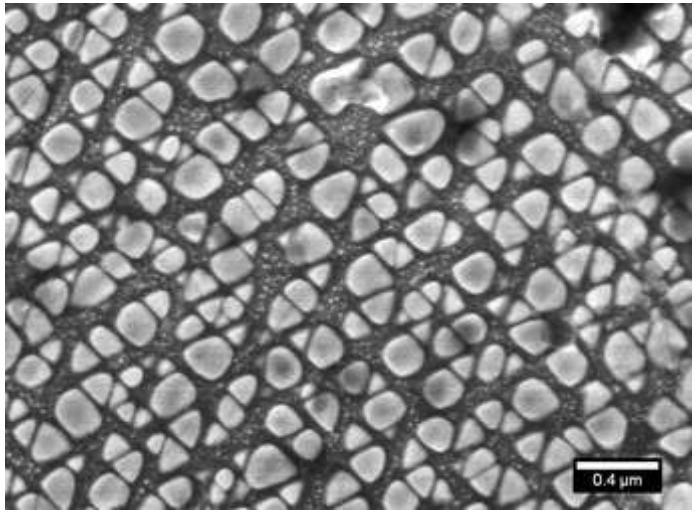
Fe

3.4

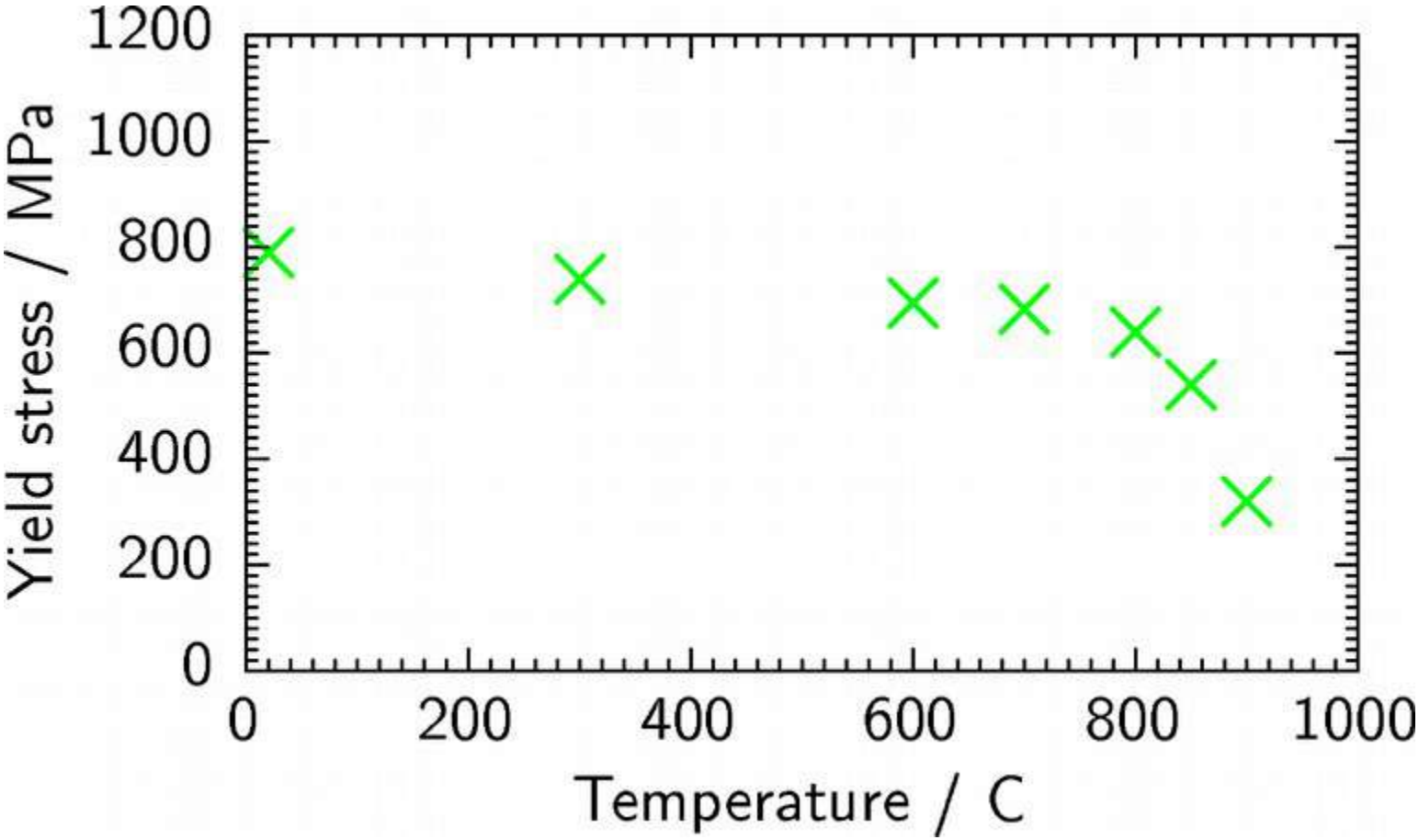
Case study: improved disc alloy



Electron micrograph



Yield stress



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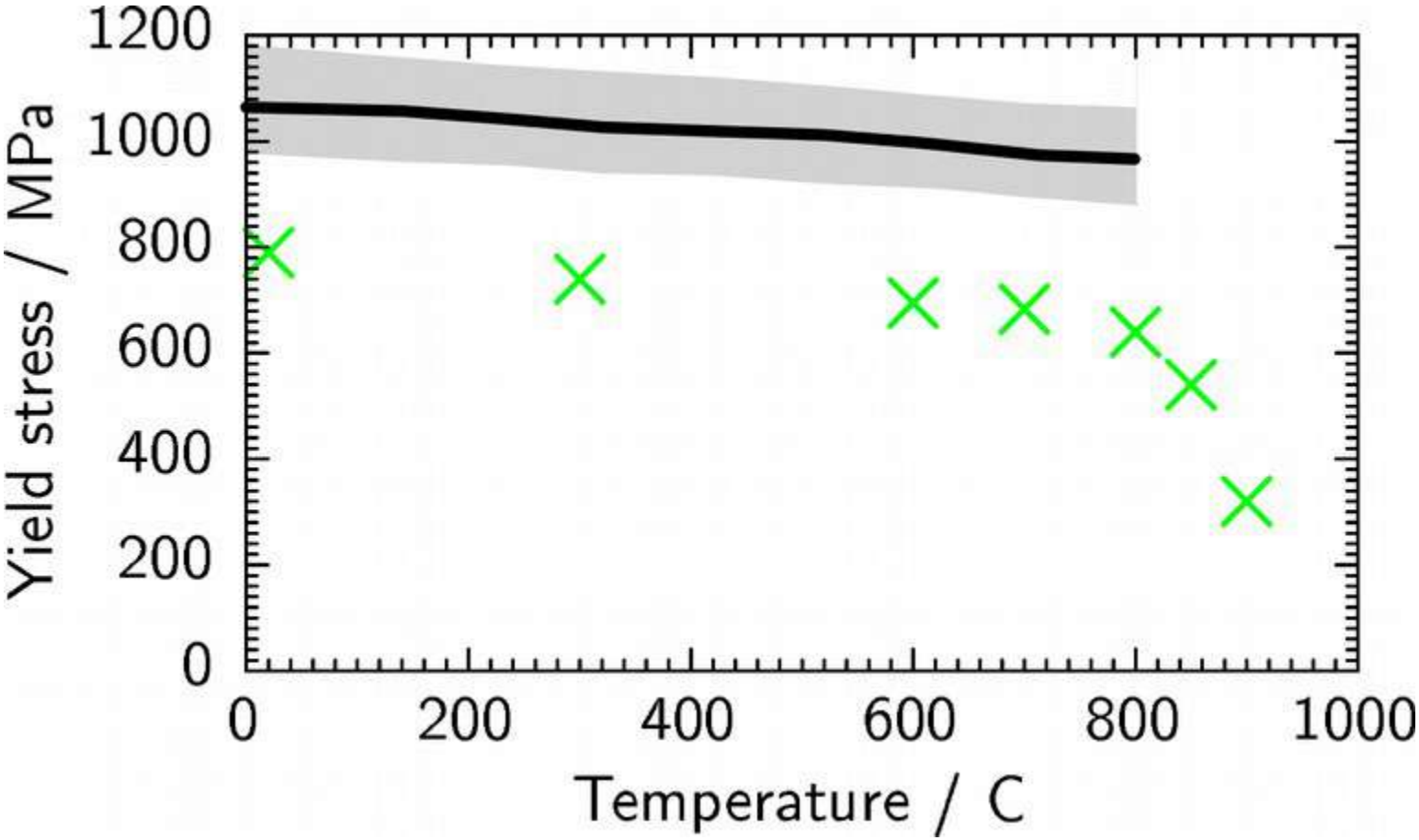

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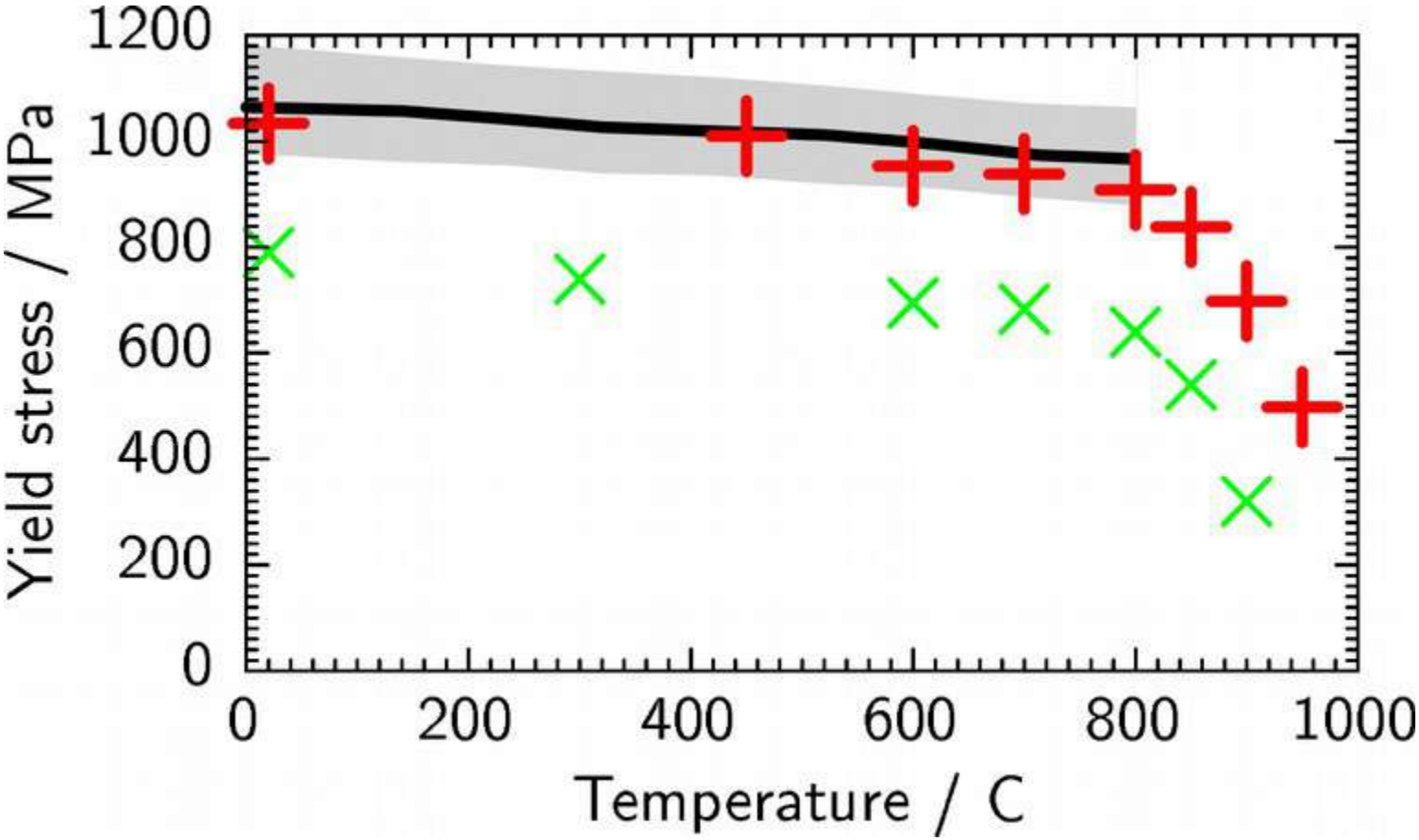
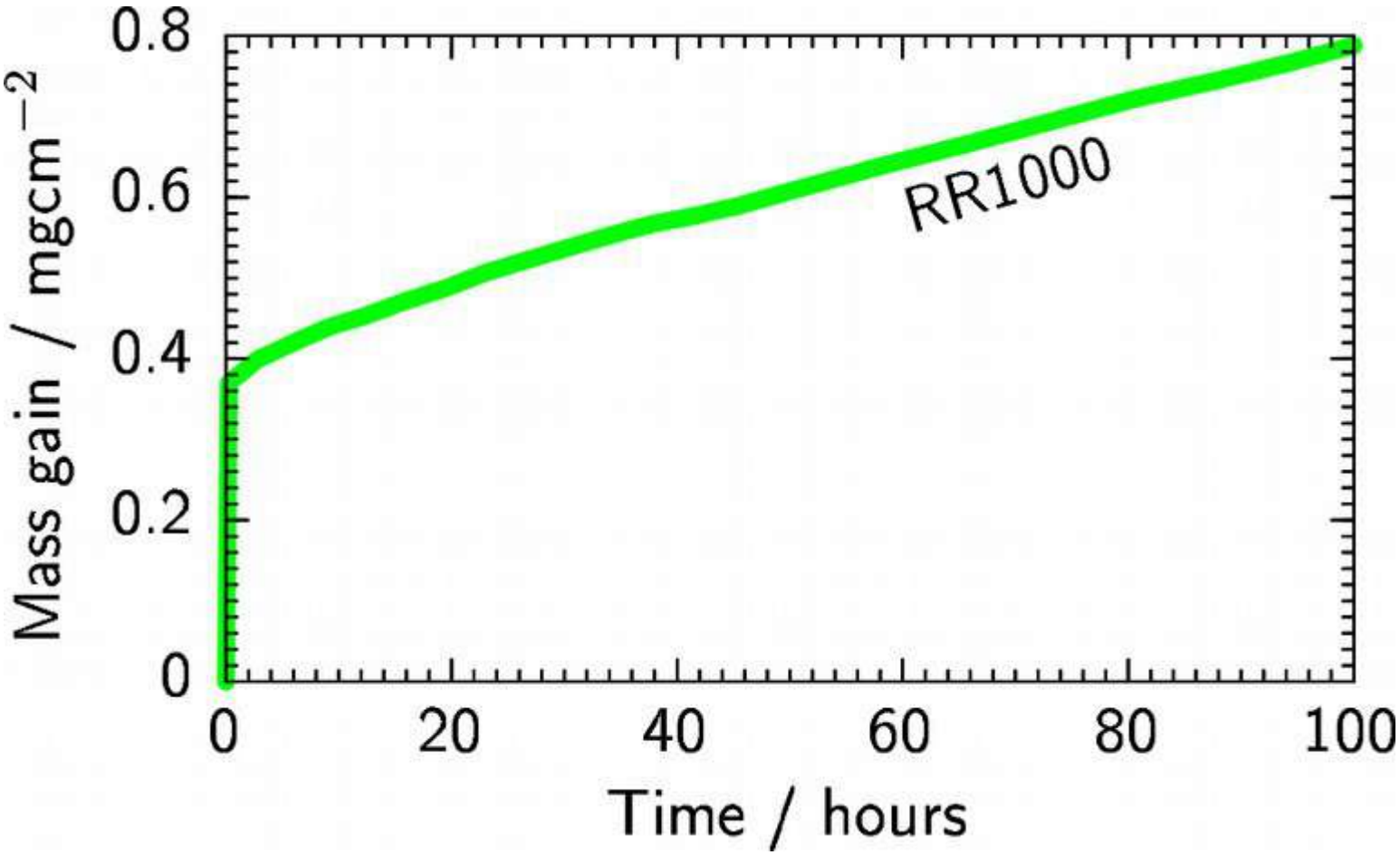


Oxidation



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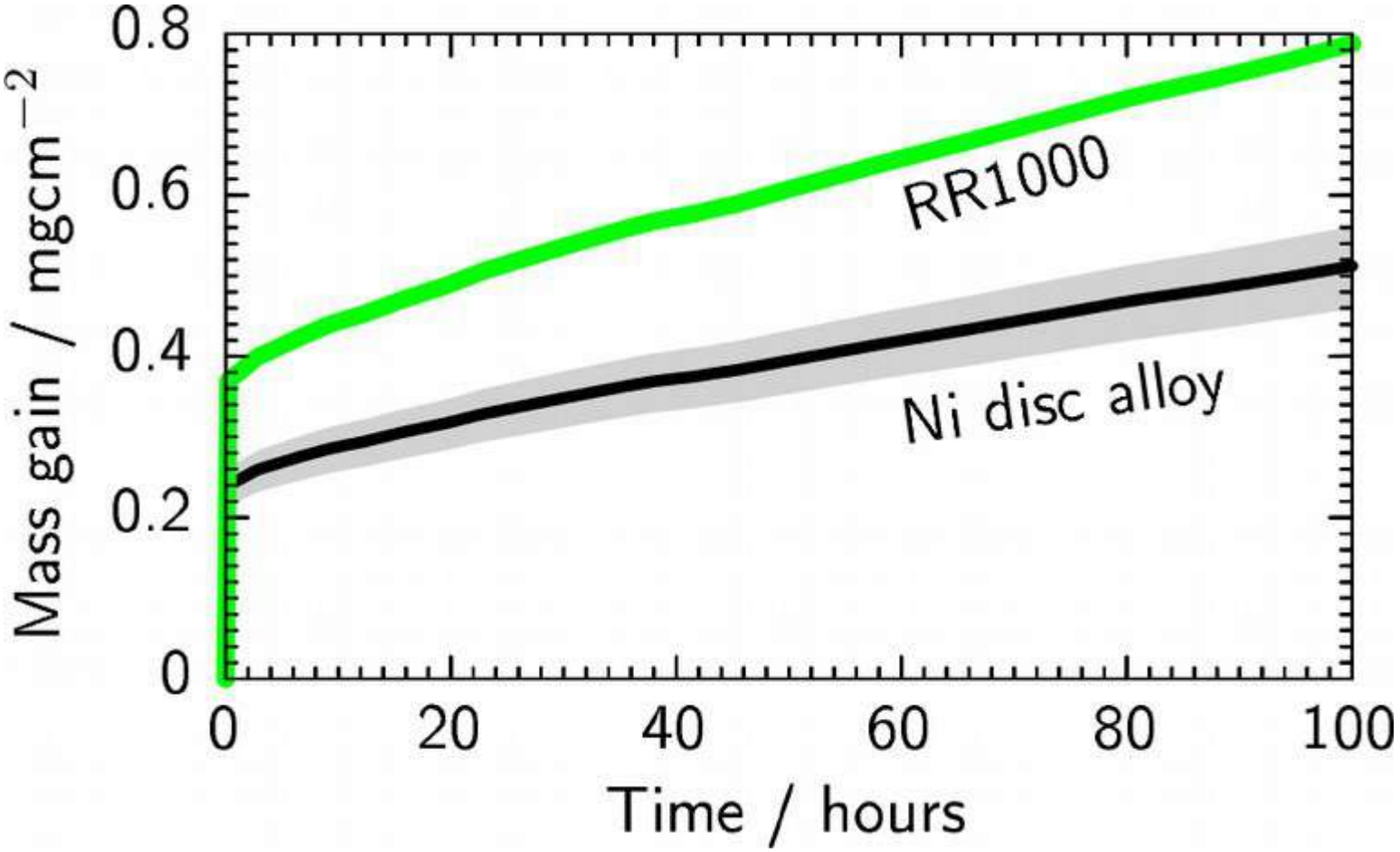
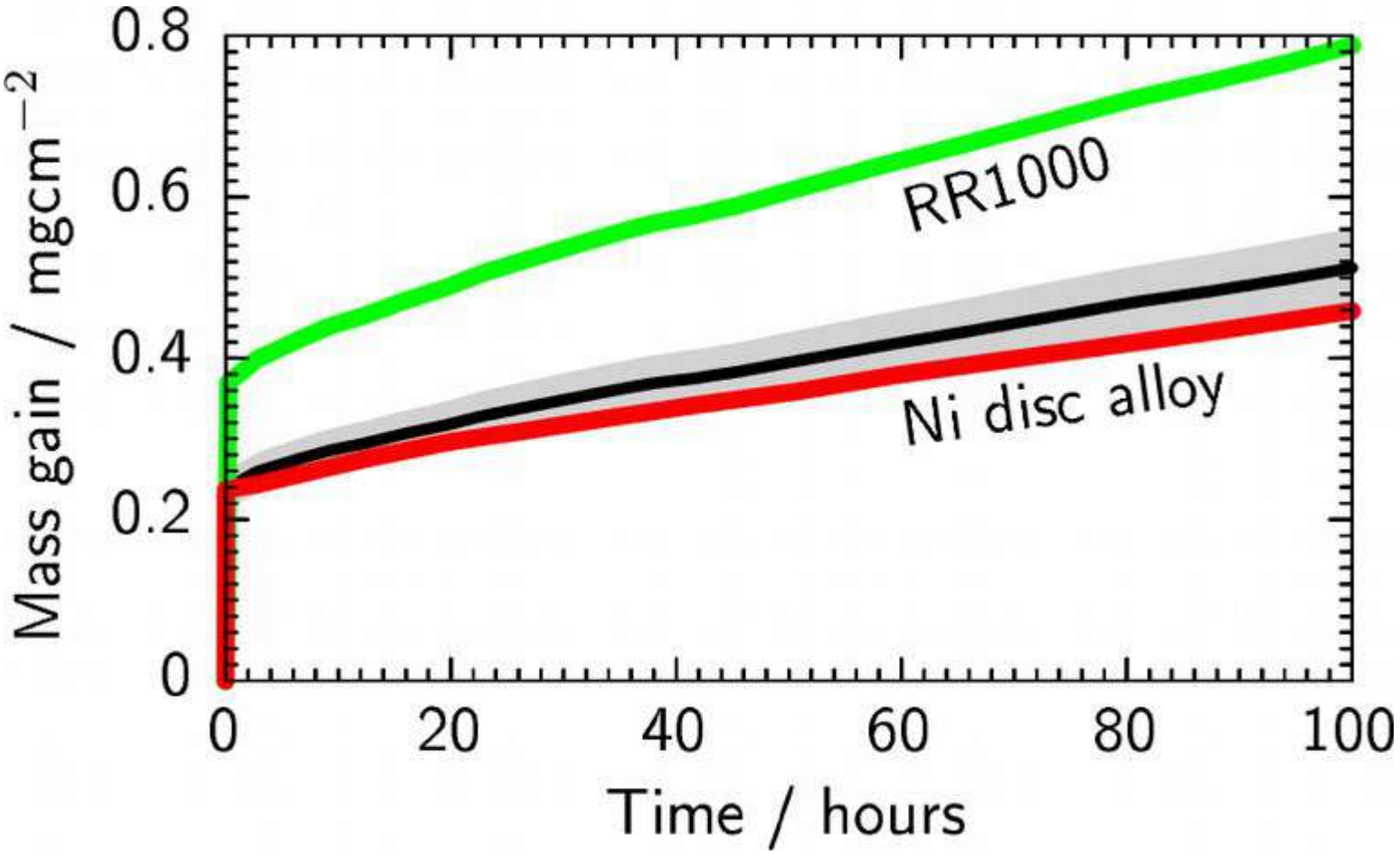

0.8
0.6
0.4
0.2
0
Mass gain / mgcm^{-2}
RR1000
Ni disc alloy
0
20
40
60
80
100
Time / hours

Oxidation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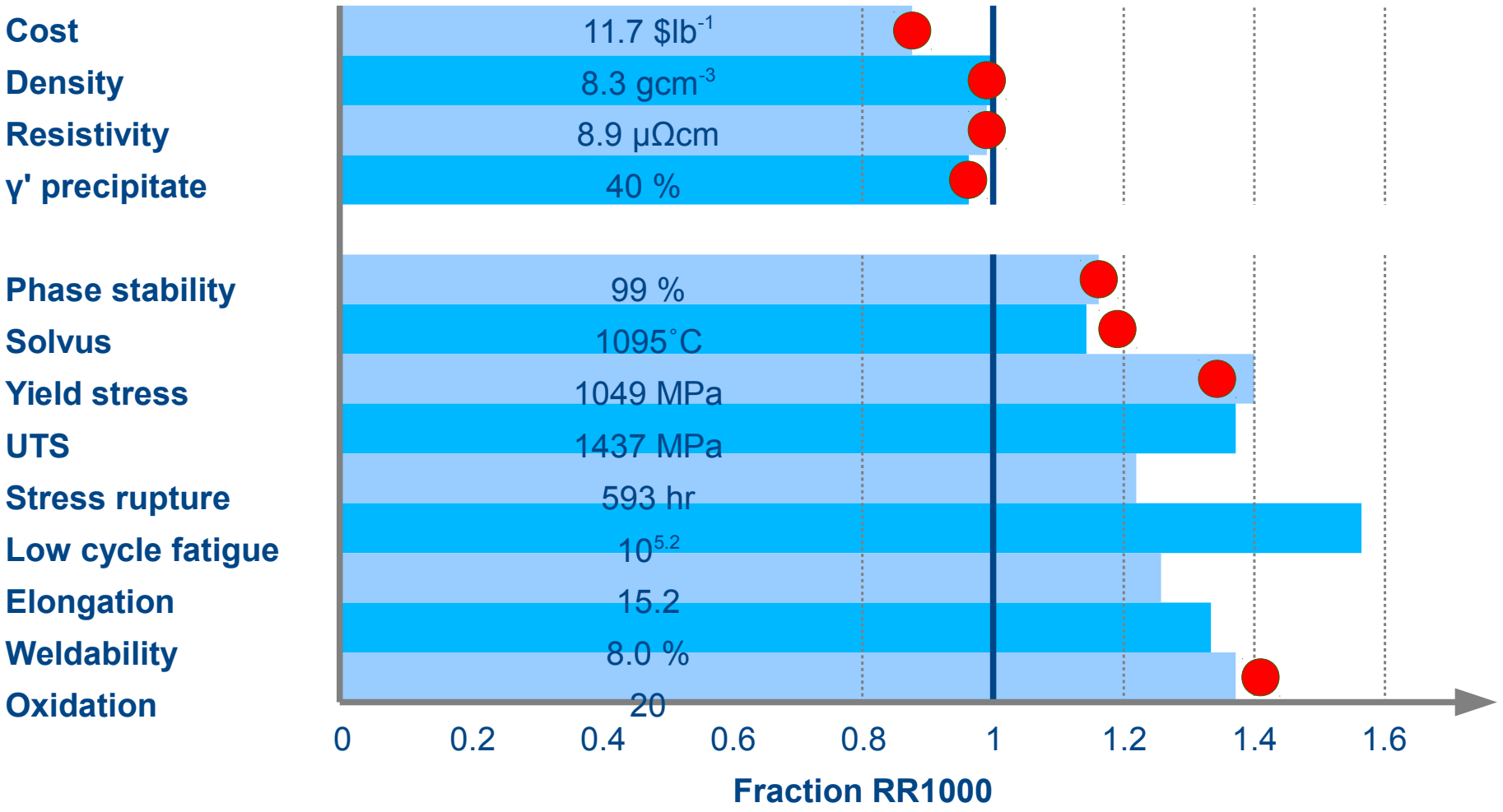

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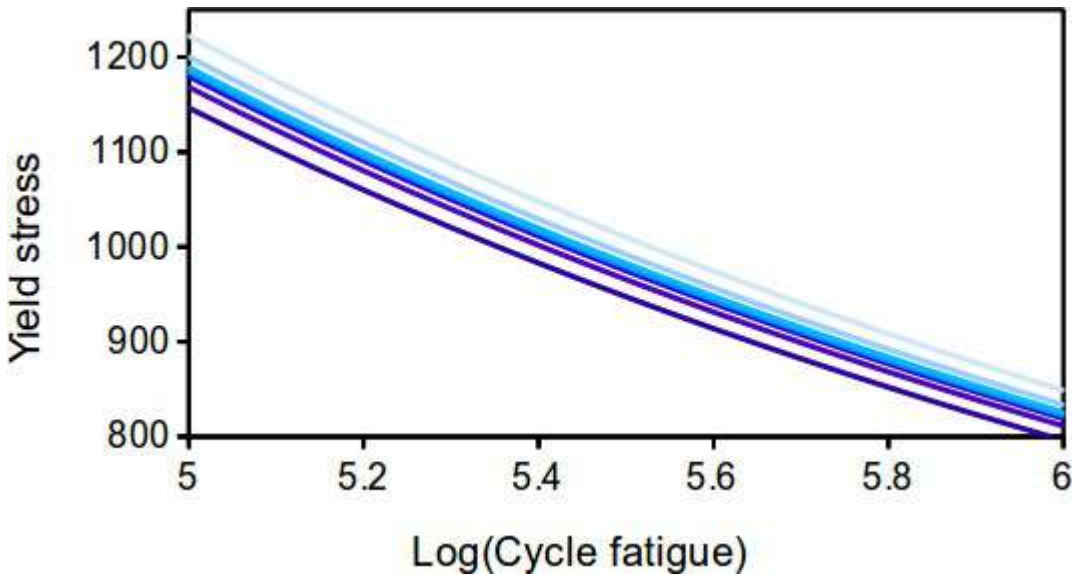

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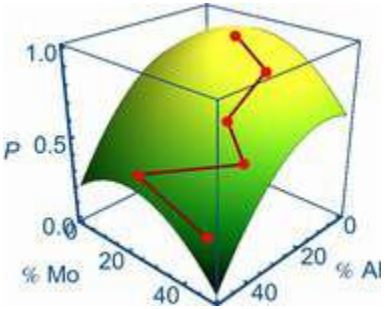
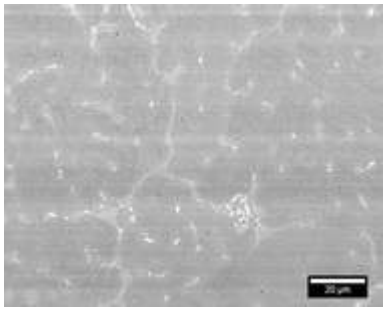
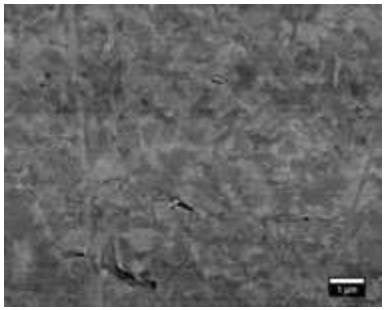
Discovery algorithm
Patent GB1302743.8 (2013)



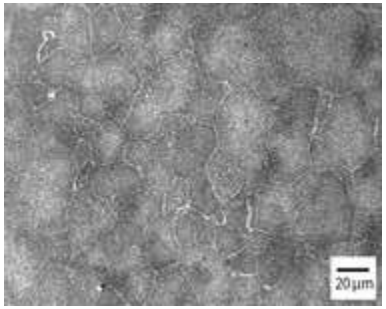
Mo-Hf forging alloy
Patent GB1307533.8 (2013)



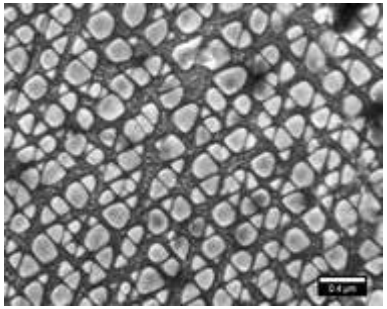
Mo-Nb forging alloy
Patent GB1307535.3 (2013)



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



Ni disc alloy
Rolls-Royce invention
NC12261 (2012)



Ni combustor liner
Rolls-Royce invention
NC13006 (2013)