UNIVERSITY OF CAMBRIDGE

Materials discovery with artificial intelligence

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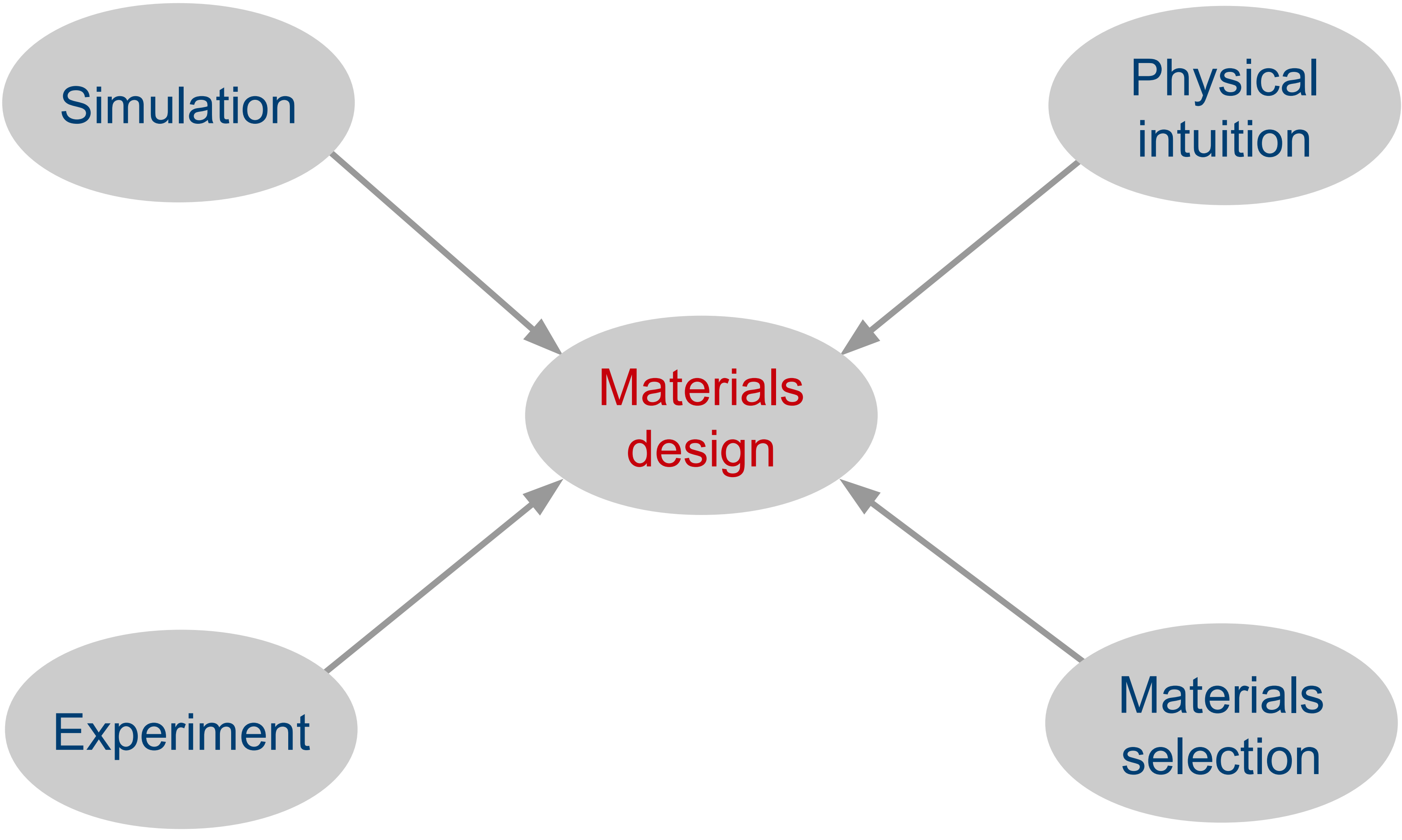
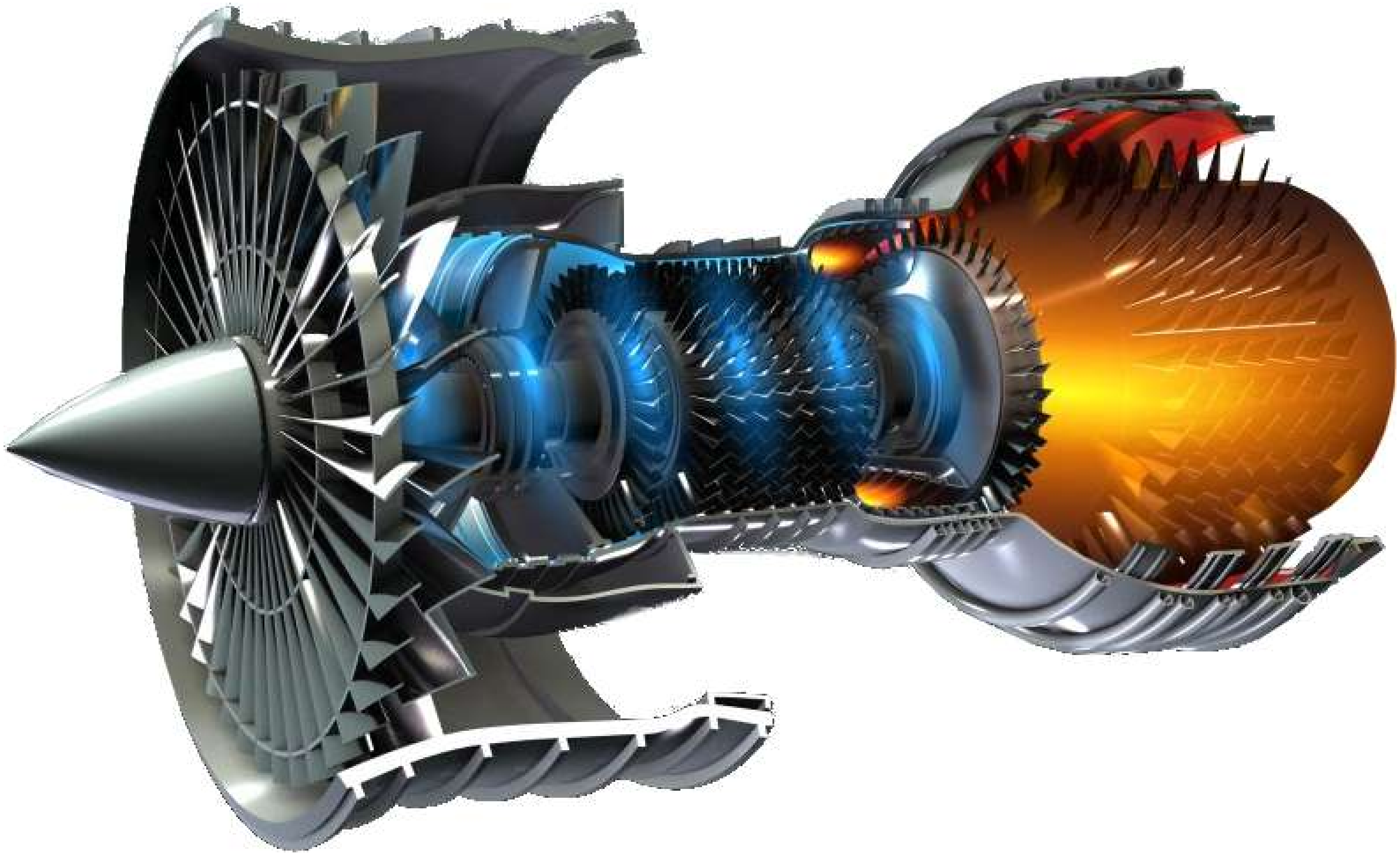
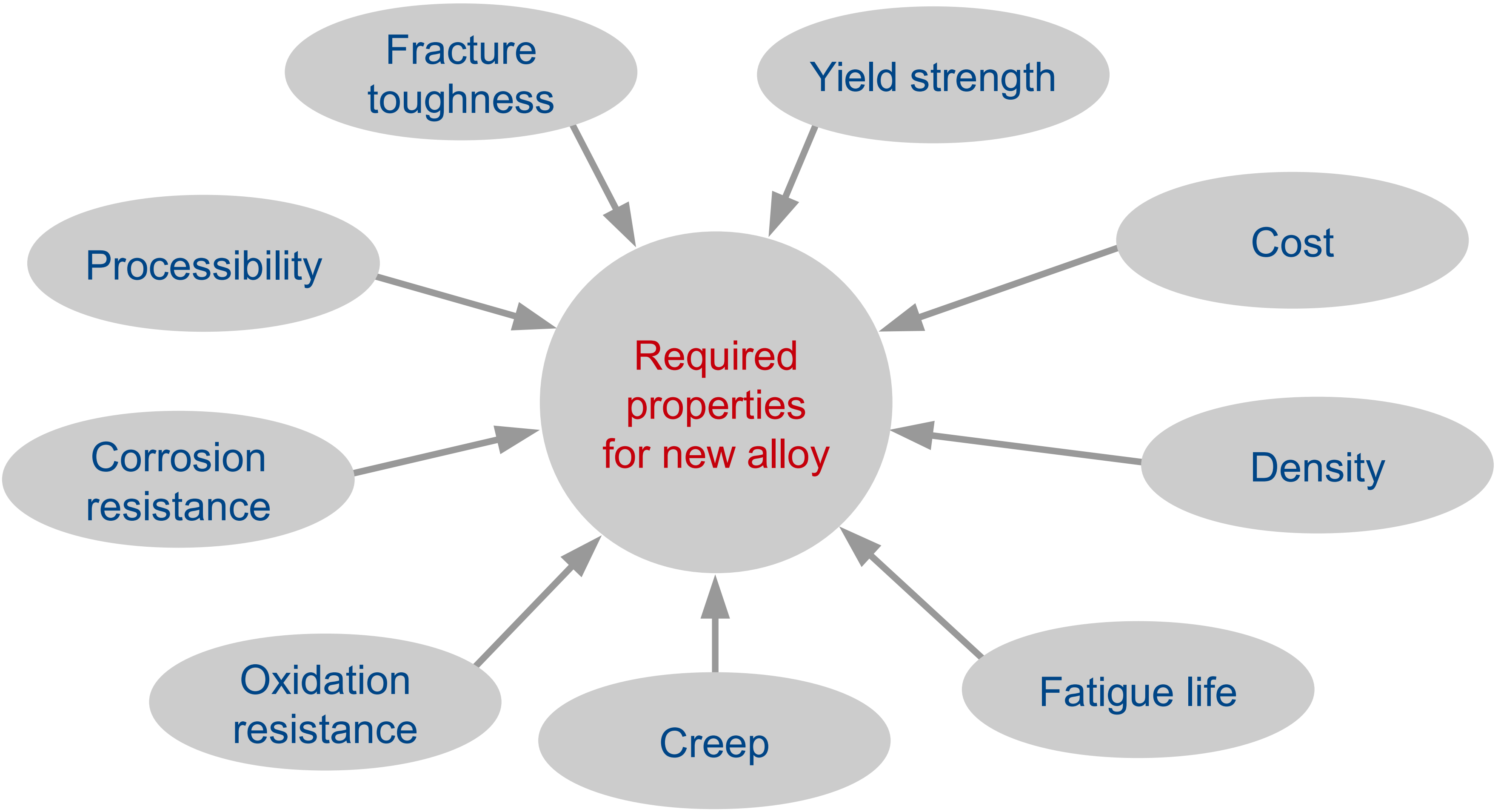
Approaches to materials design



Schematic of a jet engine



Designing a new alloy: what is required?



Multidimensional design space

Cr

Co

Mo

W

Ta

Nb

Al

Ti

Fe

Mn

Si

C

B

Zr

Cu

N

P

V

Hf

Mg

Ni

and 4 different manufacturing processes

Artificial intelligence

Composition

Artificial intelligence

Yield stress

Hardness

Melting point

Oxidation resistance

Cost

Density

Fatigue life

Fracture toughness

Creep

Processibility

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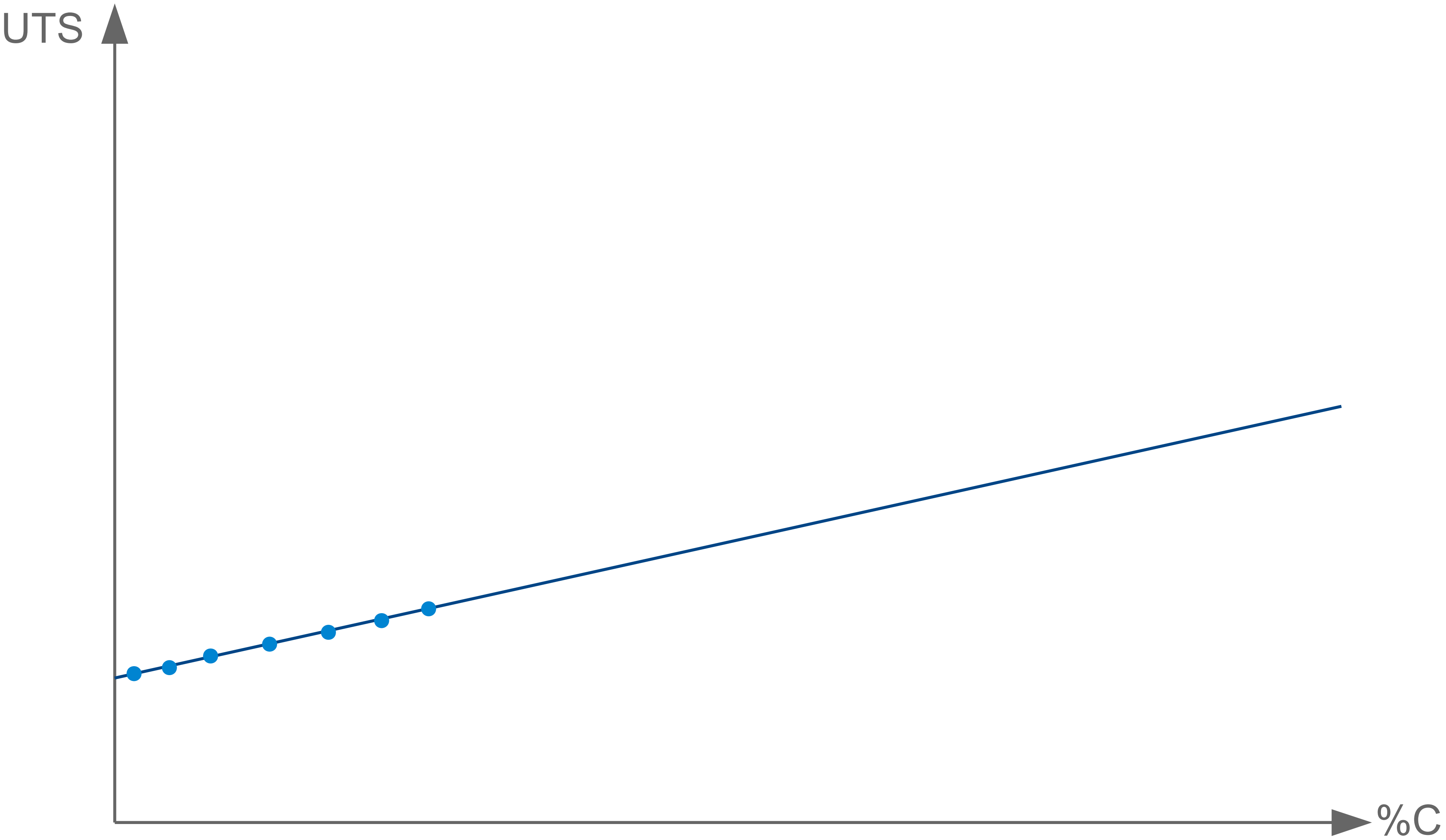
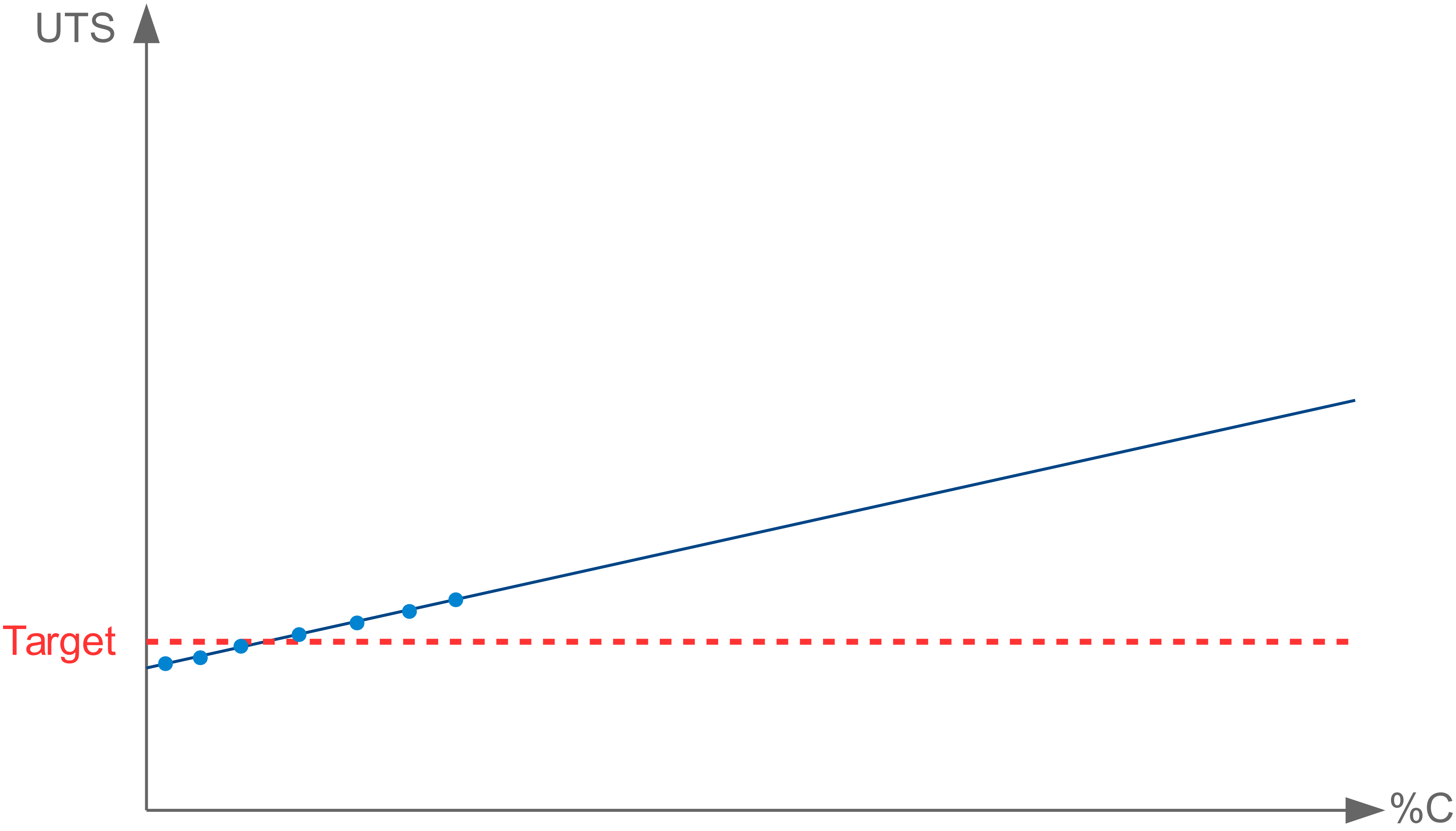
Sample data

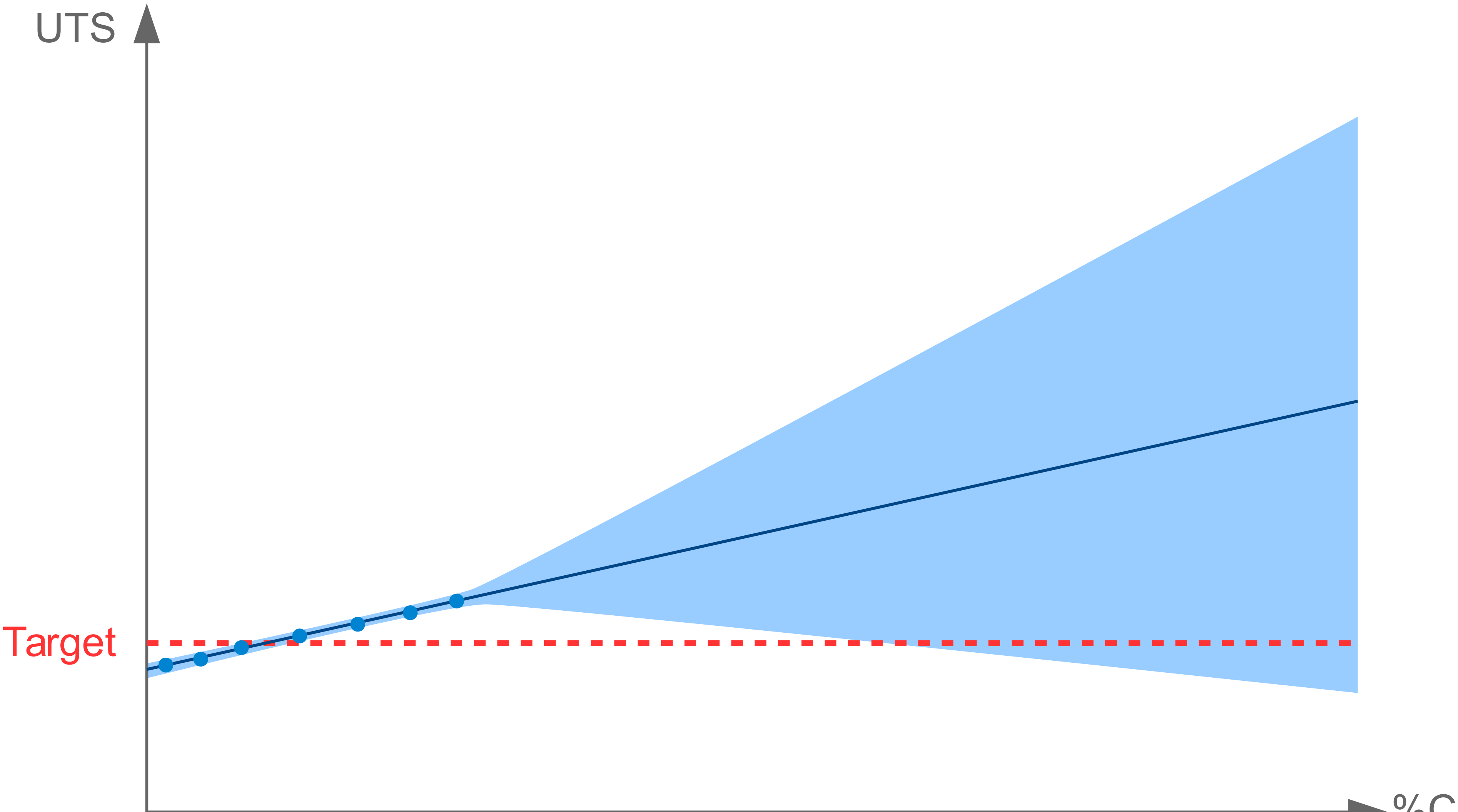
Modeling the data



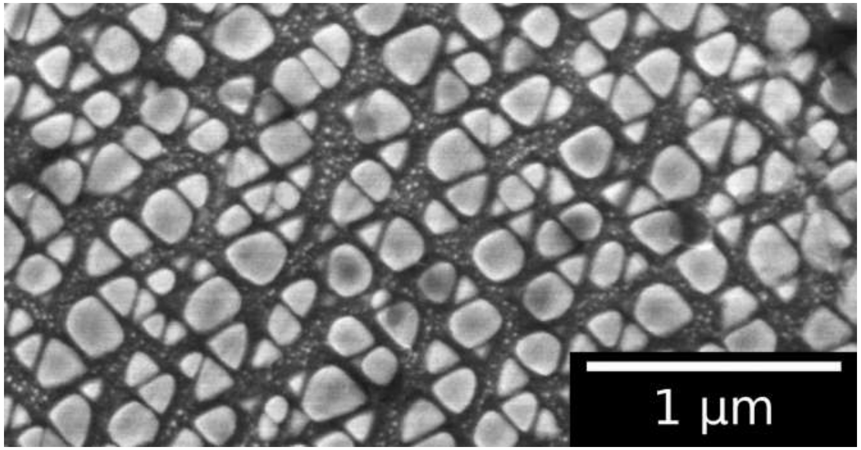
Exceeding the target



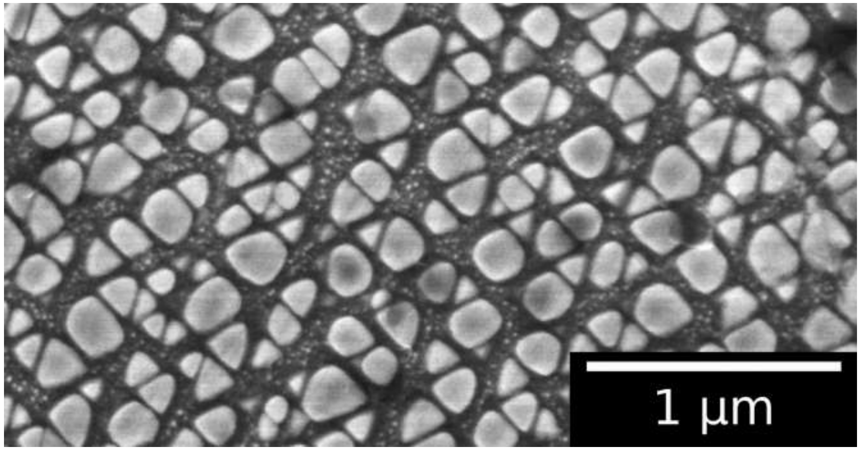
Maximizing likelihood of exceeding the target



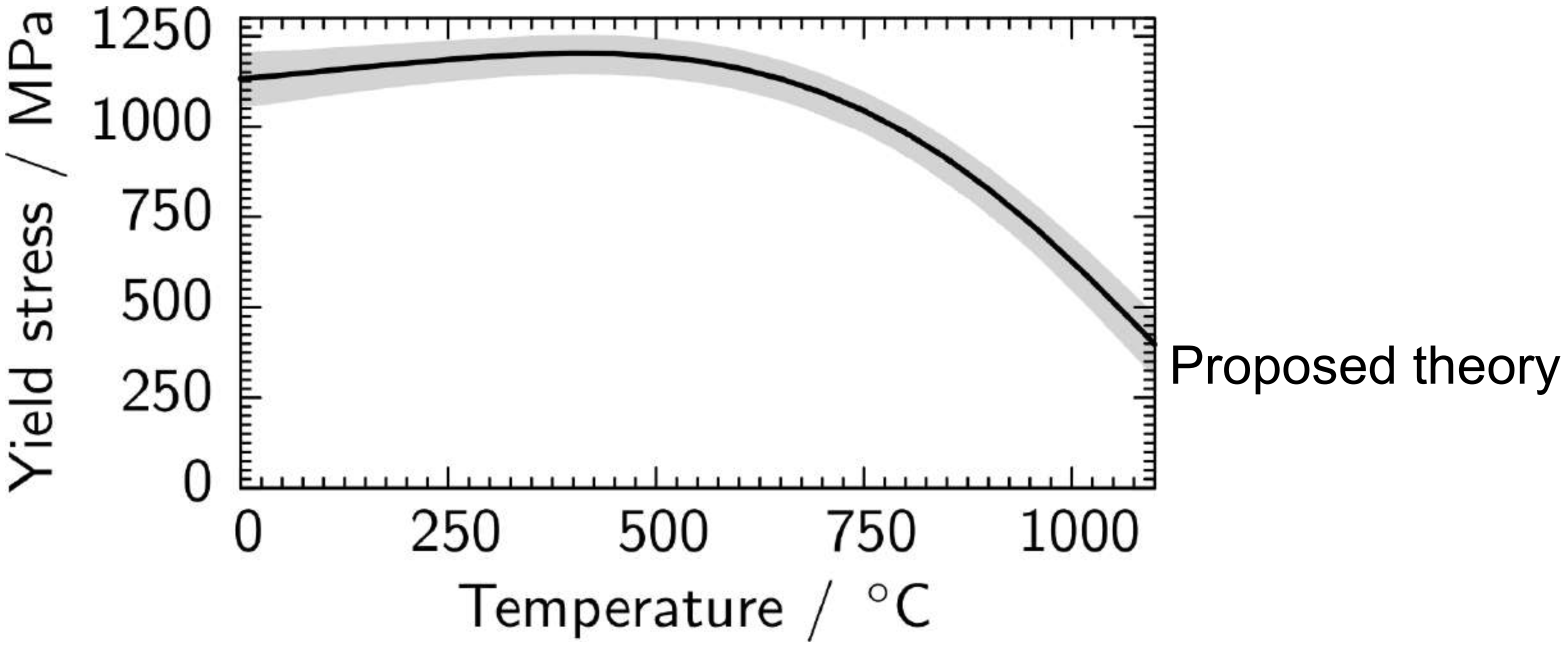
Microstructure



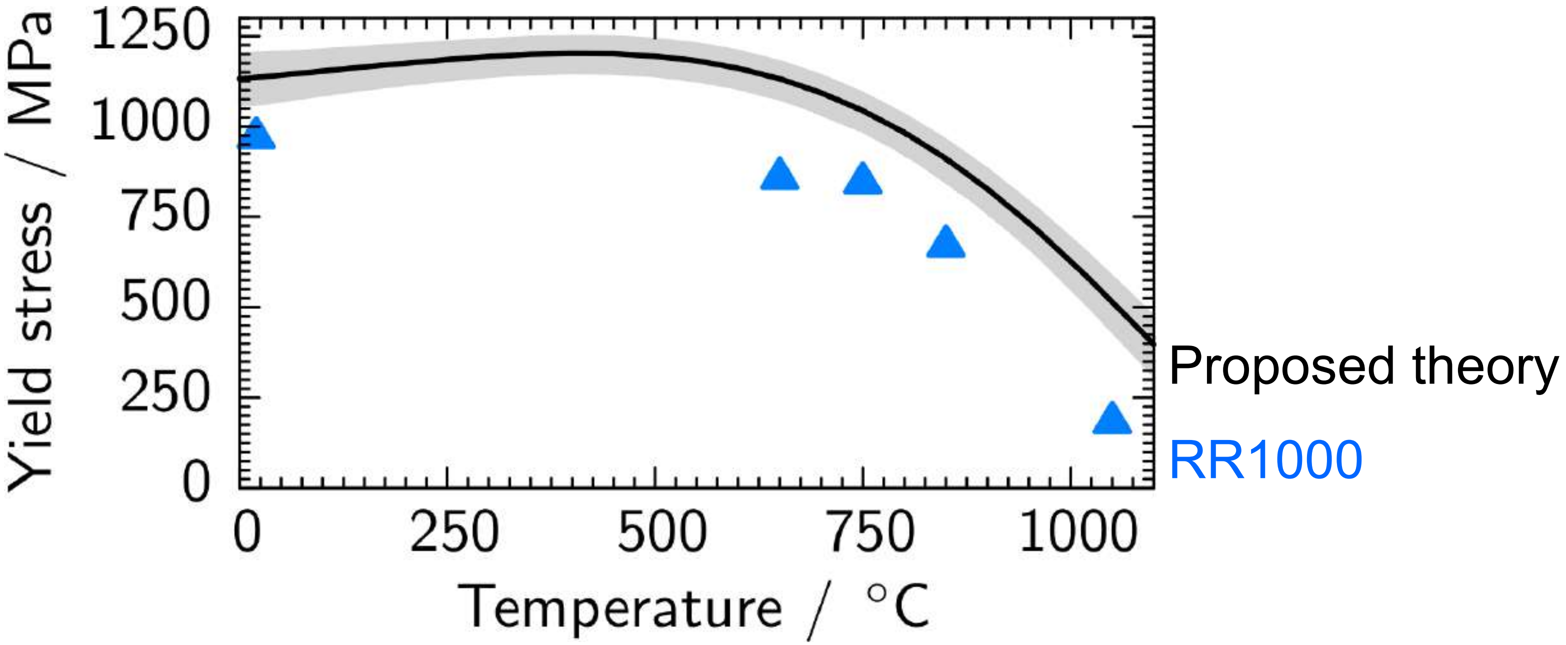
Microstructure



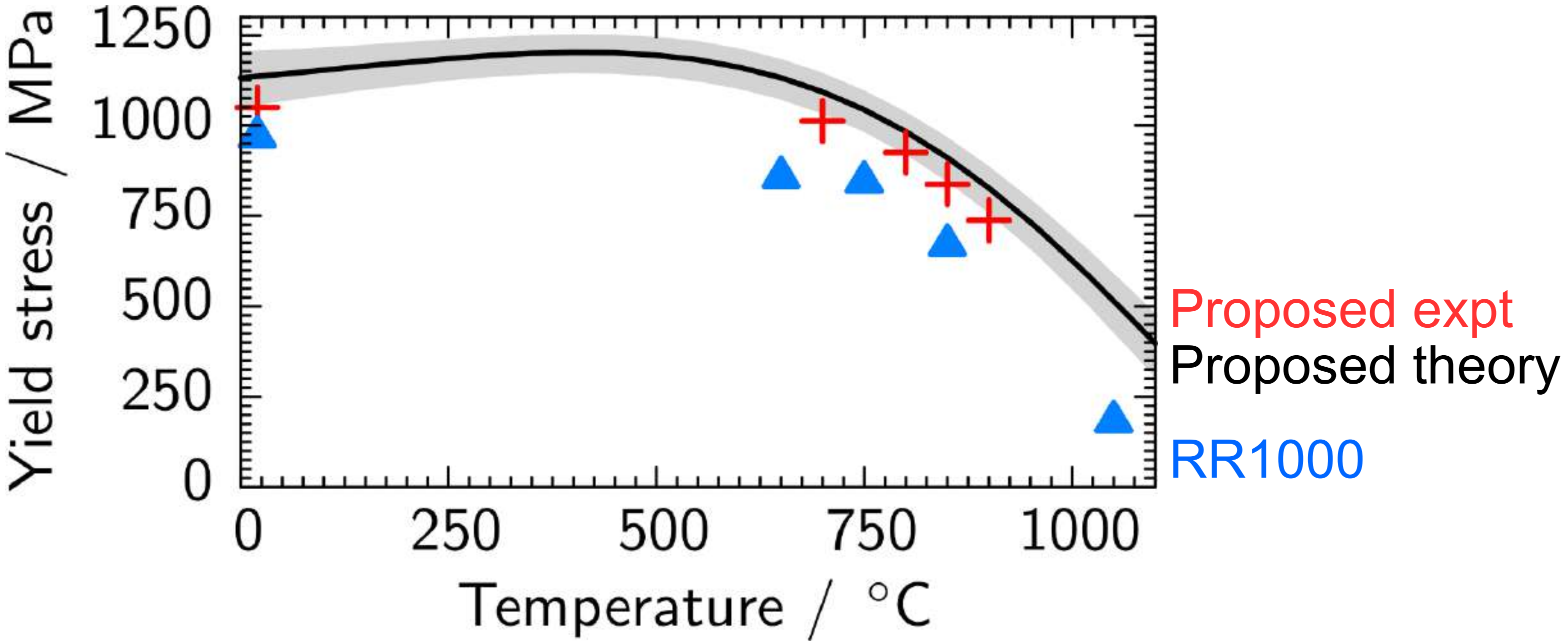
Testing the yield stress



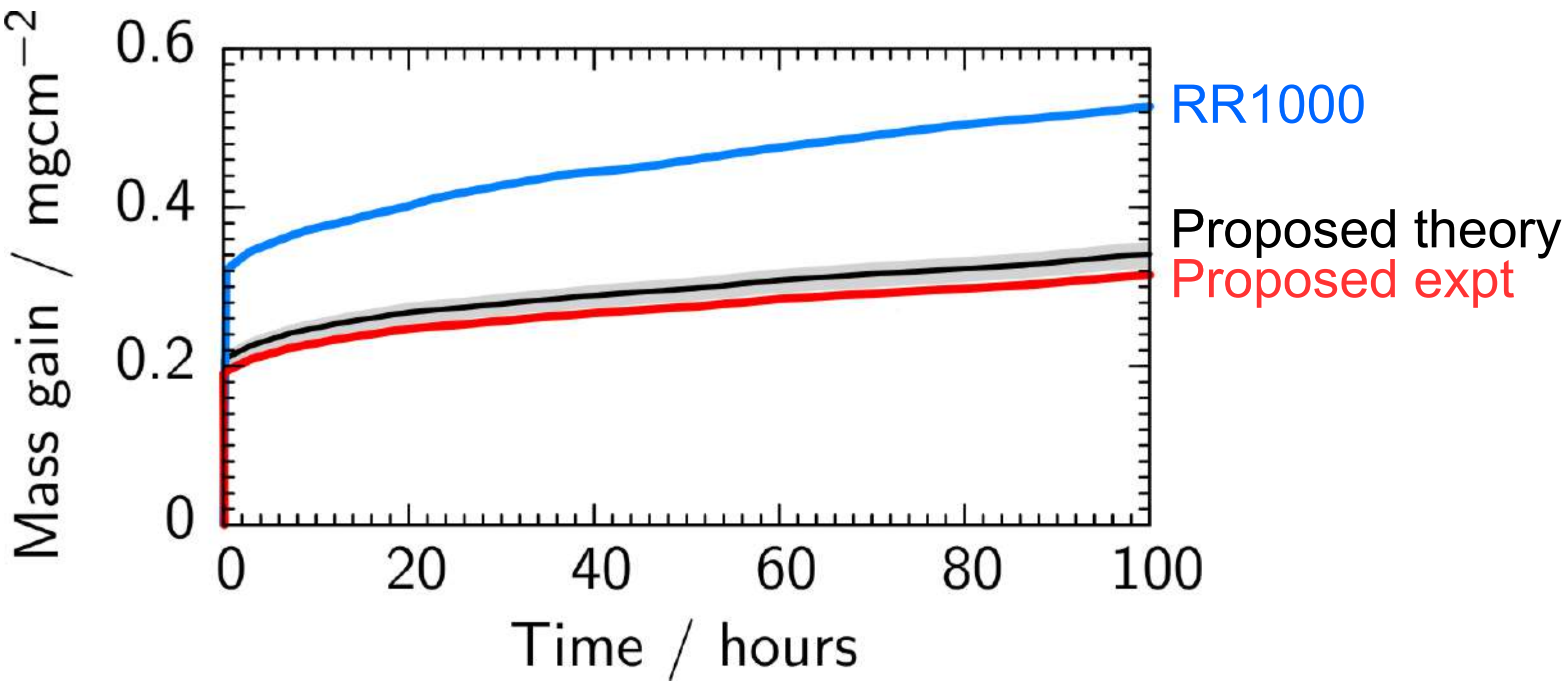
Testing the yield stress



Testing the yield stress

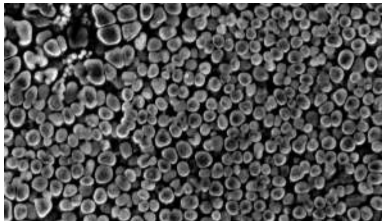


Testing the oxidation resistance



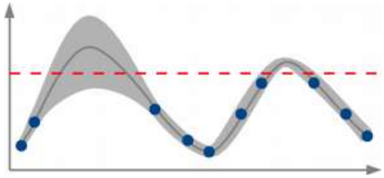
Alloys discovered

Ni disc alloy
EP14157622
US 2013/0052077 A2

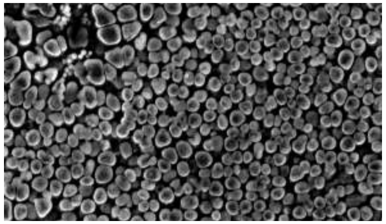


Alloys discovered

Discovery algorithm
EP14153898
US 2014/177578

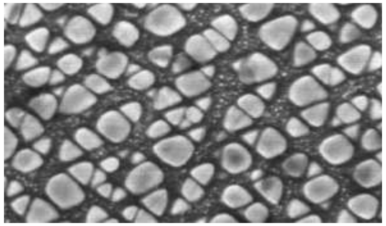


Ni disc alloy
EP14157622
US 2013/0052077 A2

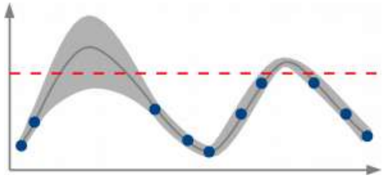


Alloys discovered

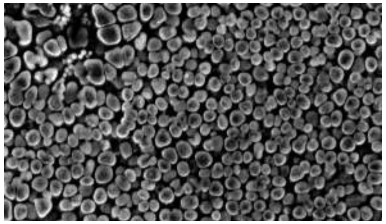
Combustor alloy
GB1408536



Discovery algorithm
EP14153898
US 2014/177578

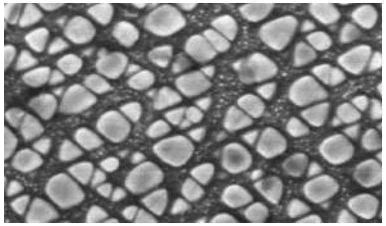


Ni disc alloy
EP14157622
US 2013/0052077 A2

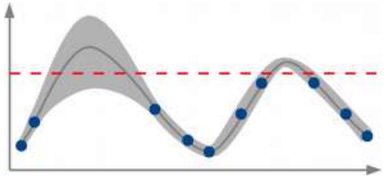


Alloys discovered

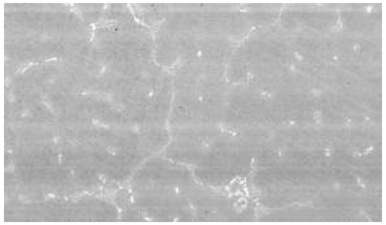
Combustor alloy
GB1408536



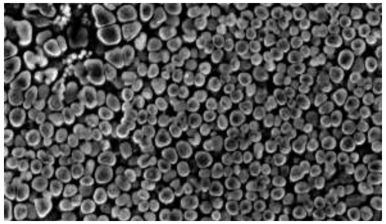
Discovery algorithm
EP14153898
US 2014/177578



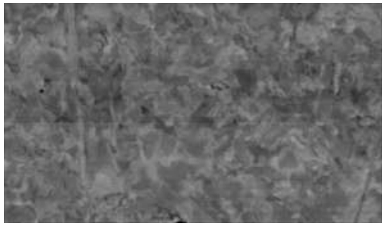
Mo-Hf forging alloy
EP14161255
US 2014/223465



Ni disc alloy
EP14157622
US 2013/0052077 A2

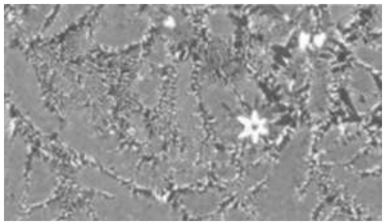


Mo-Nb forging alloy
EP14161529
US 2014/224885

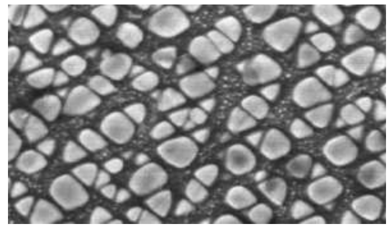


Alloys discovered

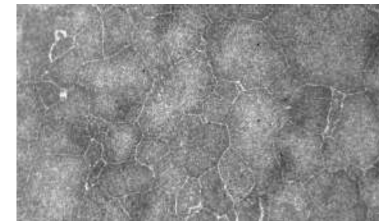
Cr-Cr_2Ta alloys
Intermetallics, 48, 62



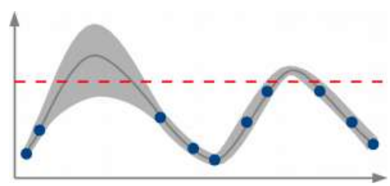
Combustor alloy
GB1408536



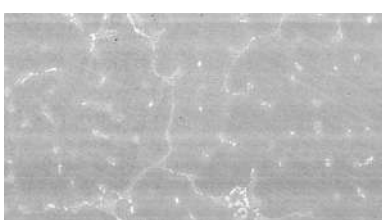
RR1000 grain growth
Acta Materialia, 61, 3378



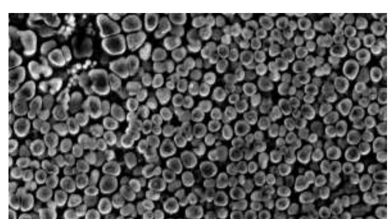
Discovery algorithm
EP14153898
US 2014/177578



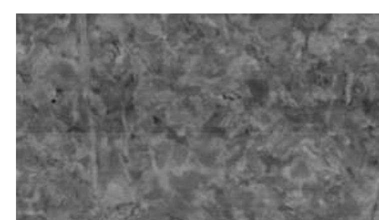
Mo-Hf forging alloy
EP14161255
US 2014/223465



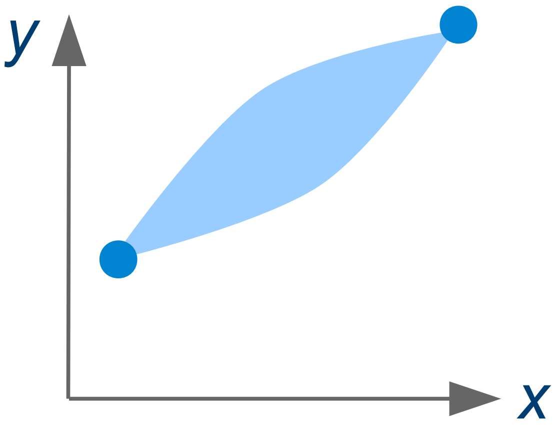
Ni disc alloy
EP14157622
US 2013/0052077 A2



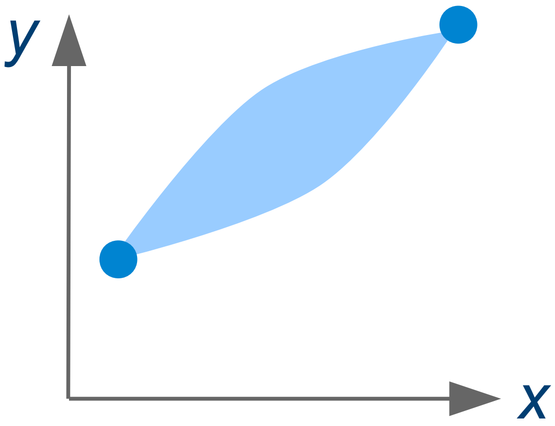
Mo-Nb forging alloy
EP14161529
US 2014/224885

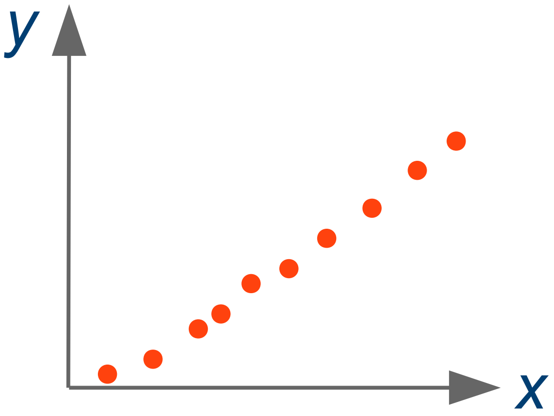


Merging simulation and experiment

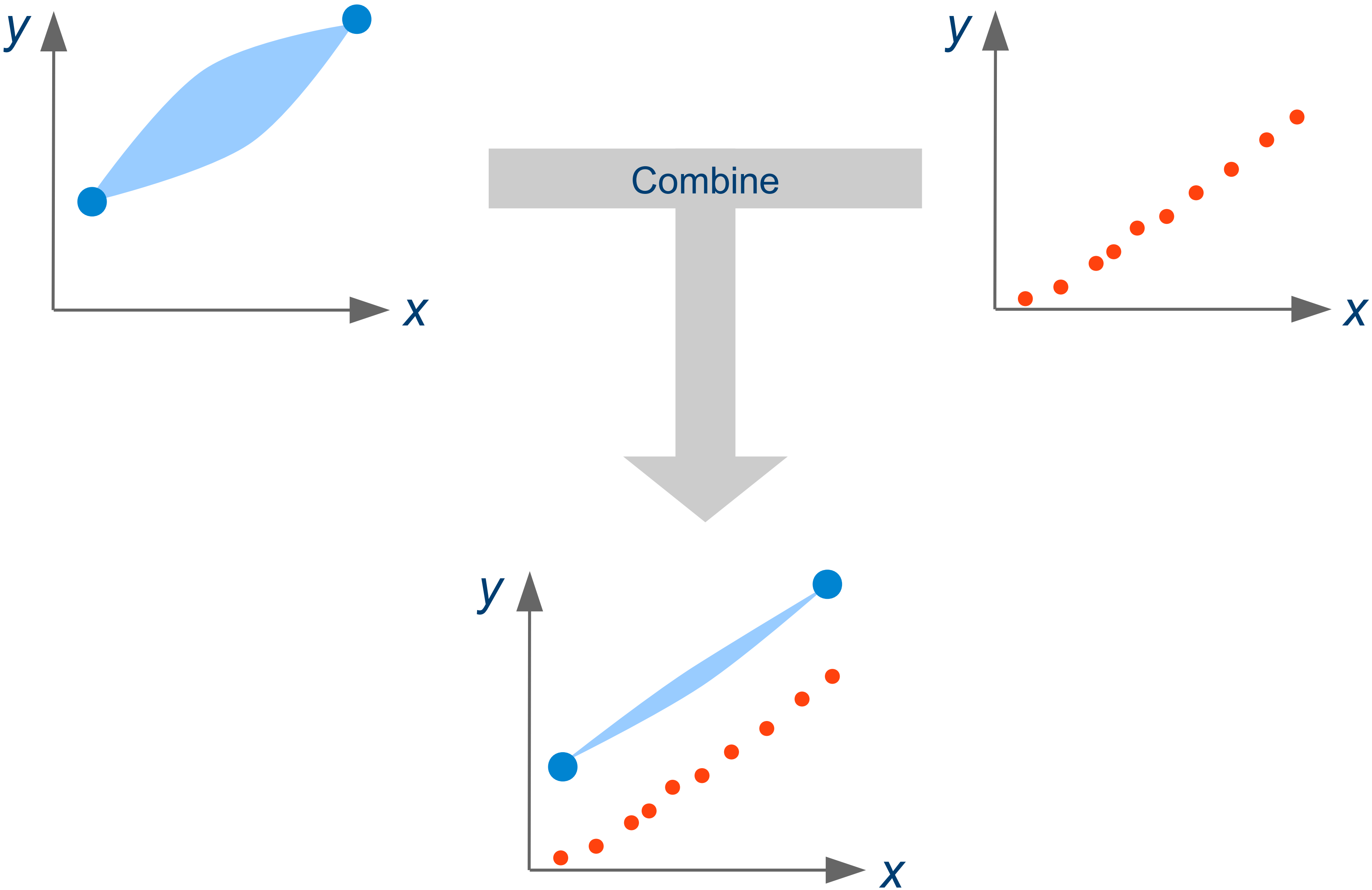


Merging simulation and experiment





Merging simulation and experiment



Artificial intelligence

Composition

Artificial intelligence

Yield stress

Hardness

Melting point

Oxidation resistance

Cost

Density

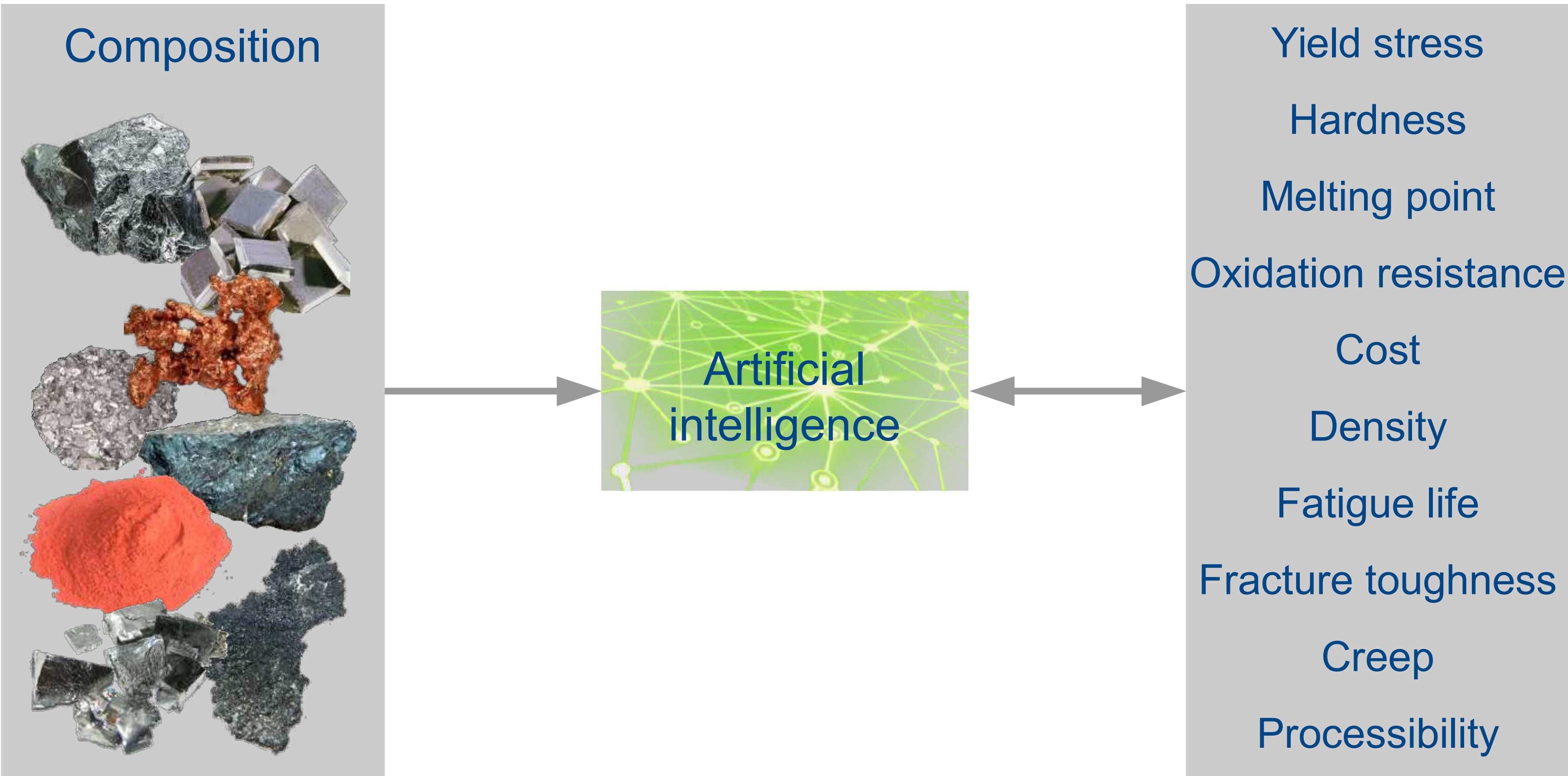
Fatigue life

Fracture toughness

Creep

Processibility

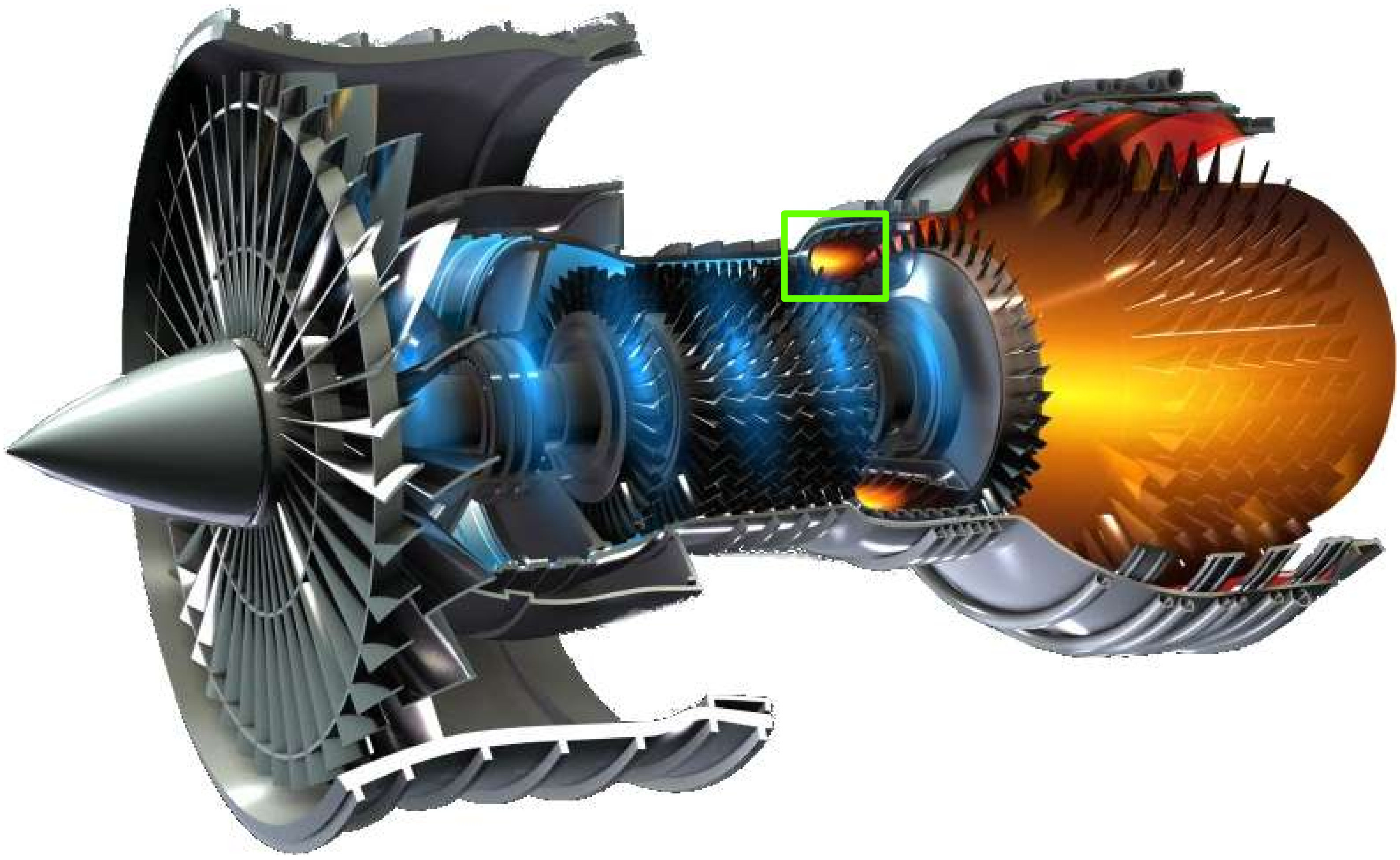
Artificial intelligence



Exploiting material correlations

Alloy for direct laser deposition

Combustor liner



Artificial intelligence

Composition

Simulations

Yield stress

Hardness

Melting point

Oxidation resistance

Cost

Density

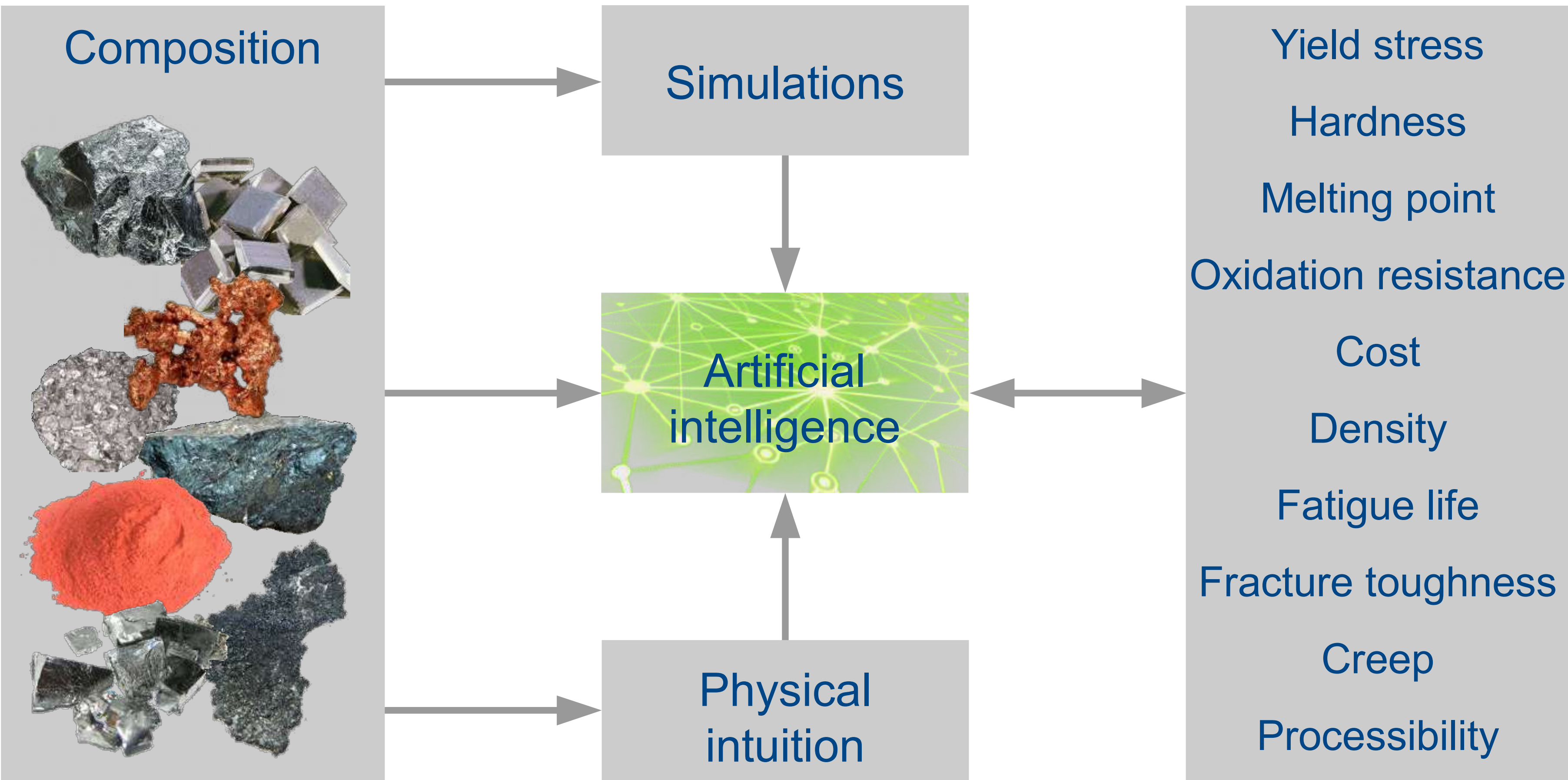
Fatigue life

Fracture toughness

Creep

Processibility

Artificial intelligence



Exploiting material correlations

Alloy for direct laser deposition

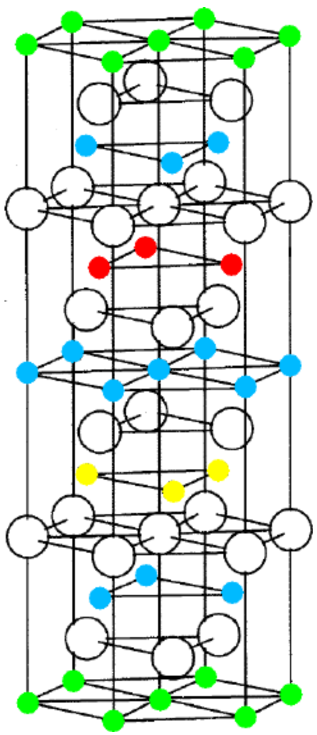
3D printability ⟷ Weldability

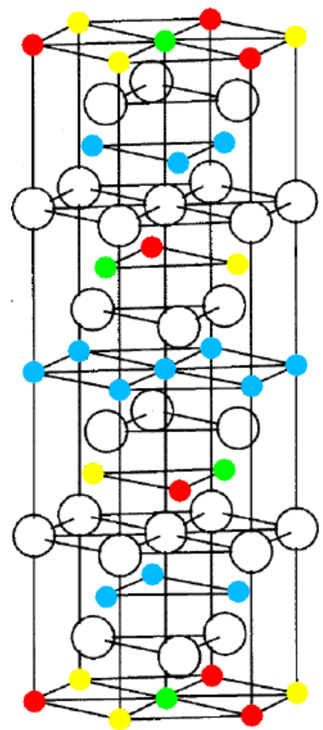
Lithium cathode materials

Experiment ⟷ DFT

Nickel-Cobalt-Manganese (NCM) battery materials

NCM-424 battery structure

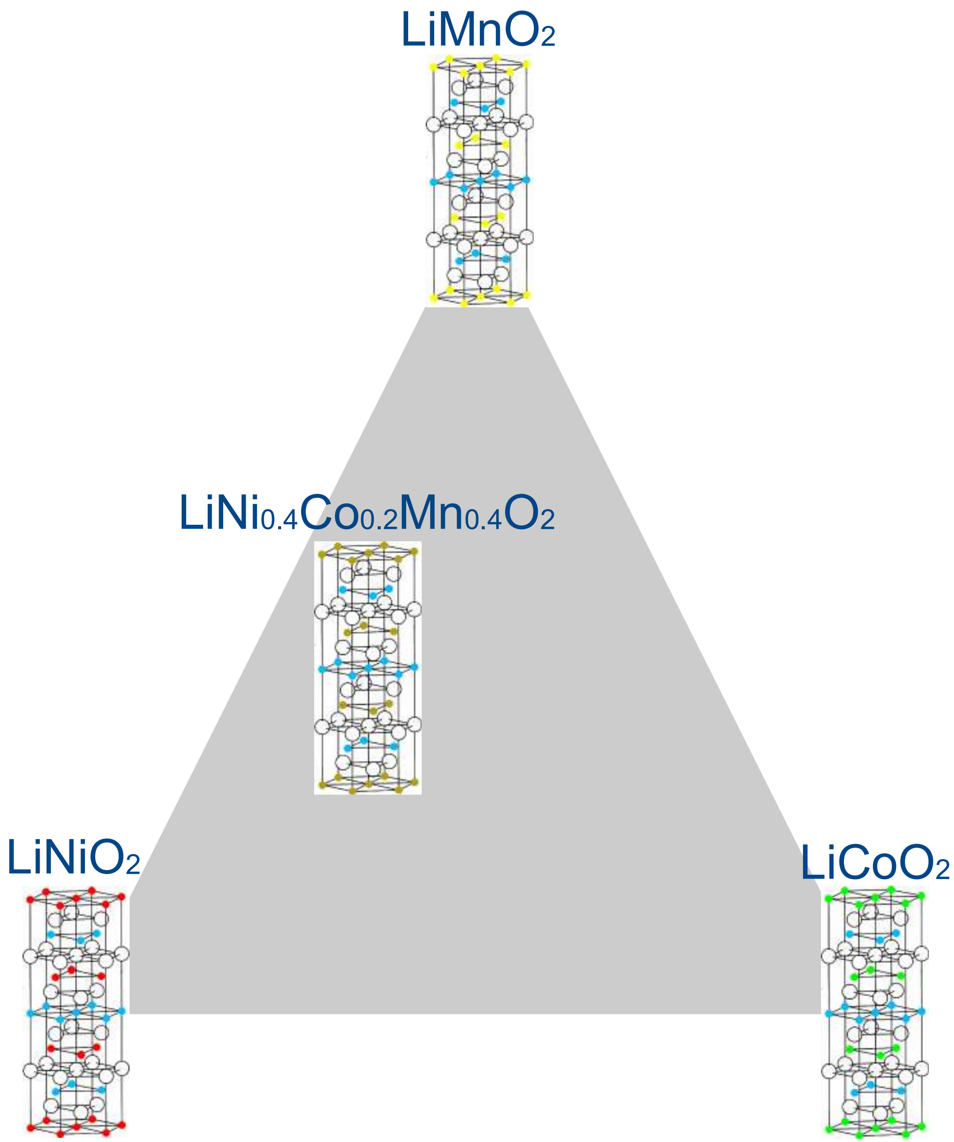




$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$

	O
	Li
	Ni
	Co
	Mn

Traditional approach



0.4Ni → 7.2 atoms
0.2Co → 3.6 atoms
0.4Mn → 7.2 atoms

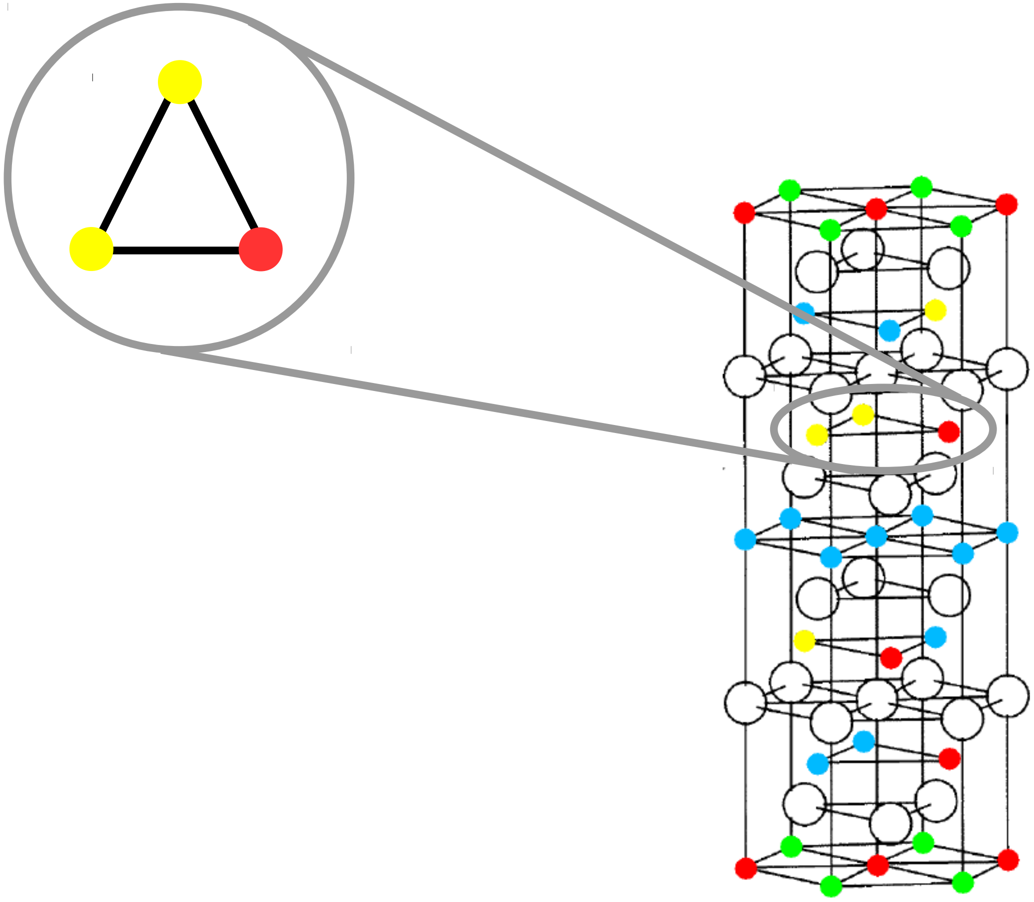
153153000
possible
permutations
=42000 years

Access any composition
Information on order
Li migration

Approach: characterize with a local order matrix

$N_{\text{yellow-yellow}}=1$

$N_{\text{yellow-red}}=2$

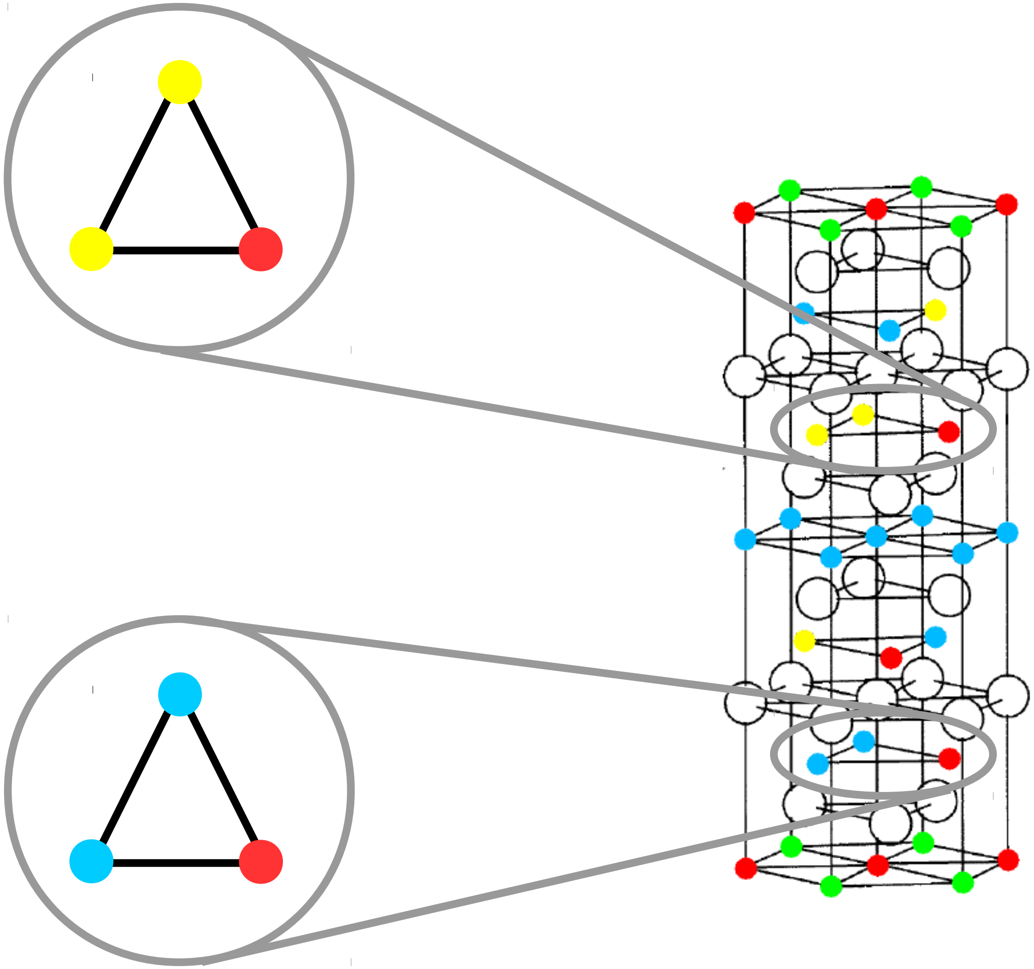


Approach: characterize with a local order matrix

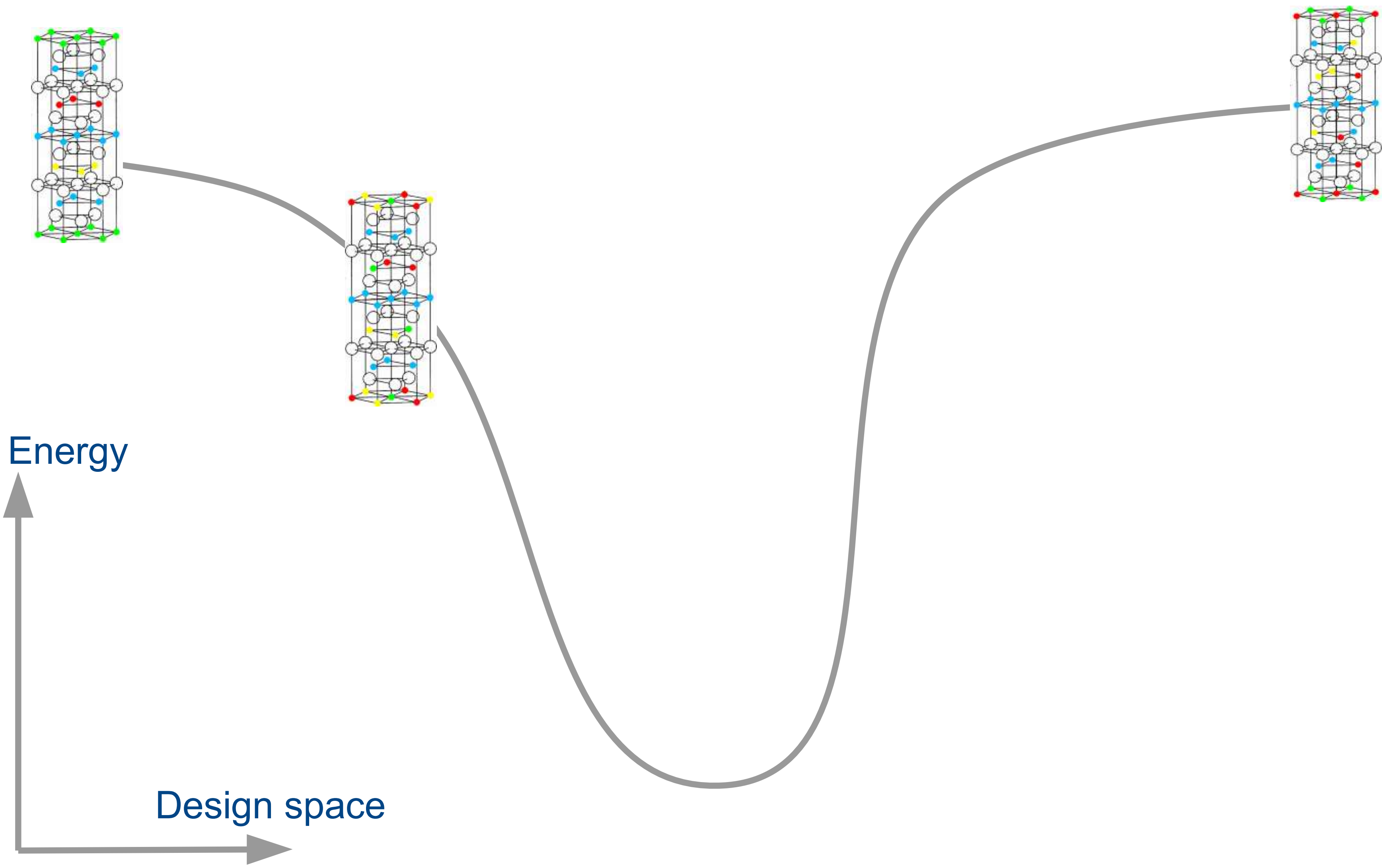
$N_{\text{yellow-yellow}}=1$

$N_{\text{yellow-red}}=2$

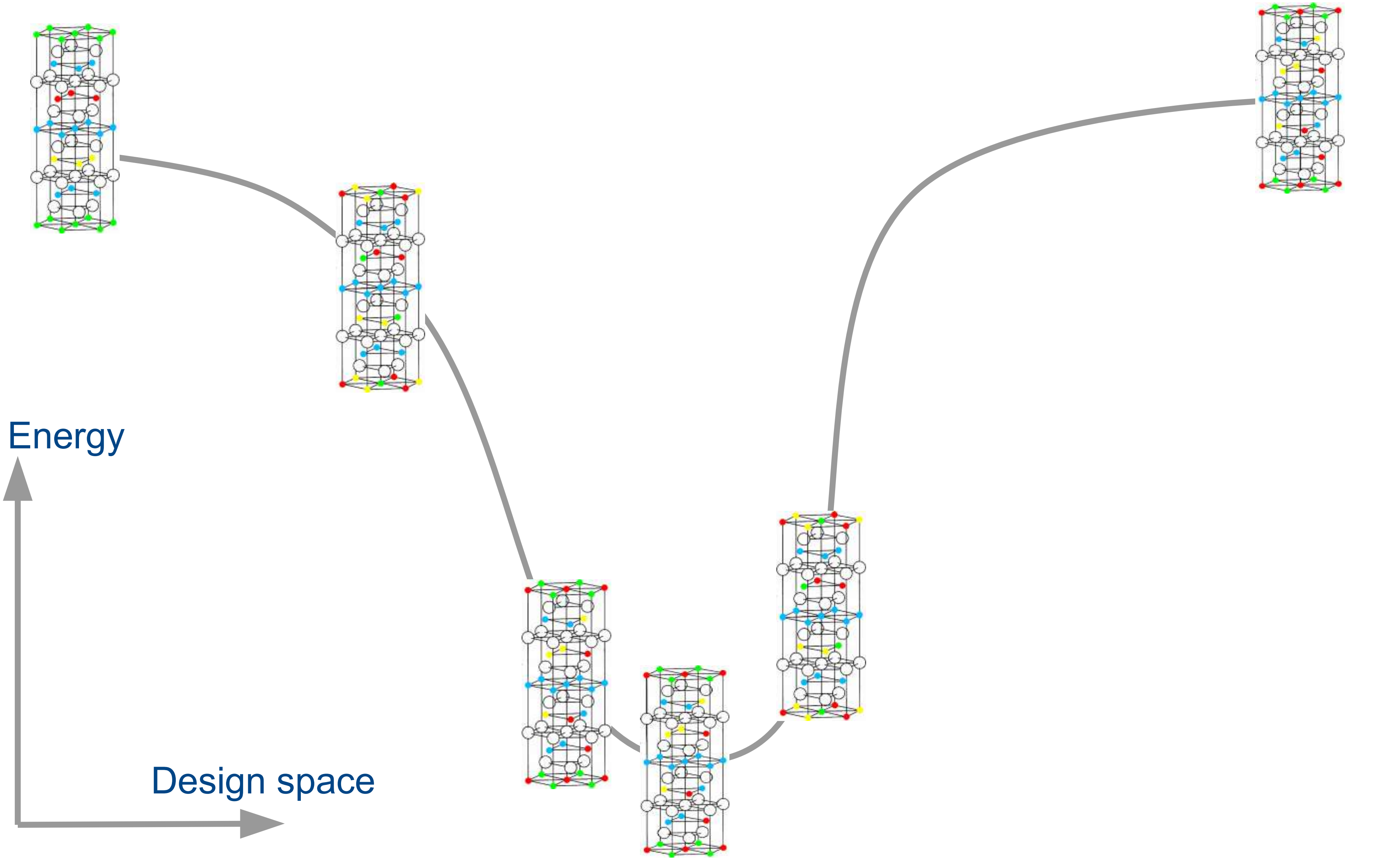
$N_{\text{red migrate}}=1$



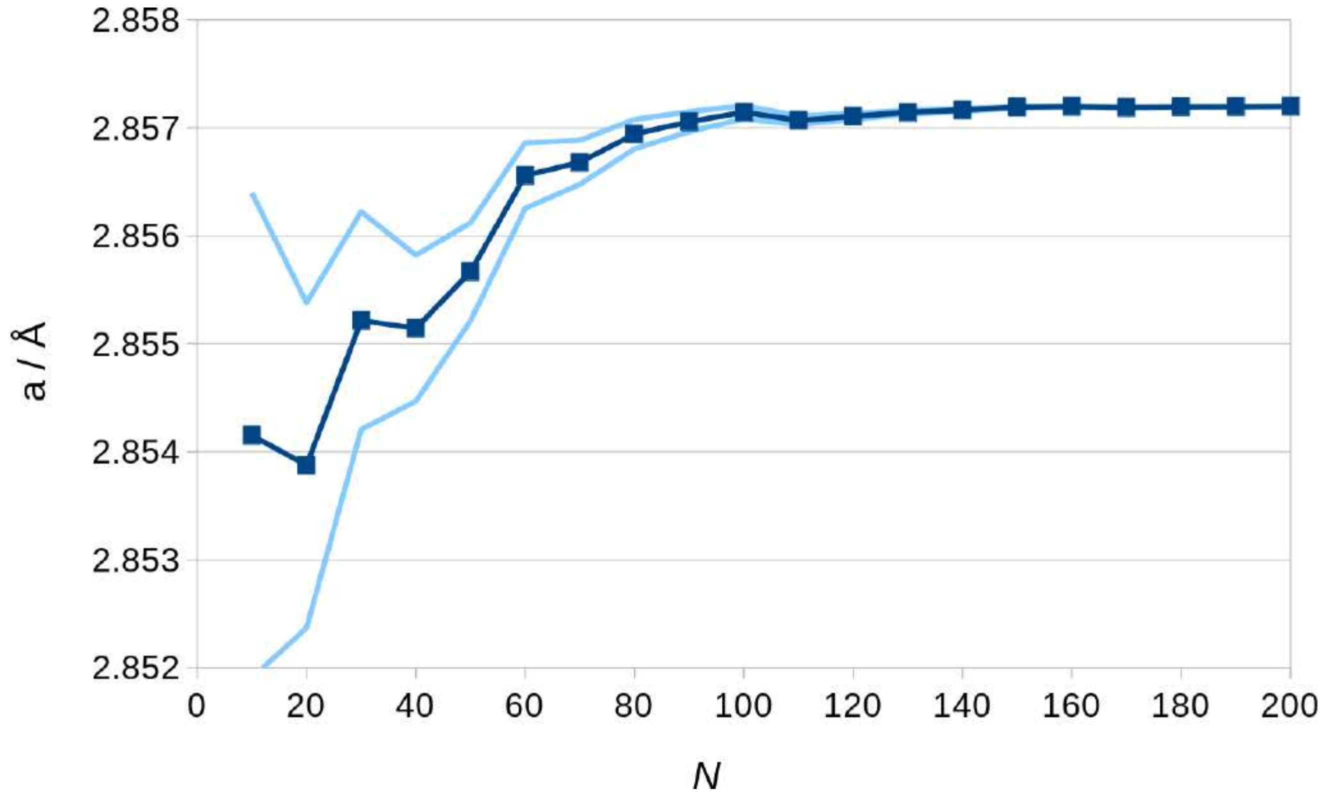
Recursive learning



Recursive learning



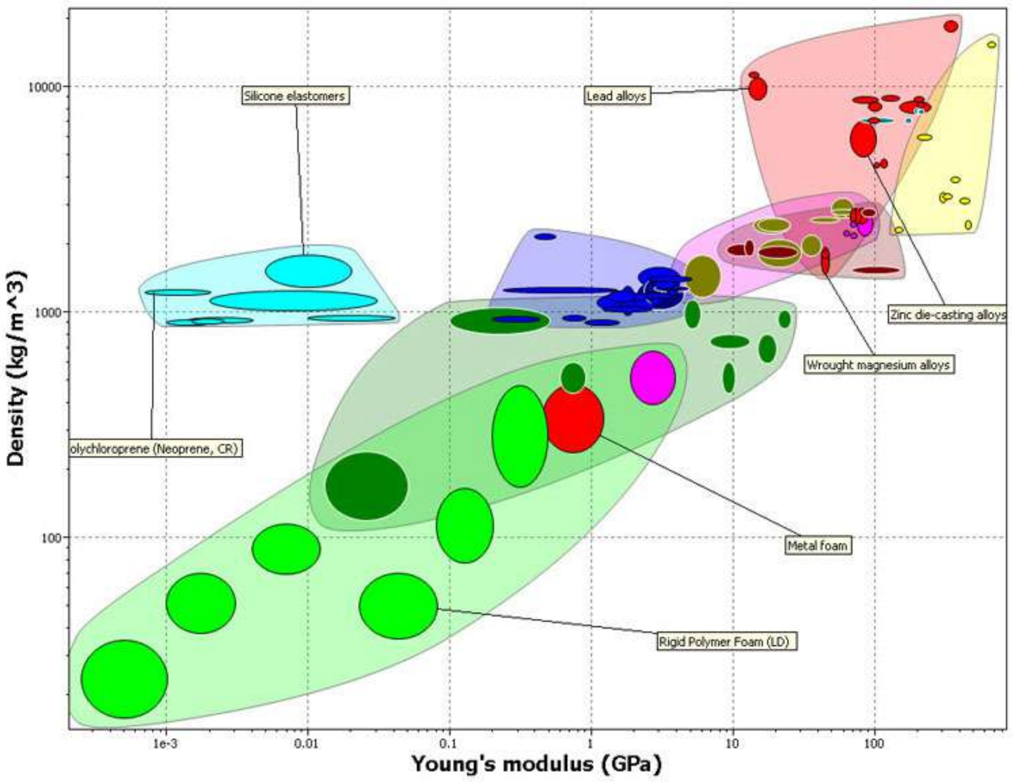
How many calculations are required



Local order matrix

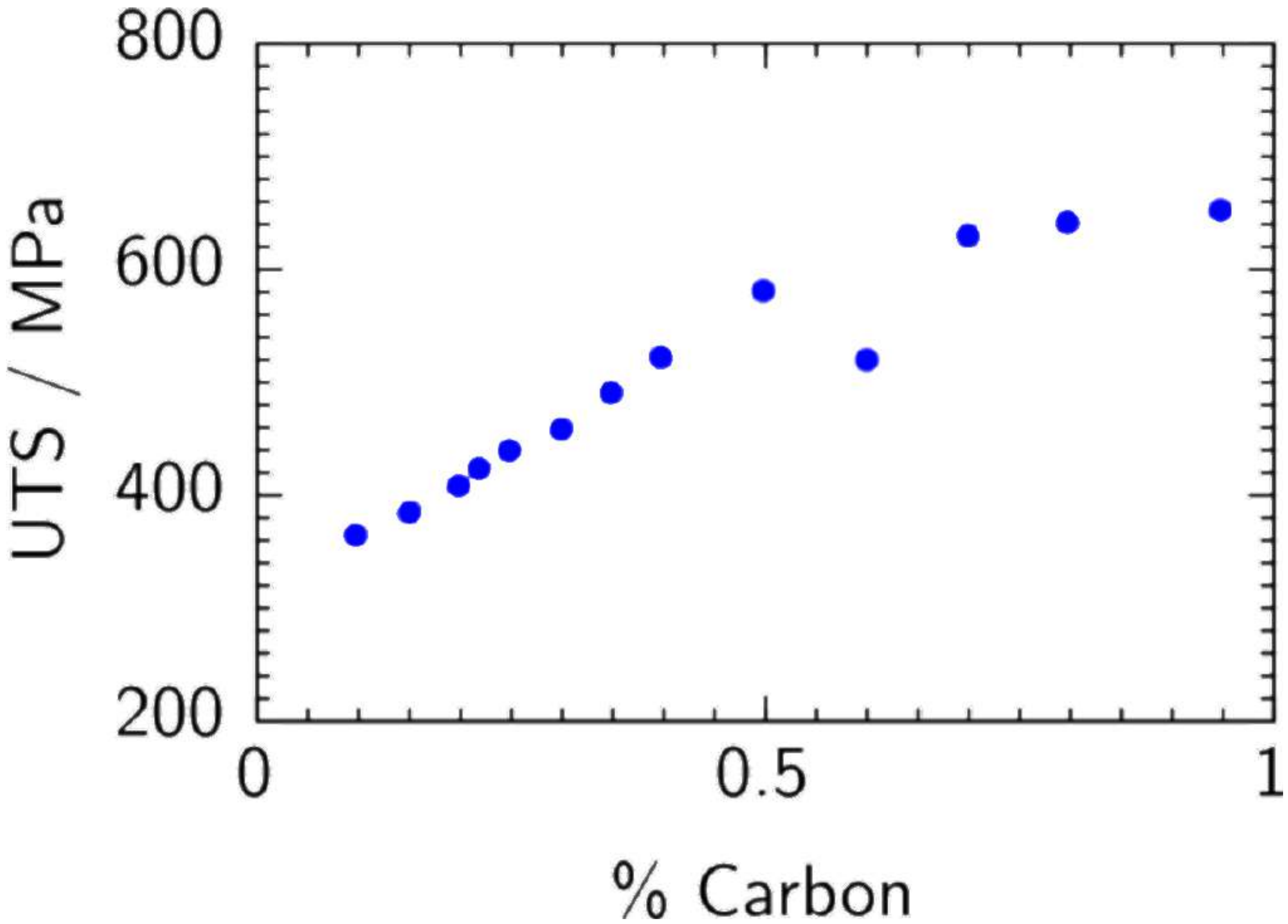
Matrix element	Optimal	From NMR
$N_{Co\text{-}Co}$	0.34	0.2
$N_{Ni\text{-}Ni}$	0.16	0.3
$N_{Mn\text{-}Mn}$	0.09	0.0
$N_{Li\text{-}Li}$	0.08	0.0
$N_{Co\text{-}Ni}$	2.5	2.1
$N_{Co\text{-}Mn}$	0.2	0.1
$N_{Ni\text{-}Mn}$	3.4	3.1
$N_{Ni\text{-}Li}$	0.32	0.2
$N_{Co\text{-}Li}$	0.21	0.1
$N_{Mn\text{-}Li}$	1.37	1.2
N_{Ni}	1.82	1.1
N_{Co}	0.02	0.3
N_{Mn}	0.01	0.1

Database verification

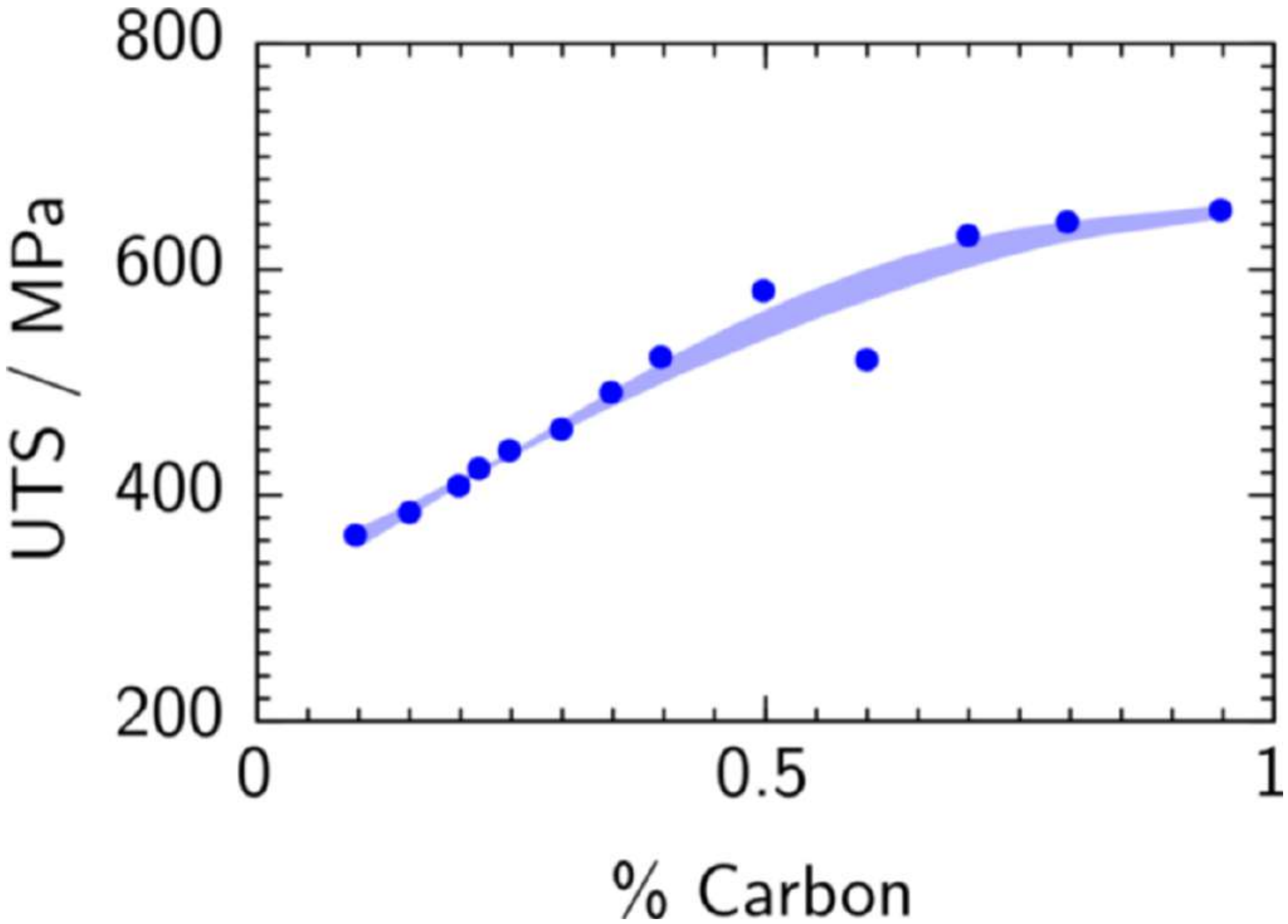


Database contains >10^7 separate entries

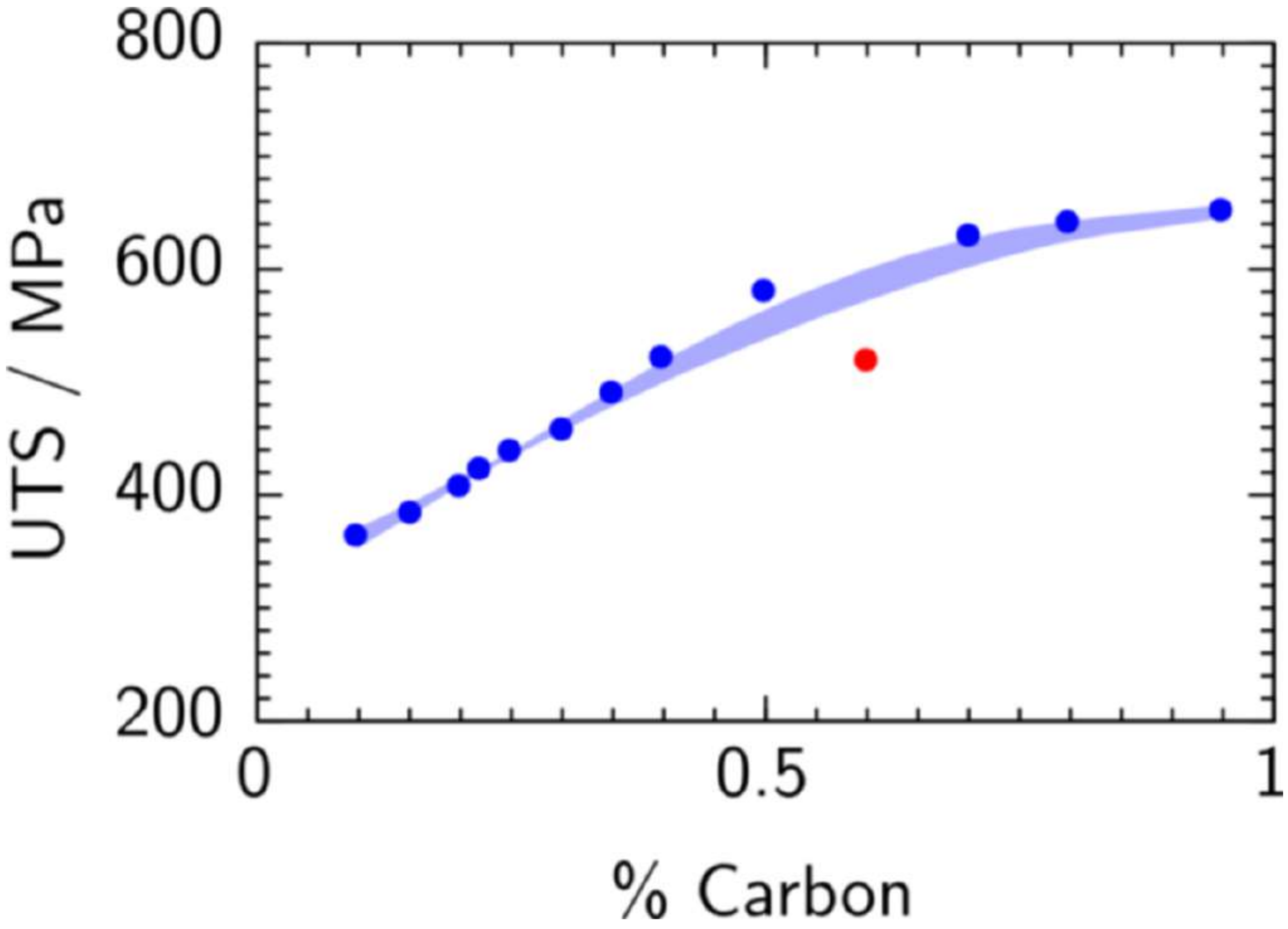
Example: steels



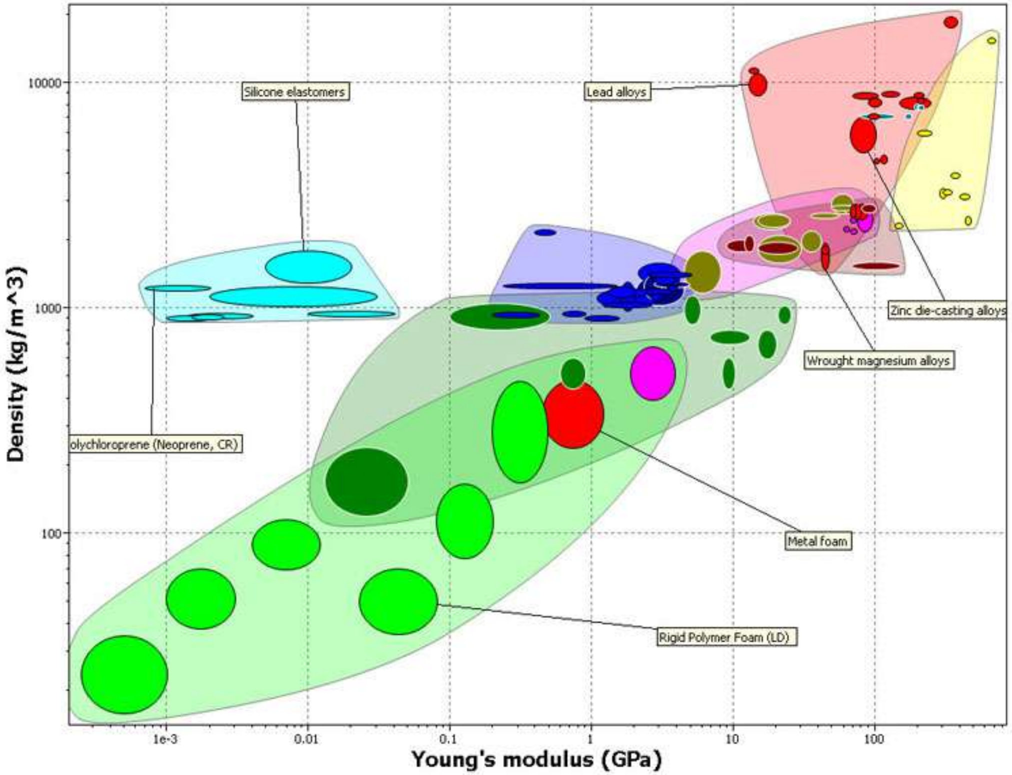
Example: steels



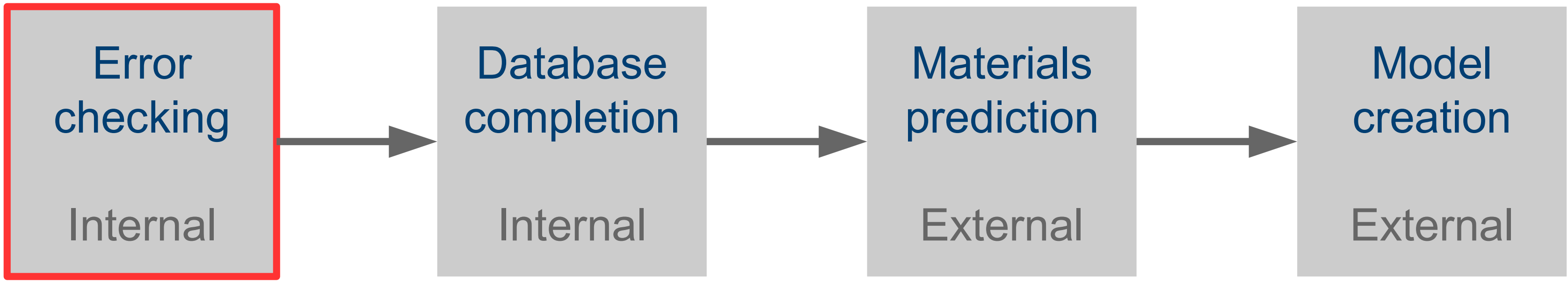
Example: steels



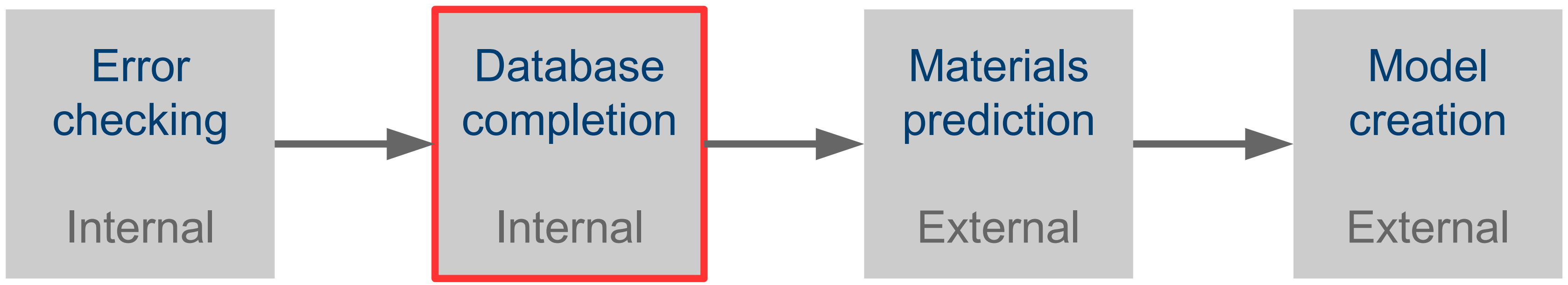
Database verification



Database verification



Database verification



Summary

Used artificial intelligence in materials discovery

Discovered four new alloys, experimentally verified, now real-world testing

Merge simulations and experiments into holistic design tool

Materials database verification and analysis