UNIVERSITY OF CAMBRIDGE

Concurrent materials design

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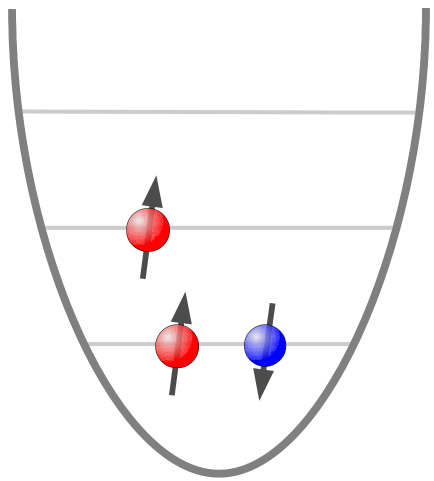
TCM Group, Department of Physics

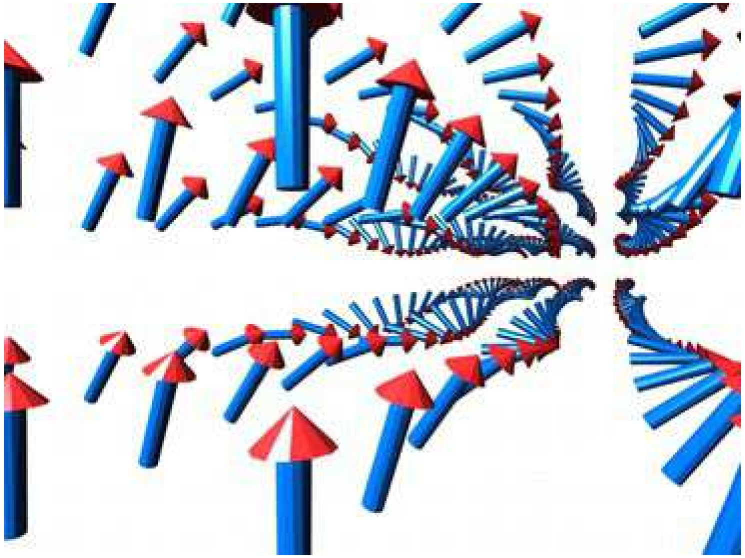
Trapped atoms



Theory P.O. Bugnion, J. Lofthouse & GJC, PRL **111**, 045301 (2013)
P.O. Bugnion & GJC, PRA **87**, 060502(R) (2013)

Experiment A.N. Wenz *et al*. arXiv:1307.3443 (2013)

Electron gas



Theory GJC, A.G. Green & B.D. Simons, PRL **103**, 207201 (2009)

Experiment S. Lausberg *et al*. PRL **109**, 216402 (2012)
Huxley group, in preparation (2013)

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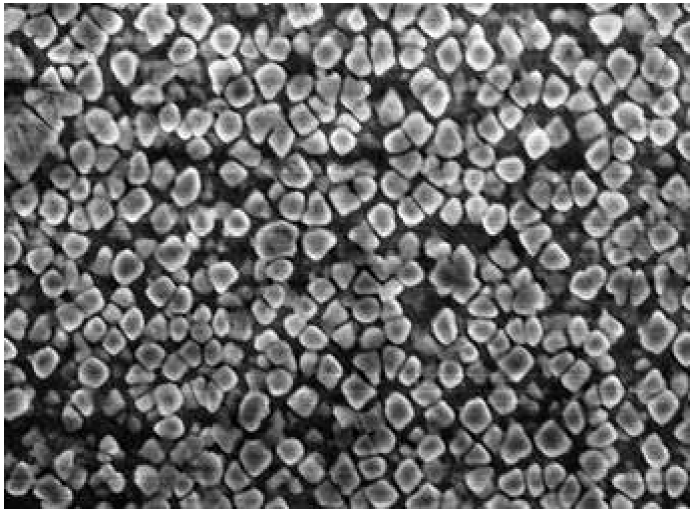
Phase equilibrium



Properties: γ' fraction

Calculate grid of

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

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Calculate grid of

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

↓

Generate neural network model and uncertainty

Properties: γ' fraction

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

↓

Generate neural network model
and uncertainty

↓

Calculate phase equilibrium
and uncertainty

Properties: γ' fraction

Calculate grid of

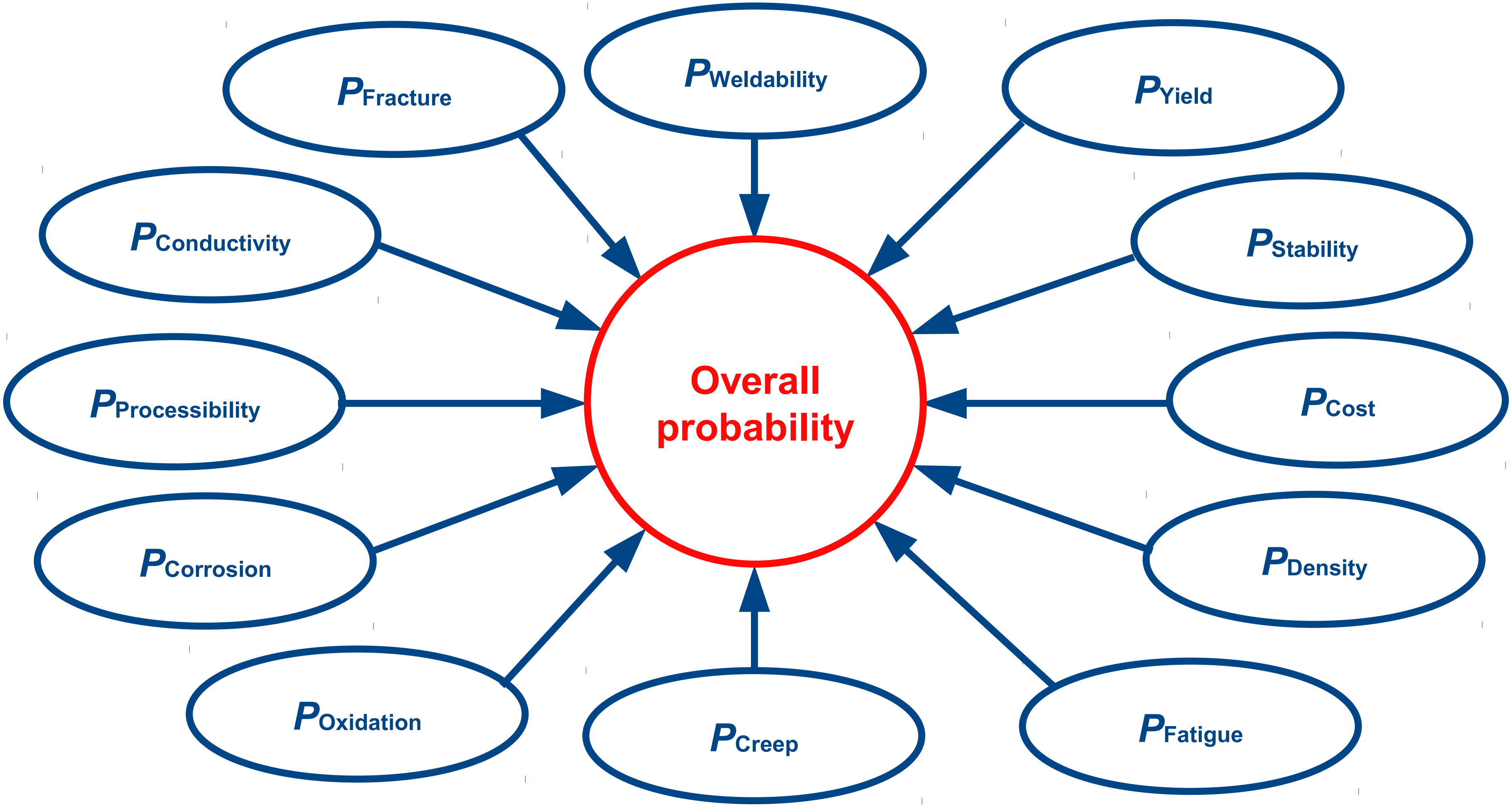
$$F_{(\gamma,\gamma')}(n_{\mathrm{ni}}, n_{\mathrm{Al}}, n_{\mathrm{Cr}}, n_{\mathrm{Co}}, n_{\mathrm{Mo}}, n_{\mathrm{Ti}})$$

Generate neural network model and uncertainty

Calculate phase equilibrium and uncertainty

Large uncertainty

Designing a new material – what is required ?



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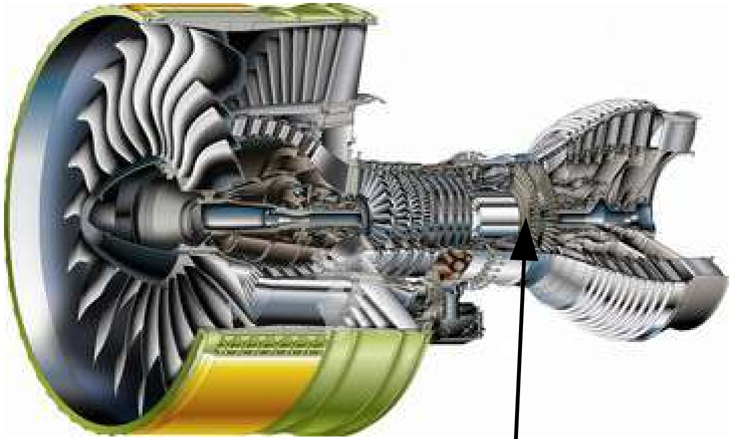


Disc
alloy

Case study: RR1000

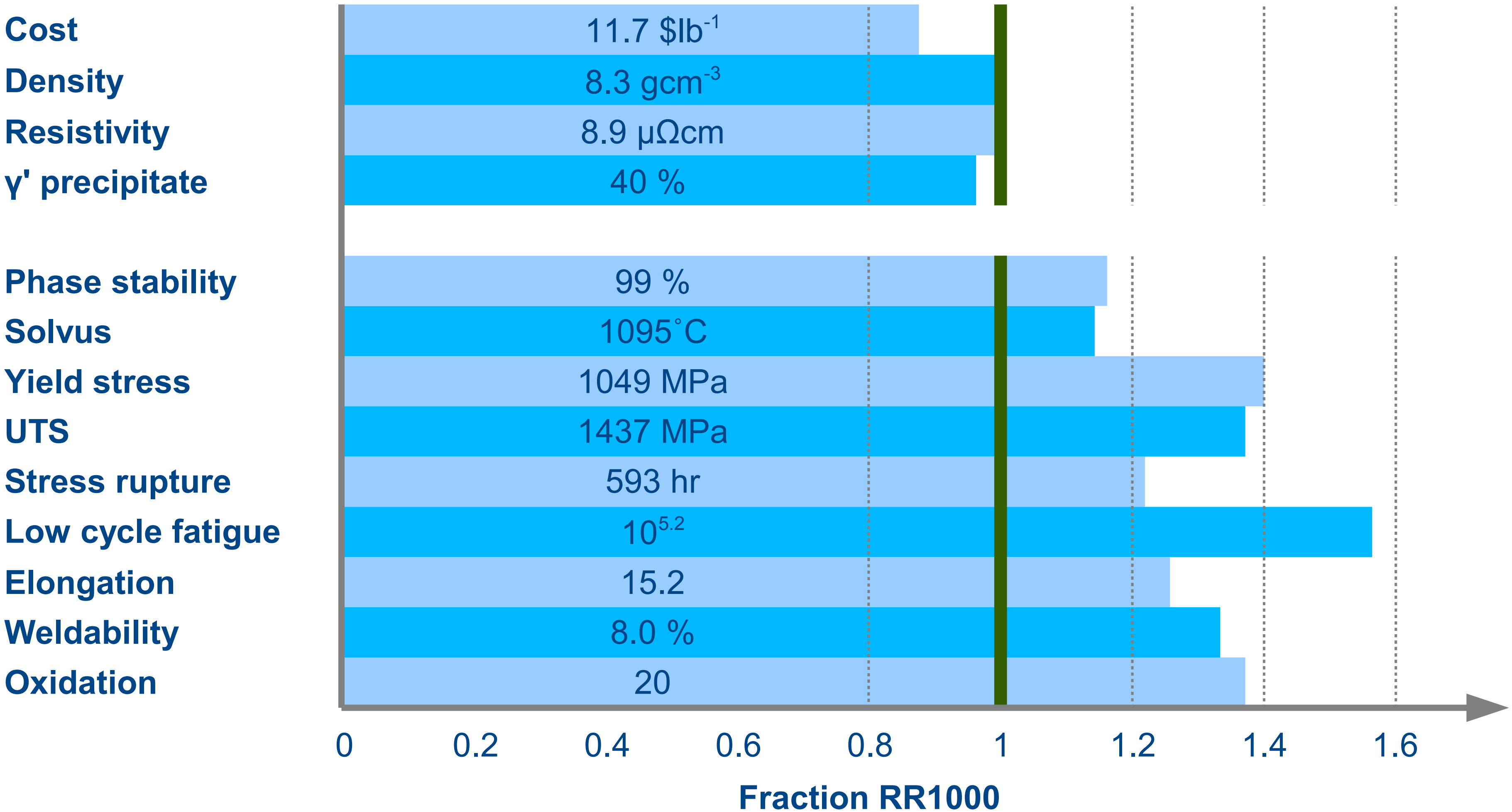
Ni	Cr	Co	Mo	Ti	Al	Ta	Hf	C	T	t
52	15	19	5	3.6	3	2	0.5	0.1	800	8

Case study: improved disc alloy

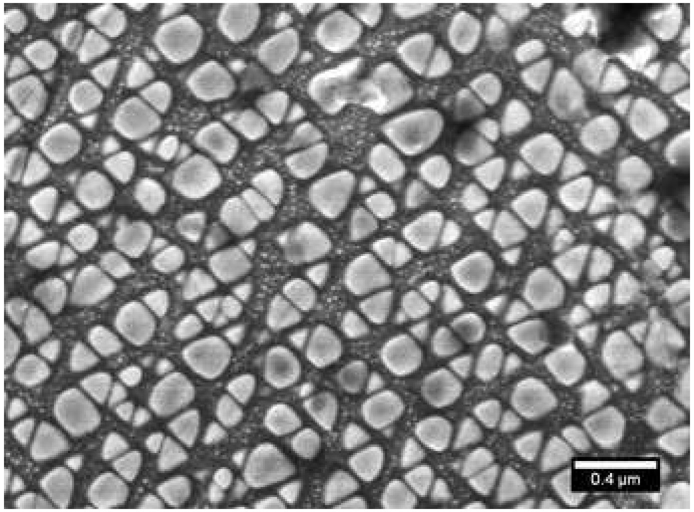
										
Ni	**Cr**	**Co**	**Mo**	**Ti**	**Al**	**Ta**	**Hf**	**C**	**T**	**t**
56	17	1.0	4.0	1.5	4.3	0.2	0.1	0.2	980	61

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

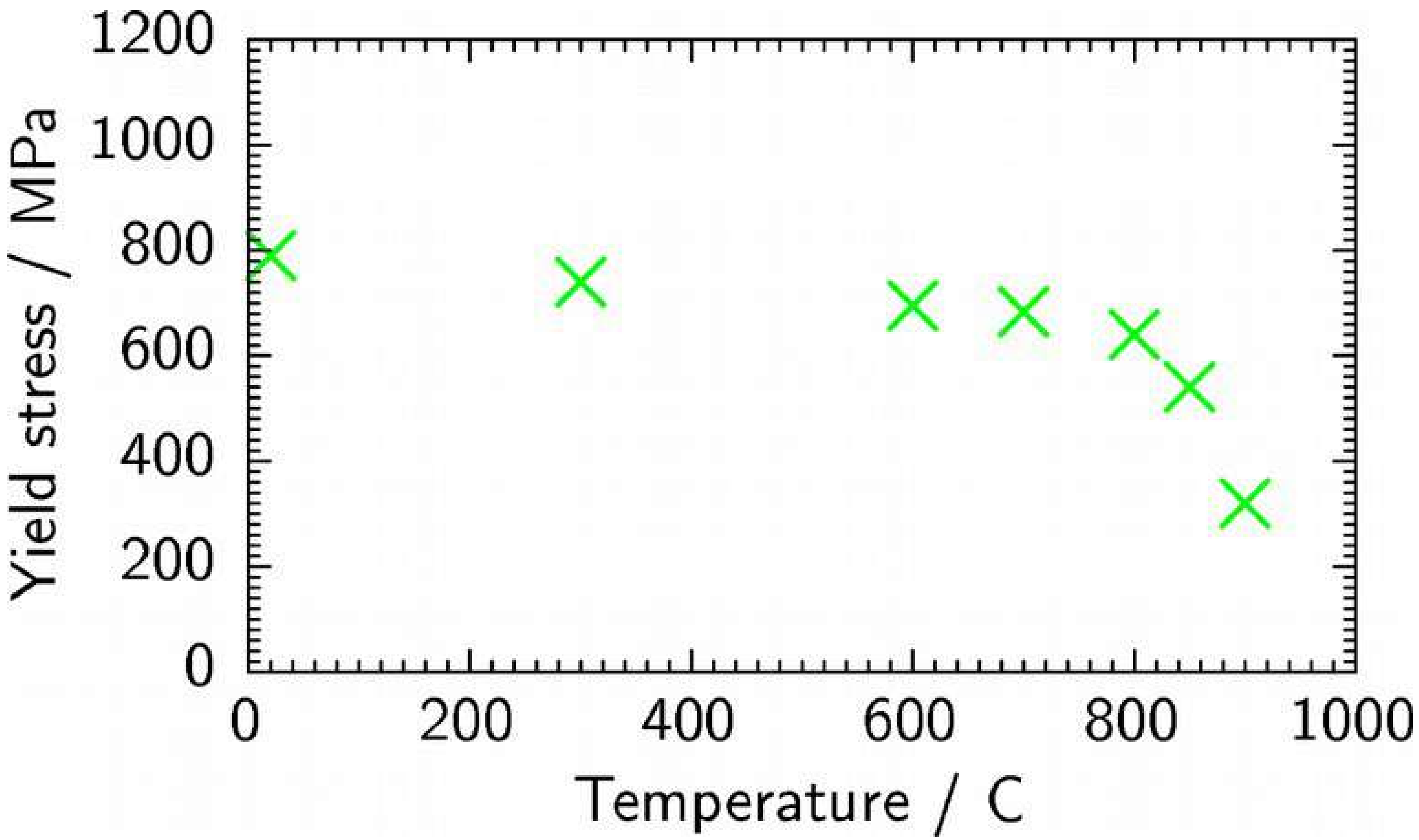
Case study: improved disc alloy



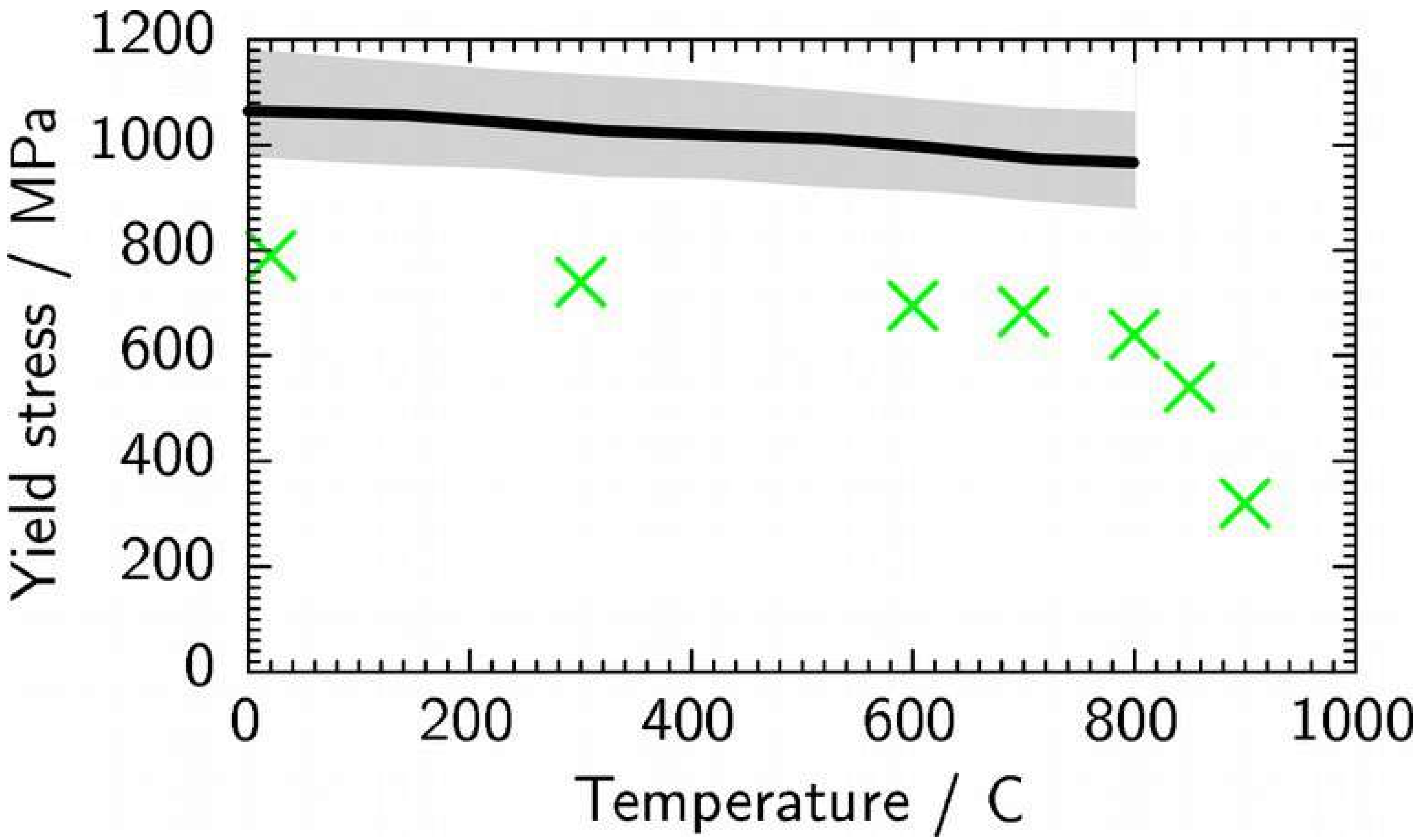
Electron micrograph



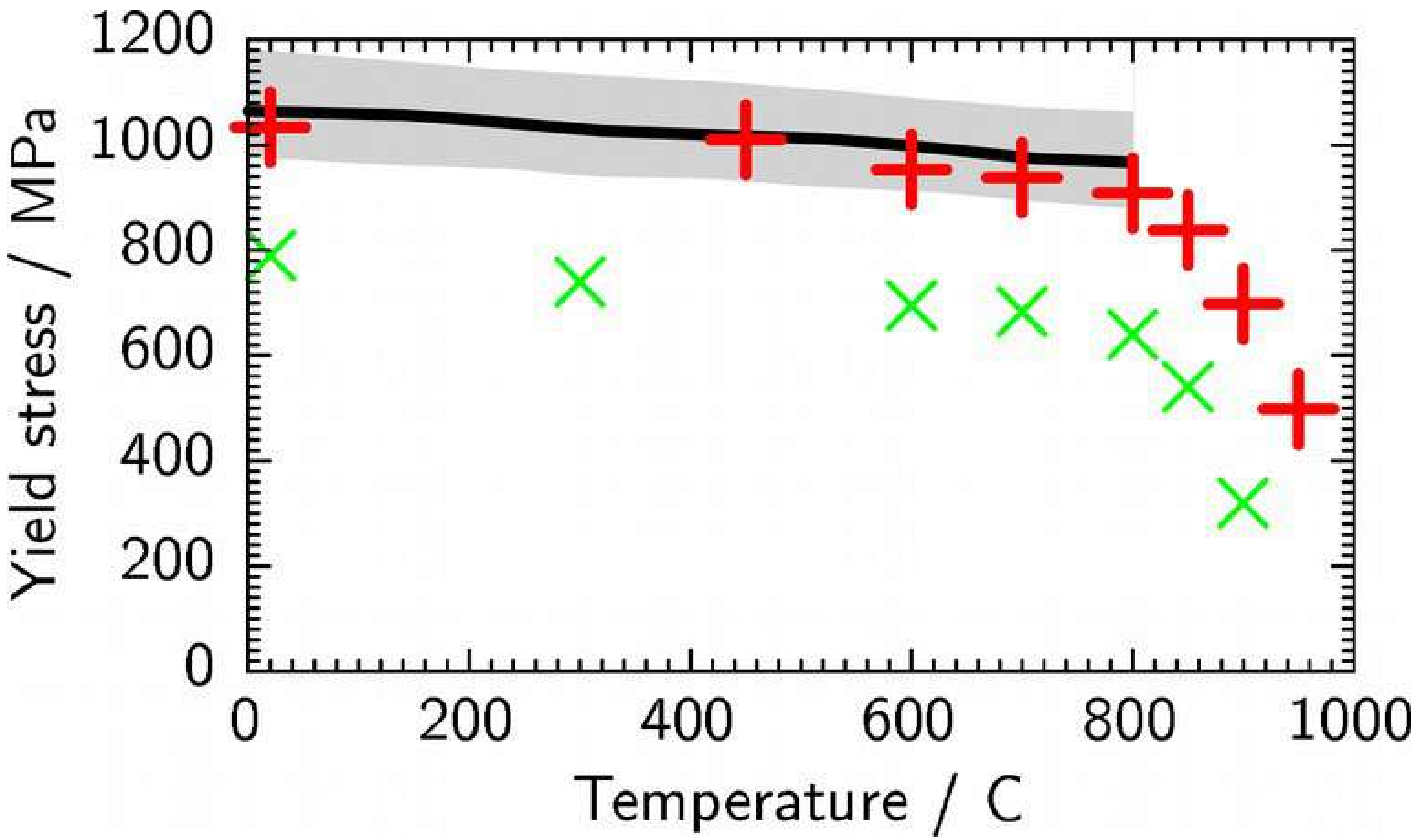
Yield stress



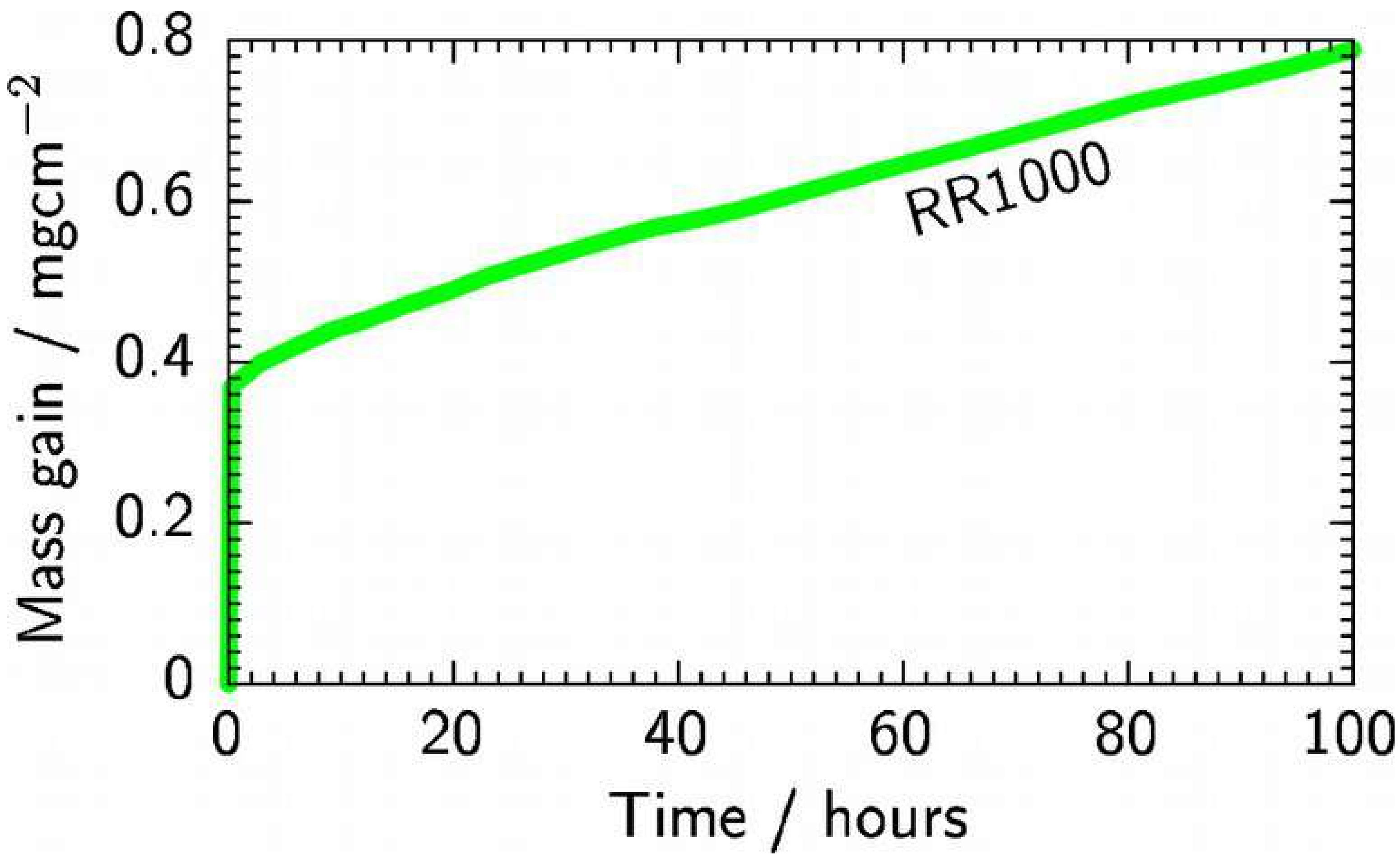
Yield stress



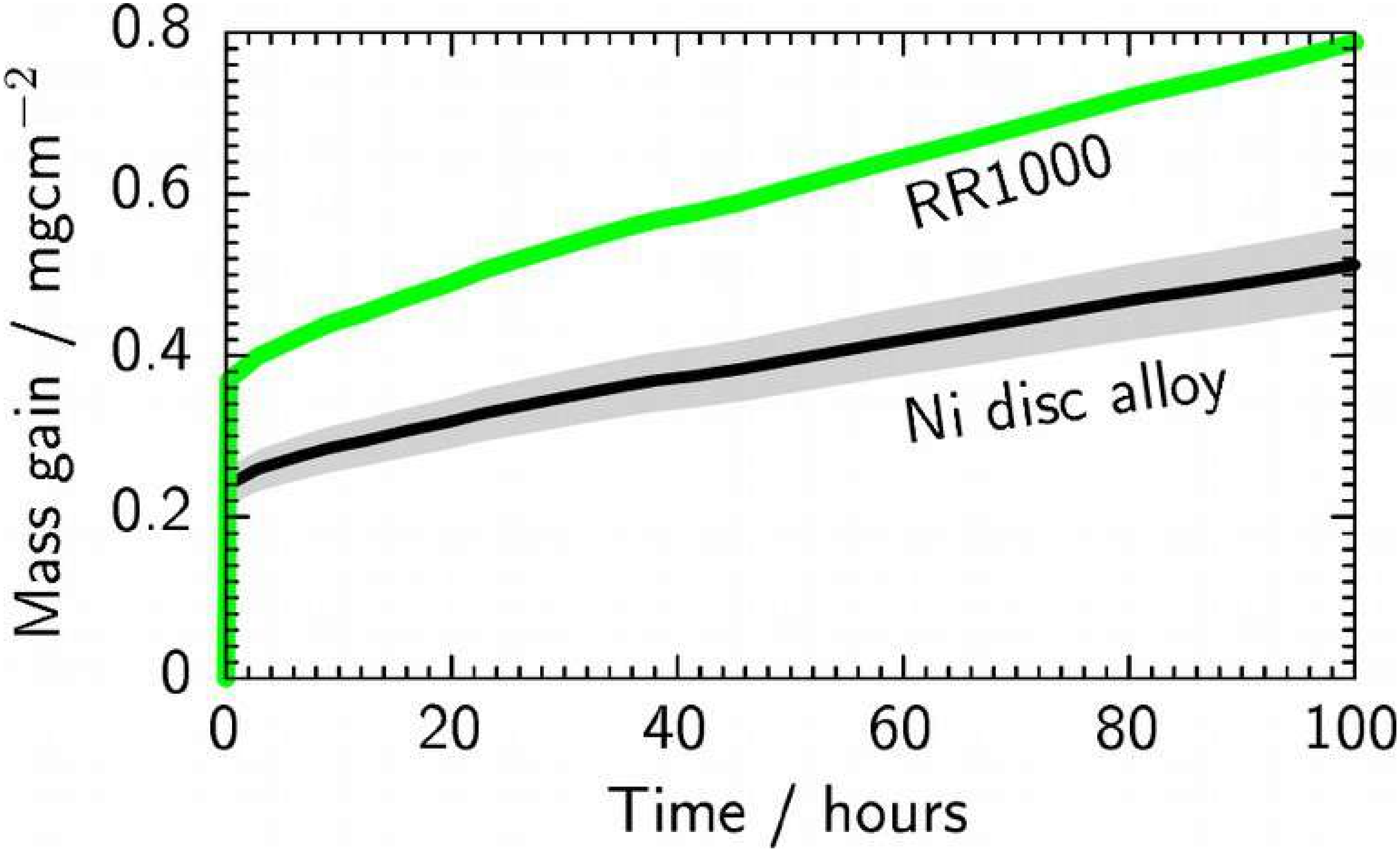
Yield stress



Oxidation

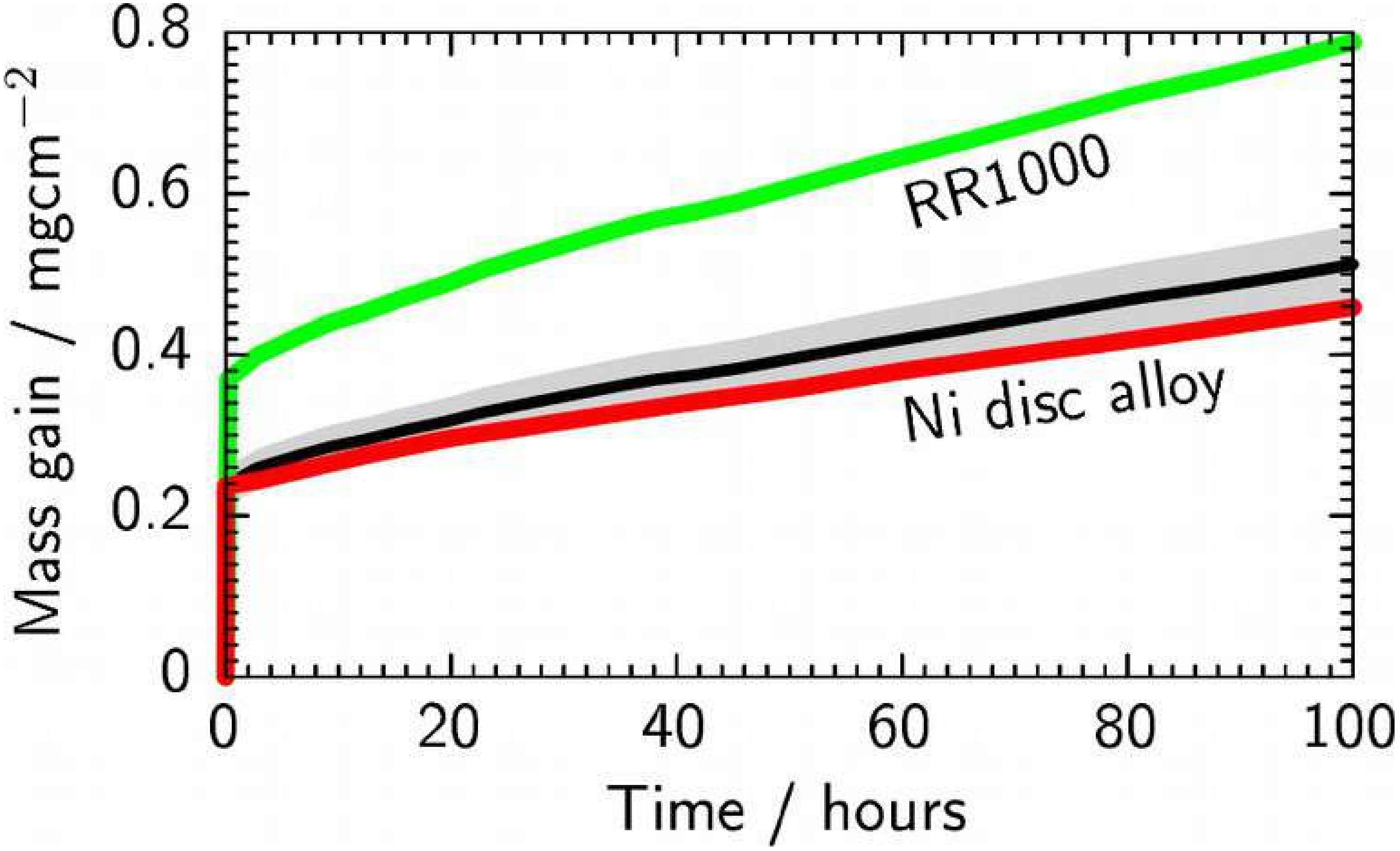


Oxidation



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

Oxidation



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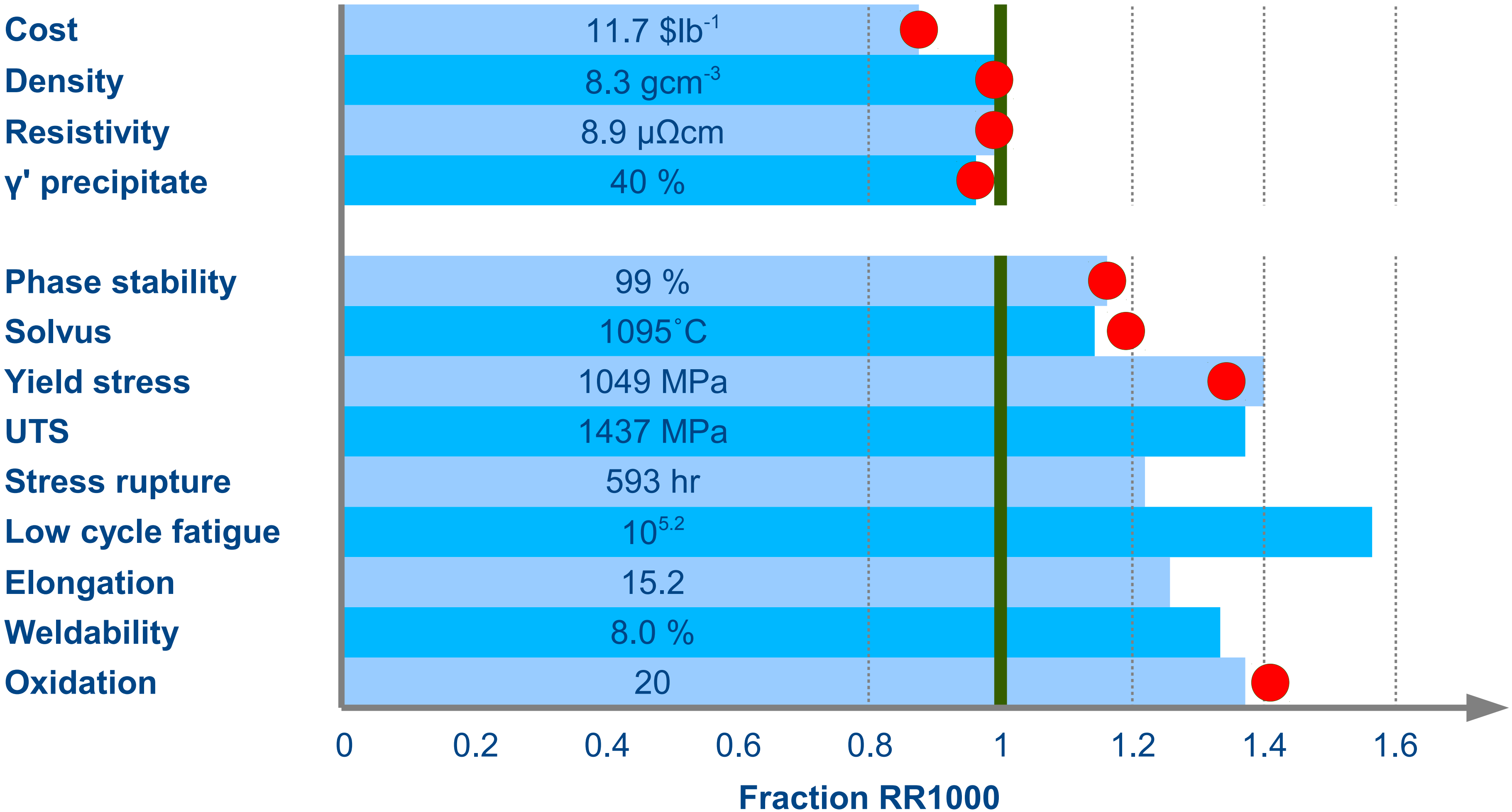
Case study: improved disc alloy



Partners

Materials Solutions

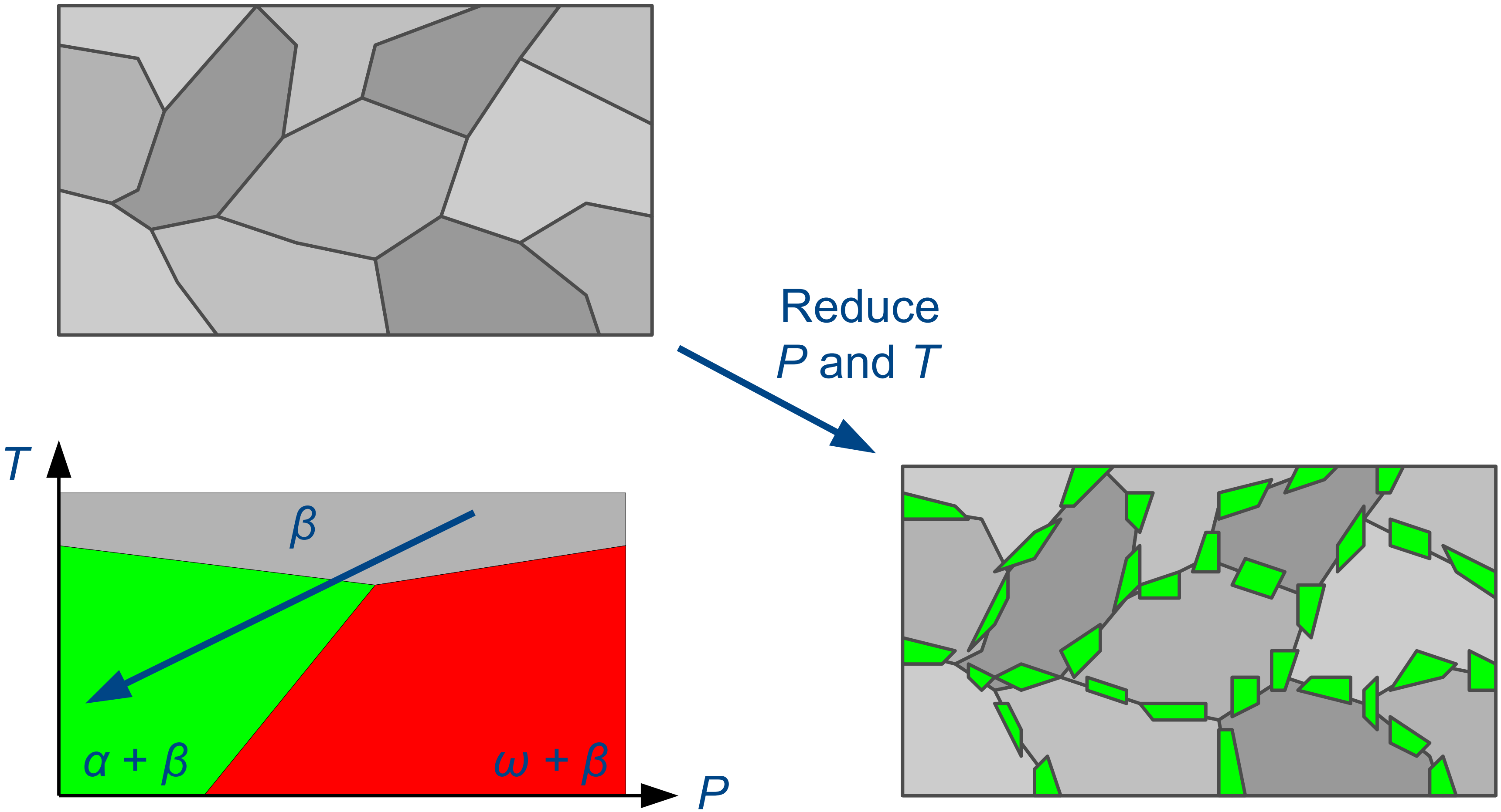
bp

SAMSUNG

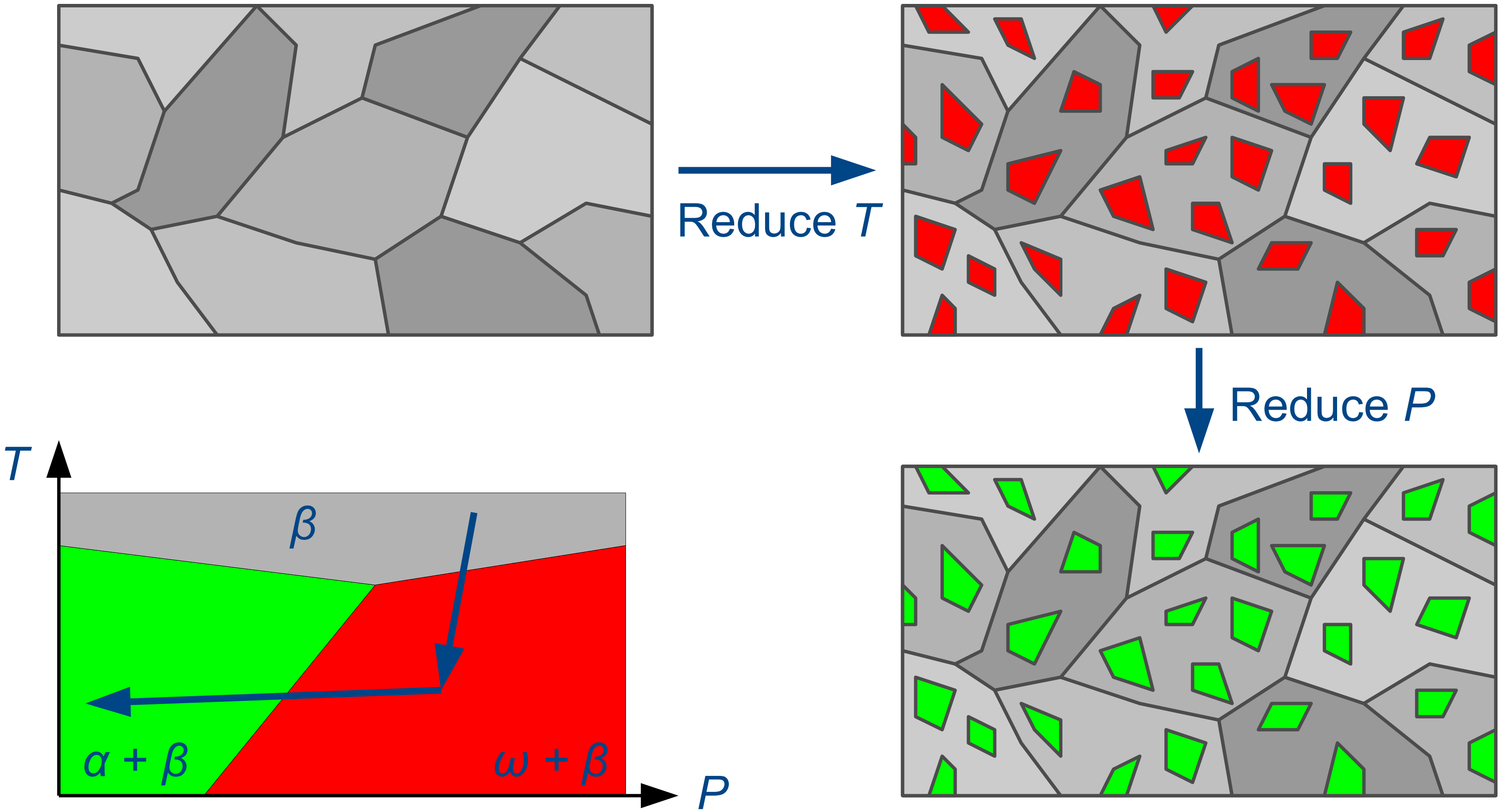
CLEANSKY

ROLLS ROYCE Rolls-Royce

Heat treatments



Heat treatments



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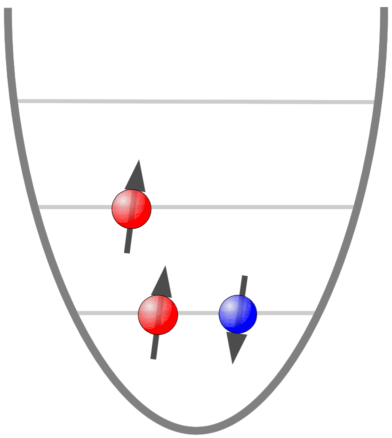
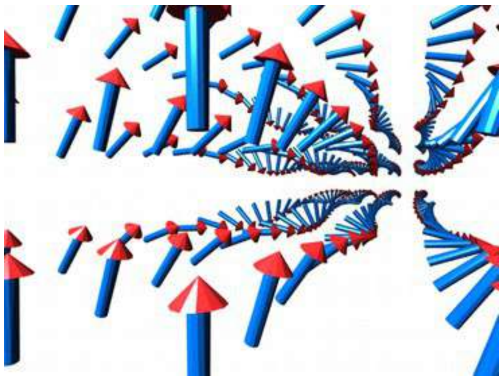
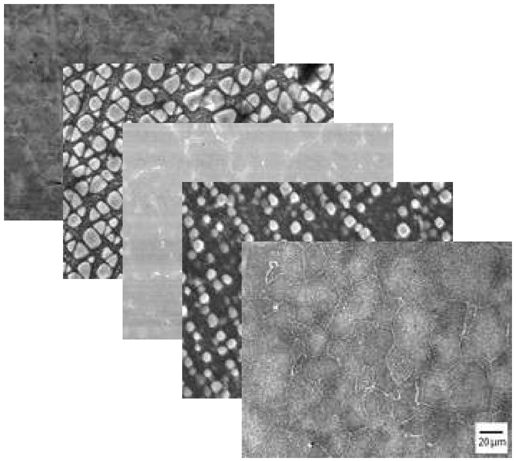


Few atoms in a trap



Electron gas



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