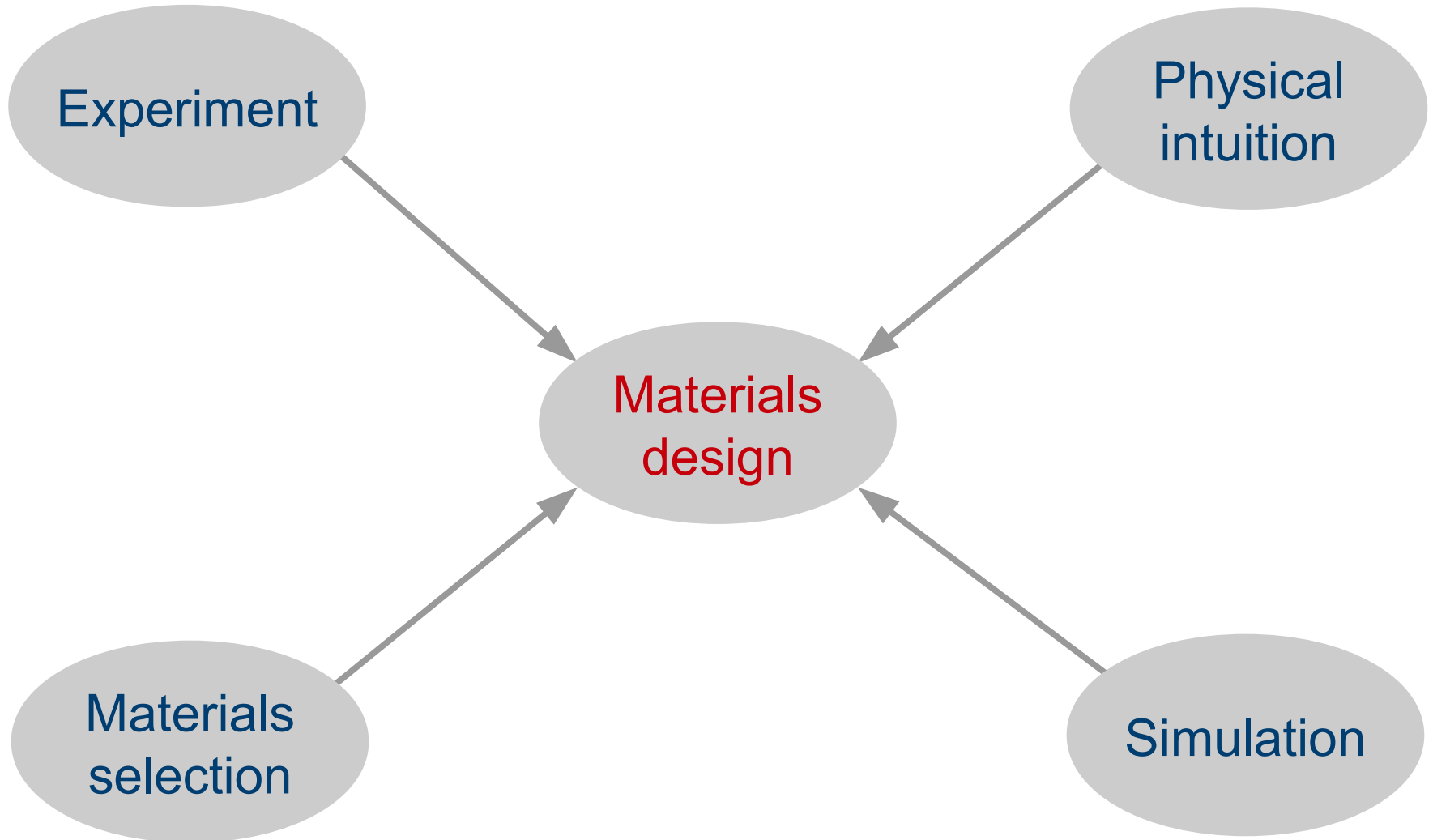


Materials discovery with artificial intelligence

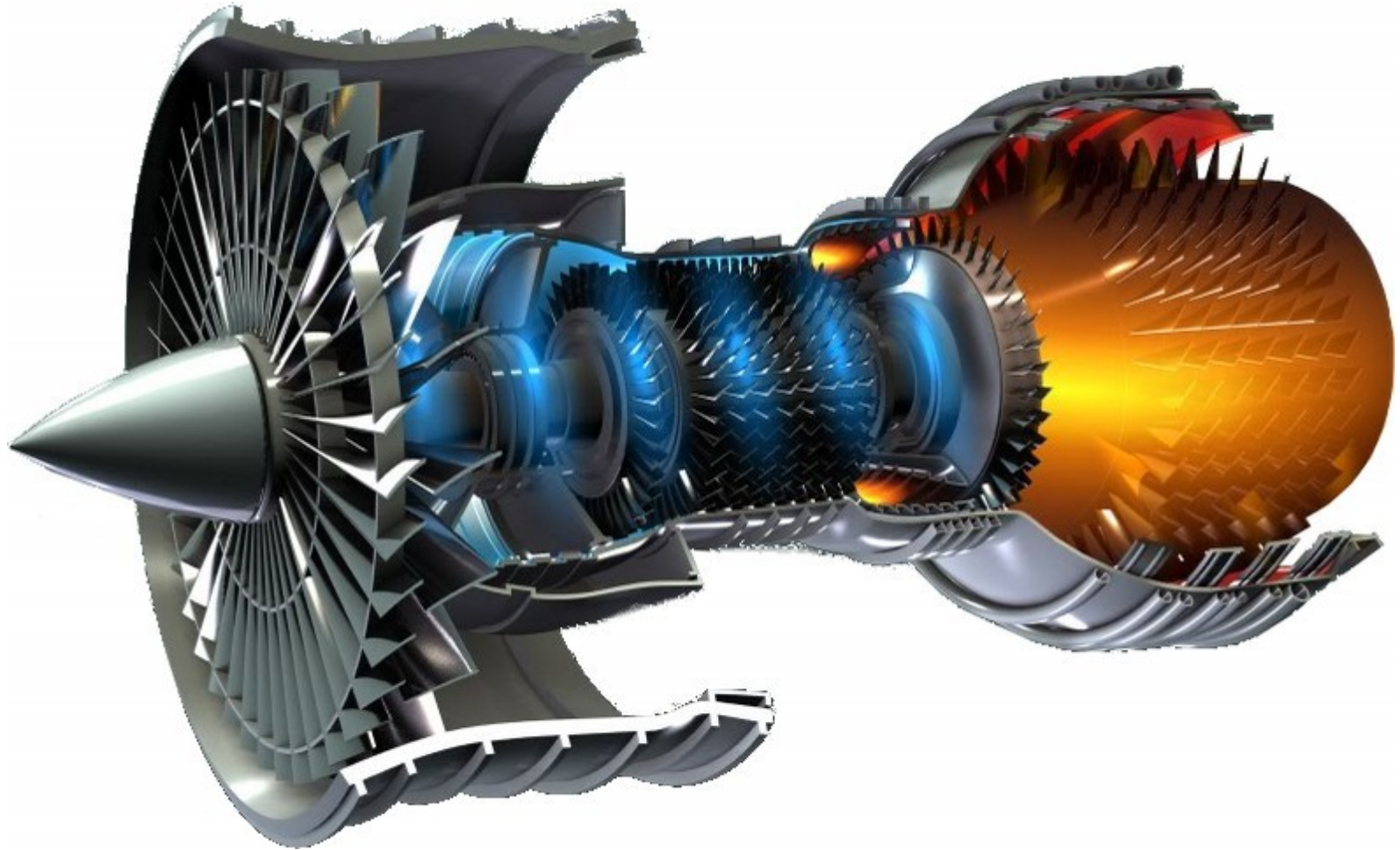
Gareth Conduit

TCM Group, Department of Physics

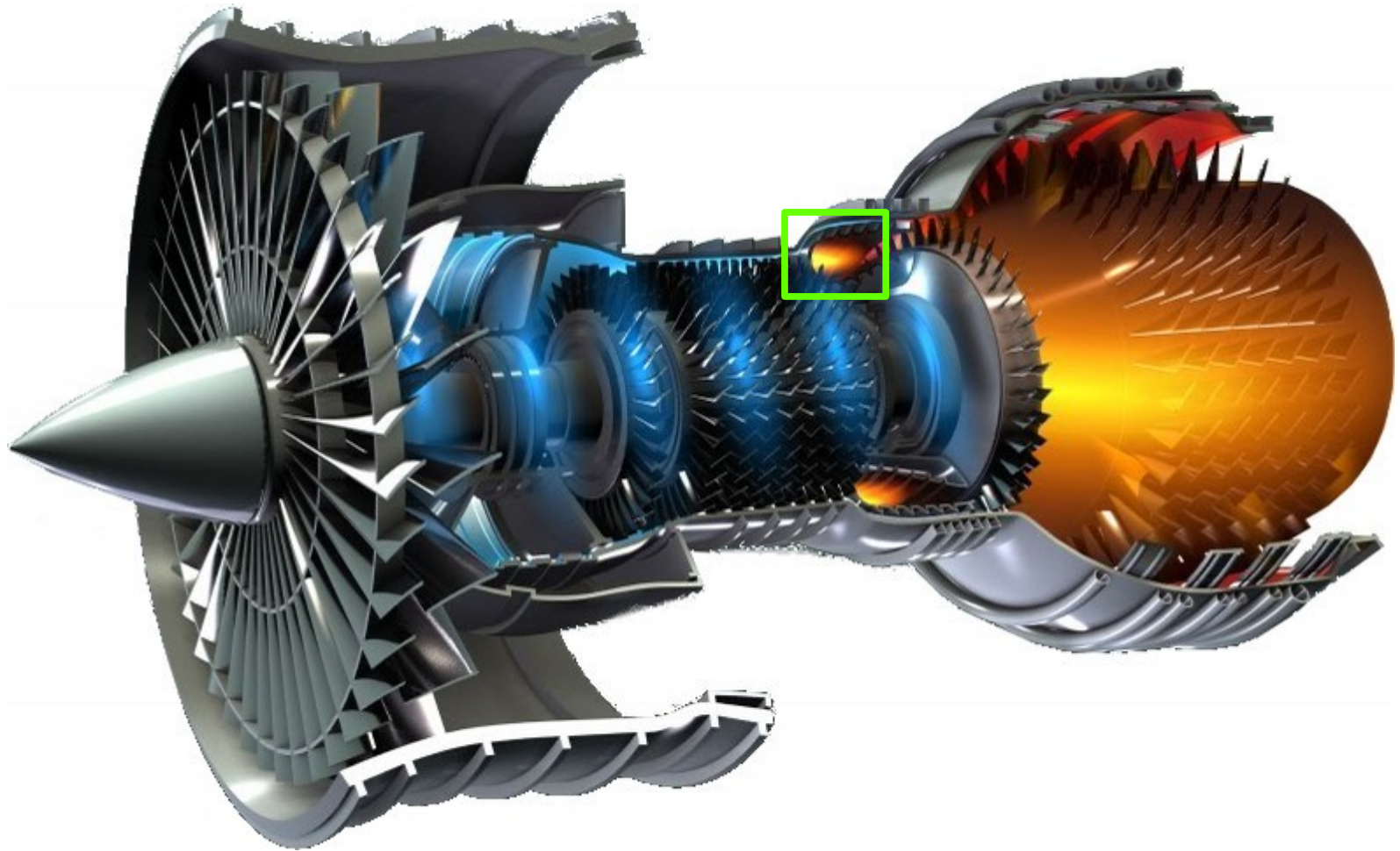
Approaches to materials design



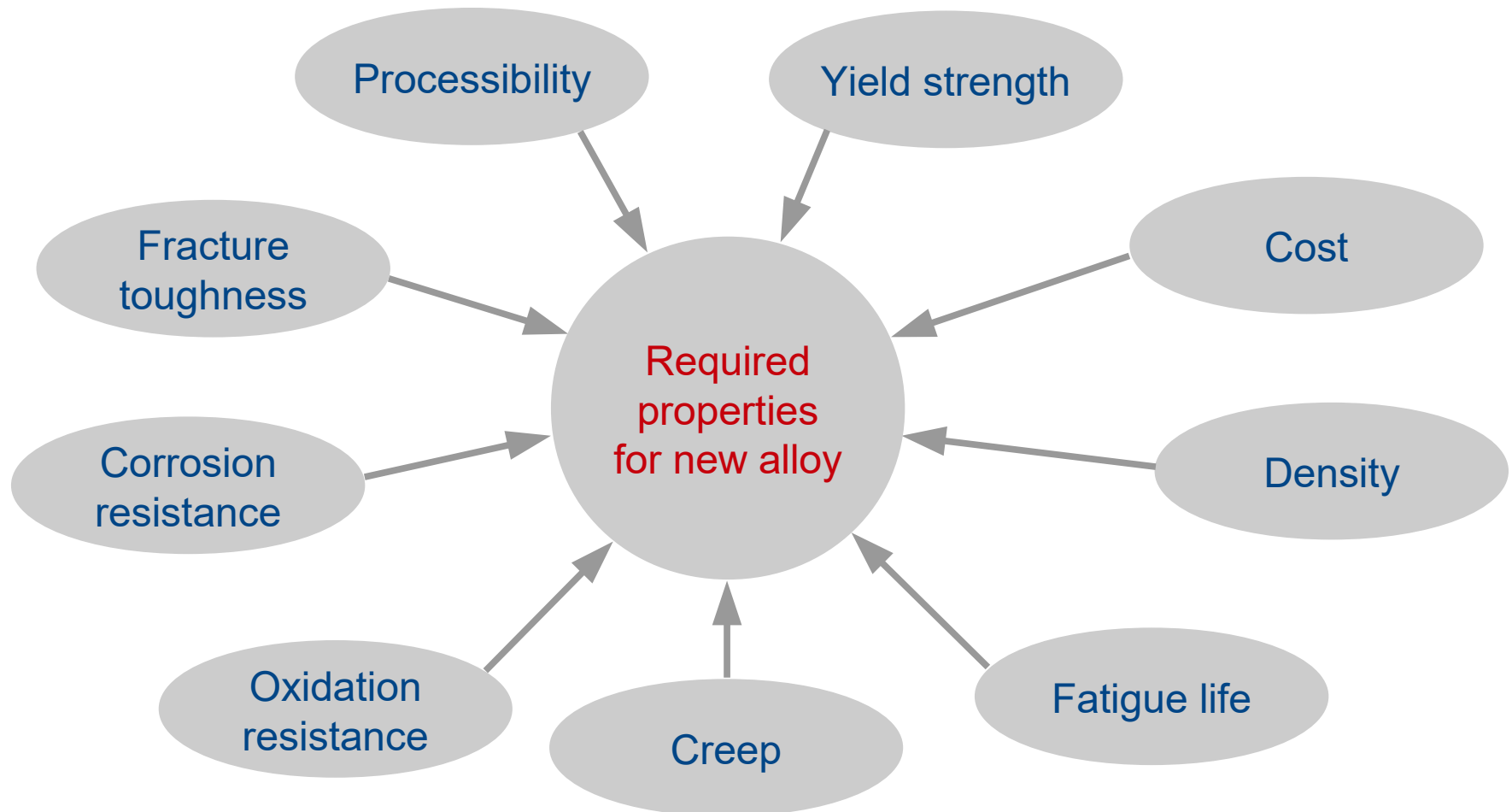
Schematic of a jet engine



Combustor liner



Designing a new alloy: what is required?

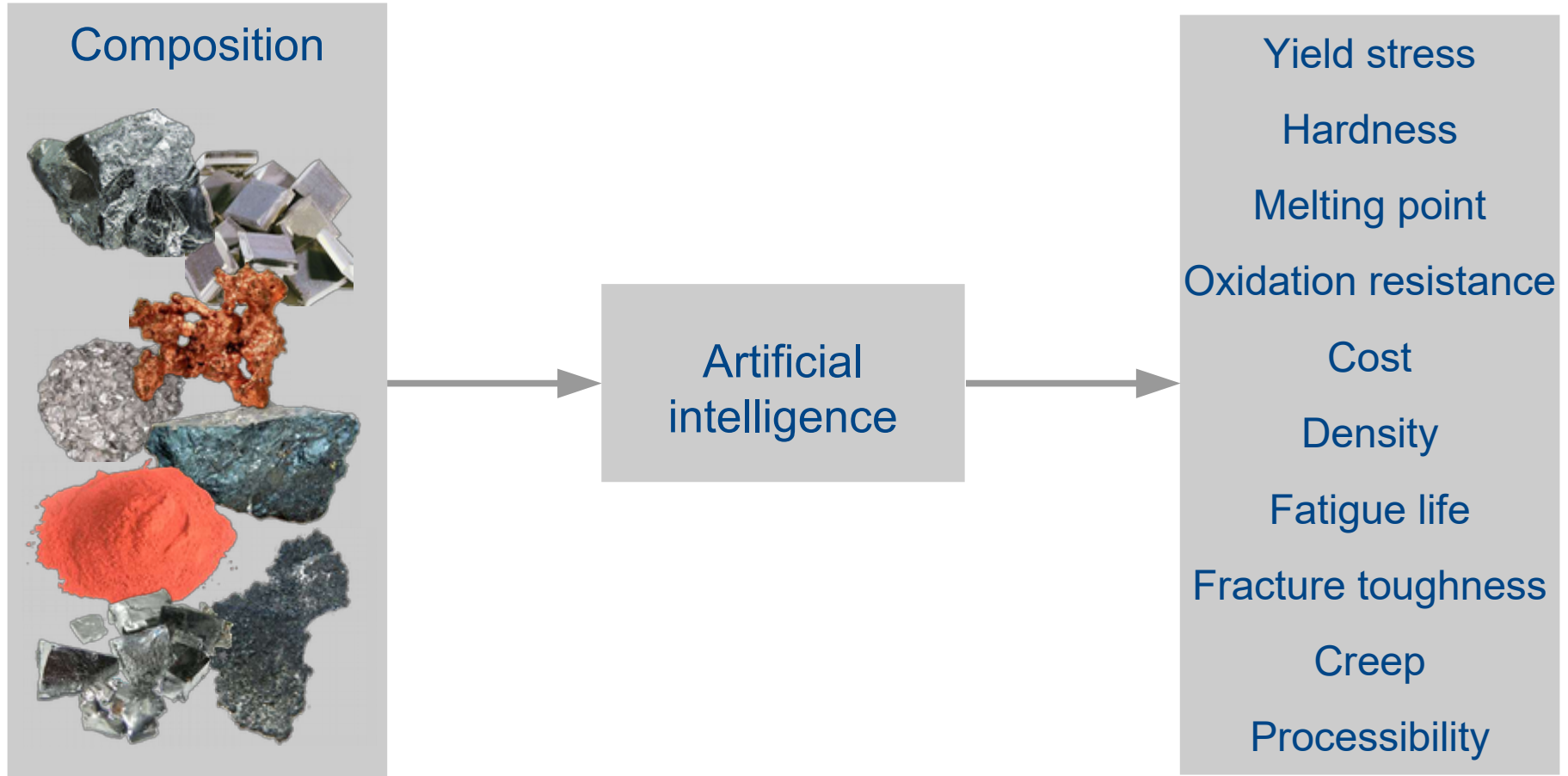


Multidimensional design space

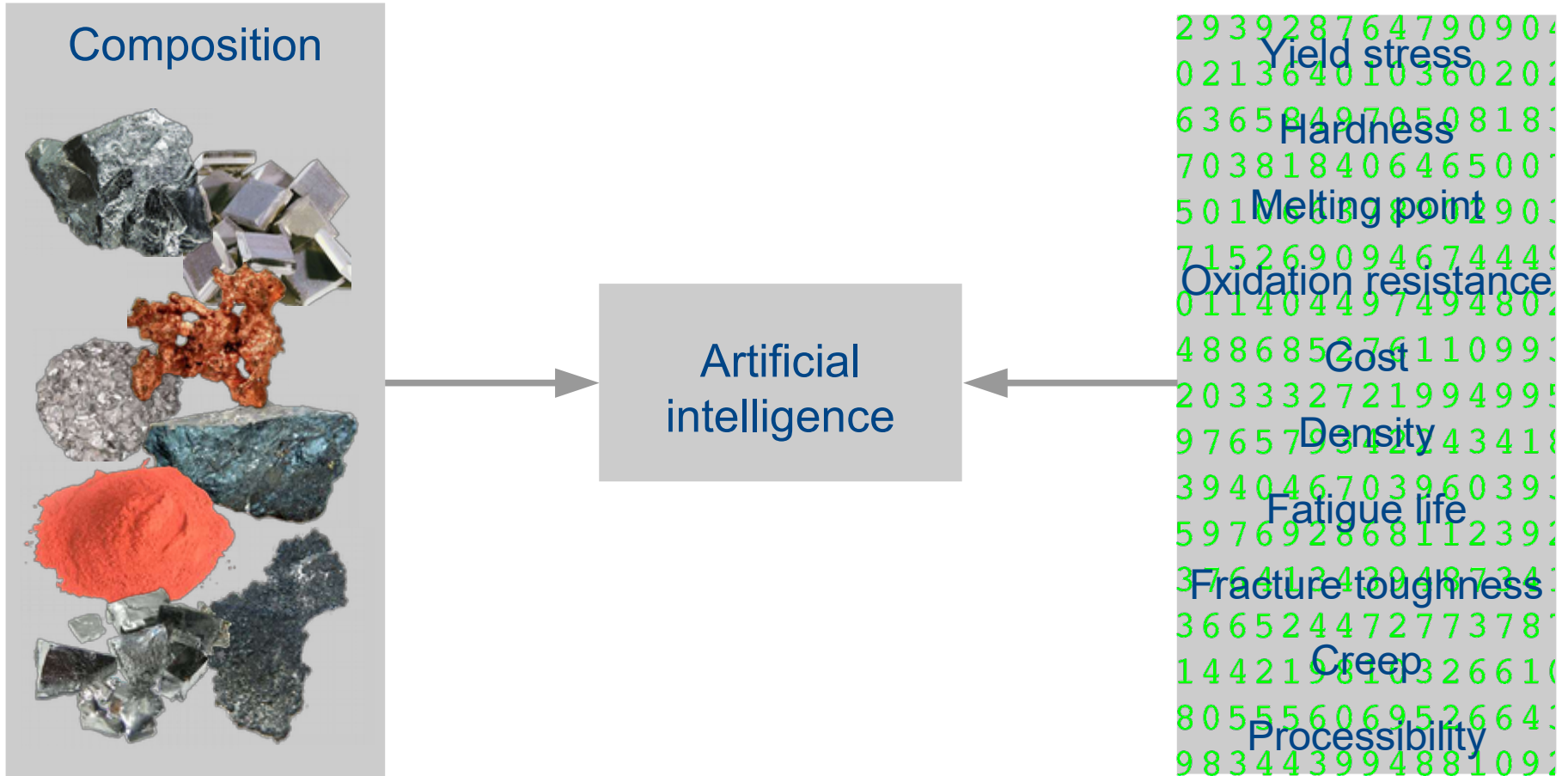


and 4 different manufacturing processes

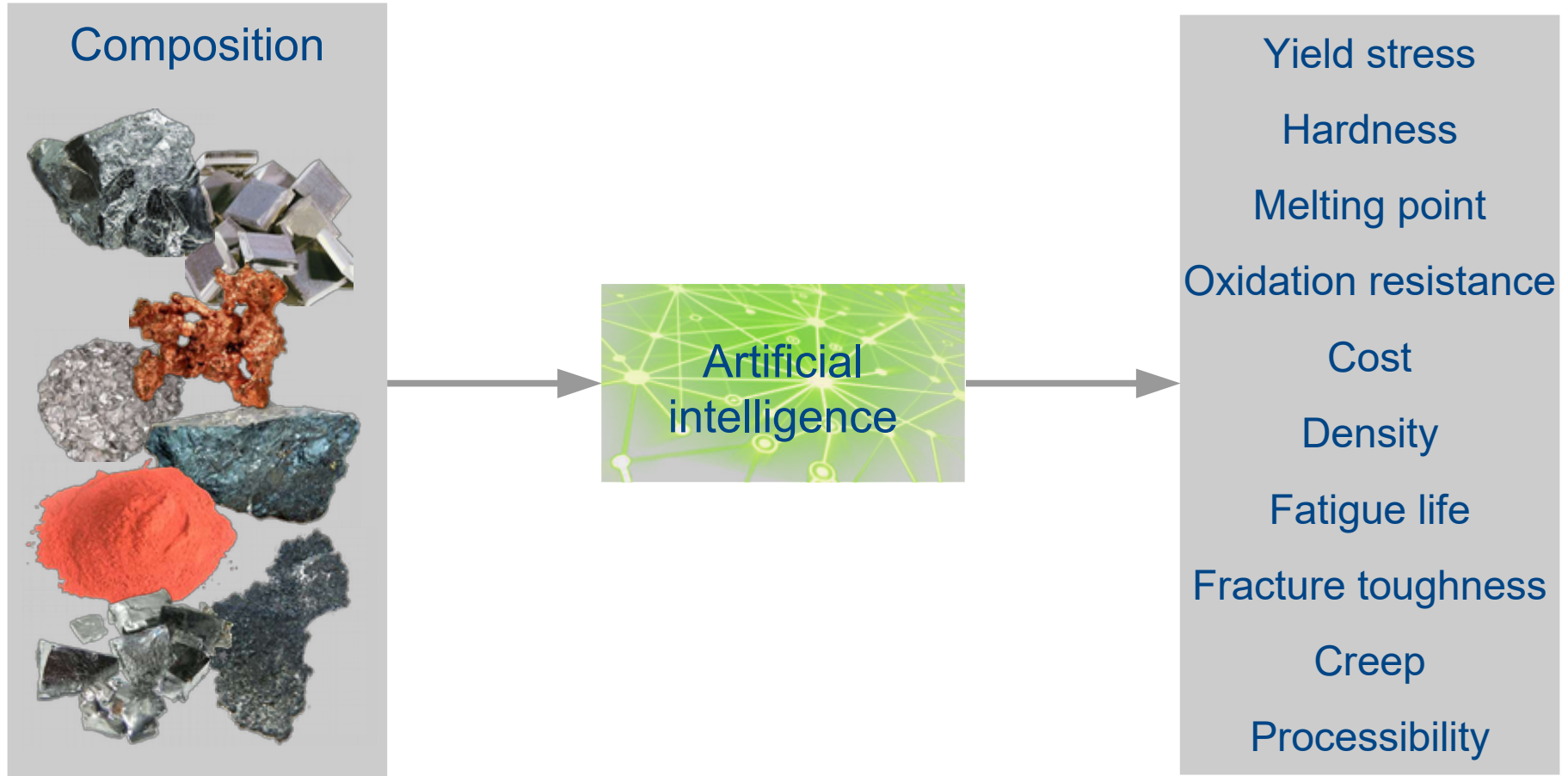
Artificial intelligence



Artificial intelligence



Artificial intelligence

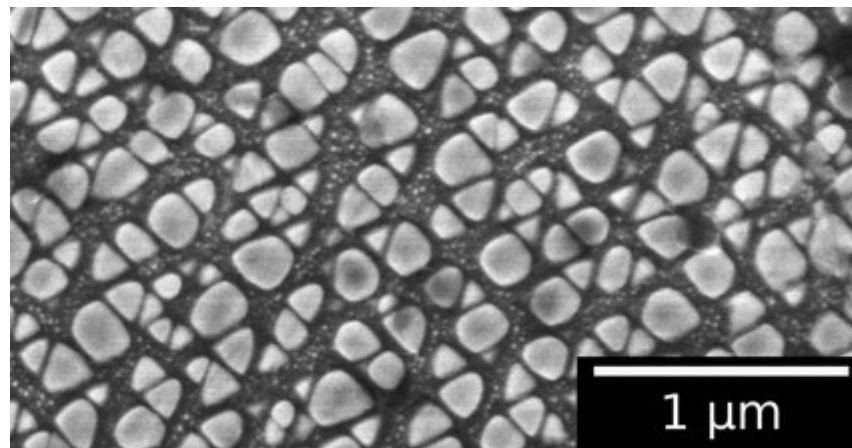


Proposed composition (wt. %)

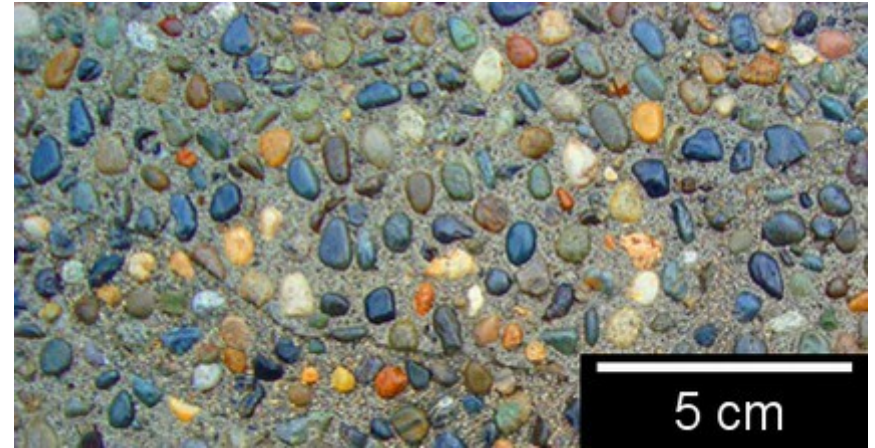
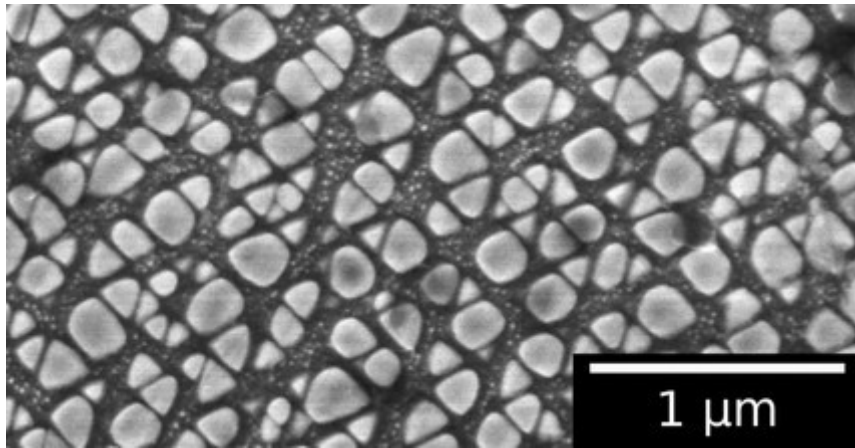
	Mn	0.2
	Co	20.0
	Mo	0.5
	W	0.5
	Ta	4.9
	Nb	1.1
	Al	2.4
	Ni	Balance
	T	900°C

	Cr	15.8
	Ti	3.0
	Fe	3.9
	Si	0.2
	Zr	0.18
	B	0.06
	C	0.02
	t	30 hr

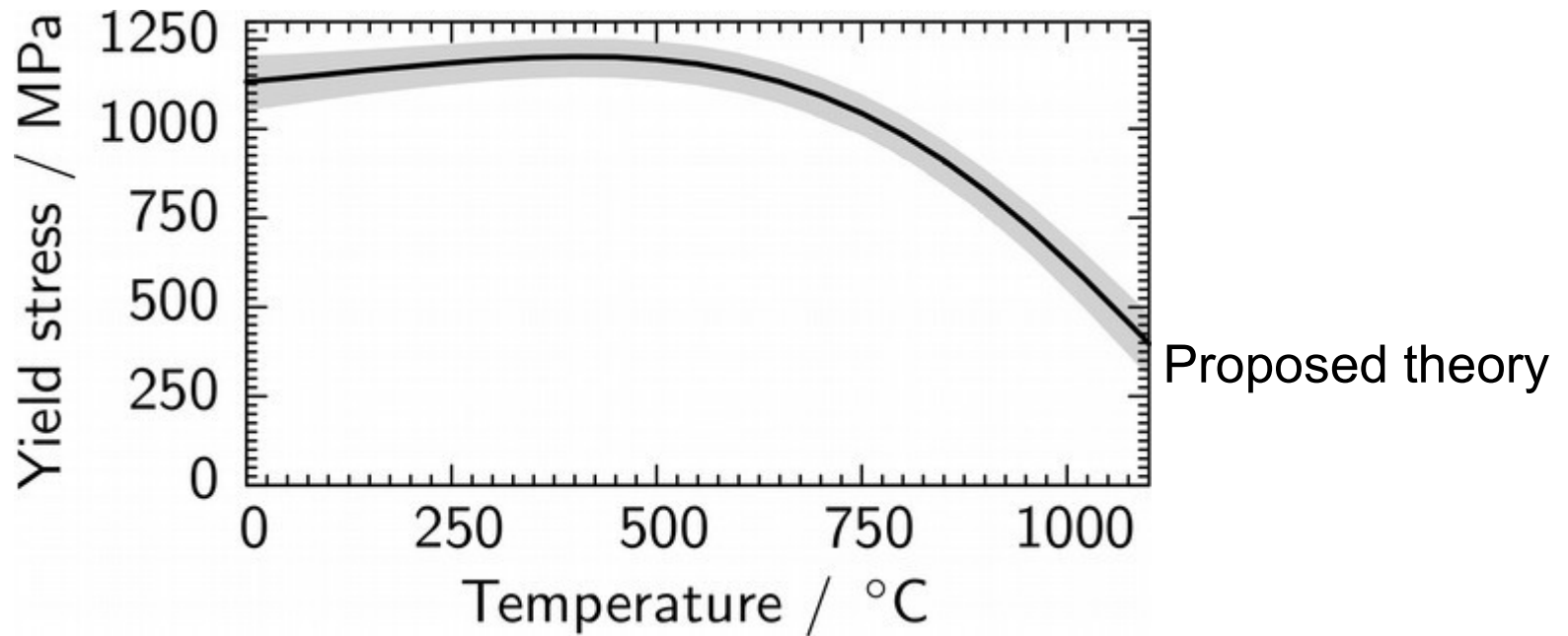
Microstructure



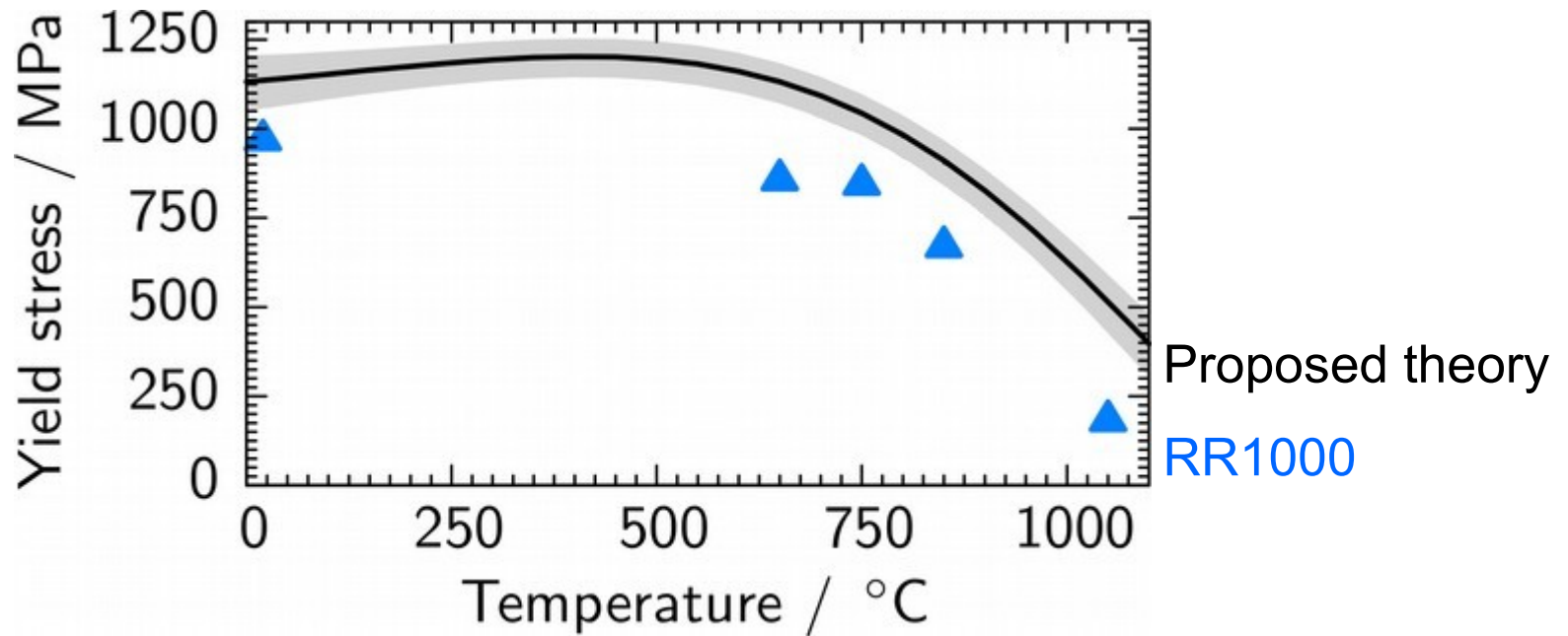
Microstructure



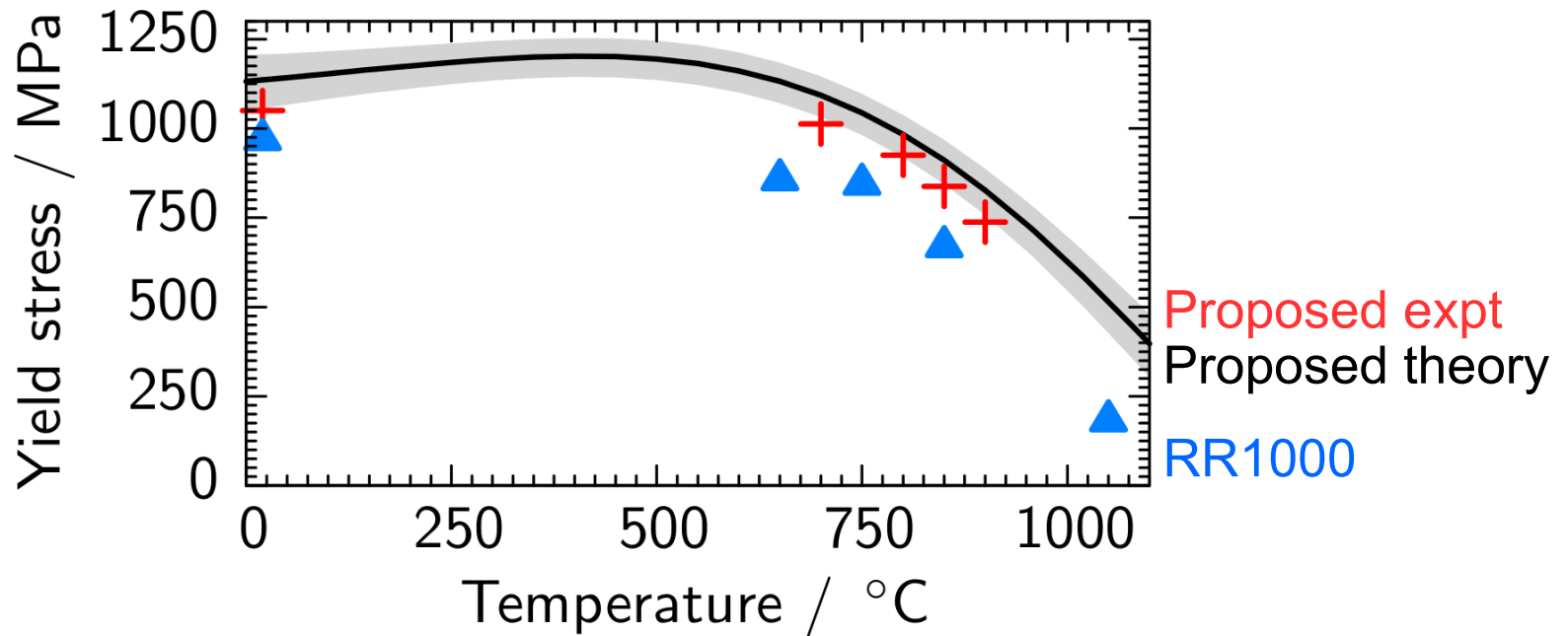
Testing the yield stress



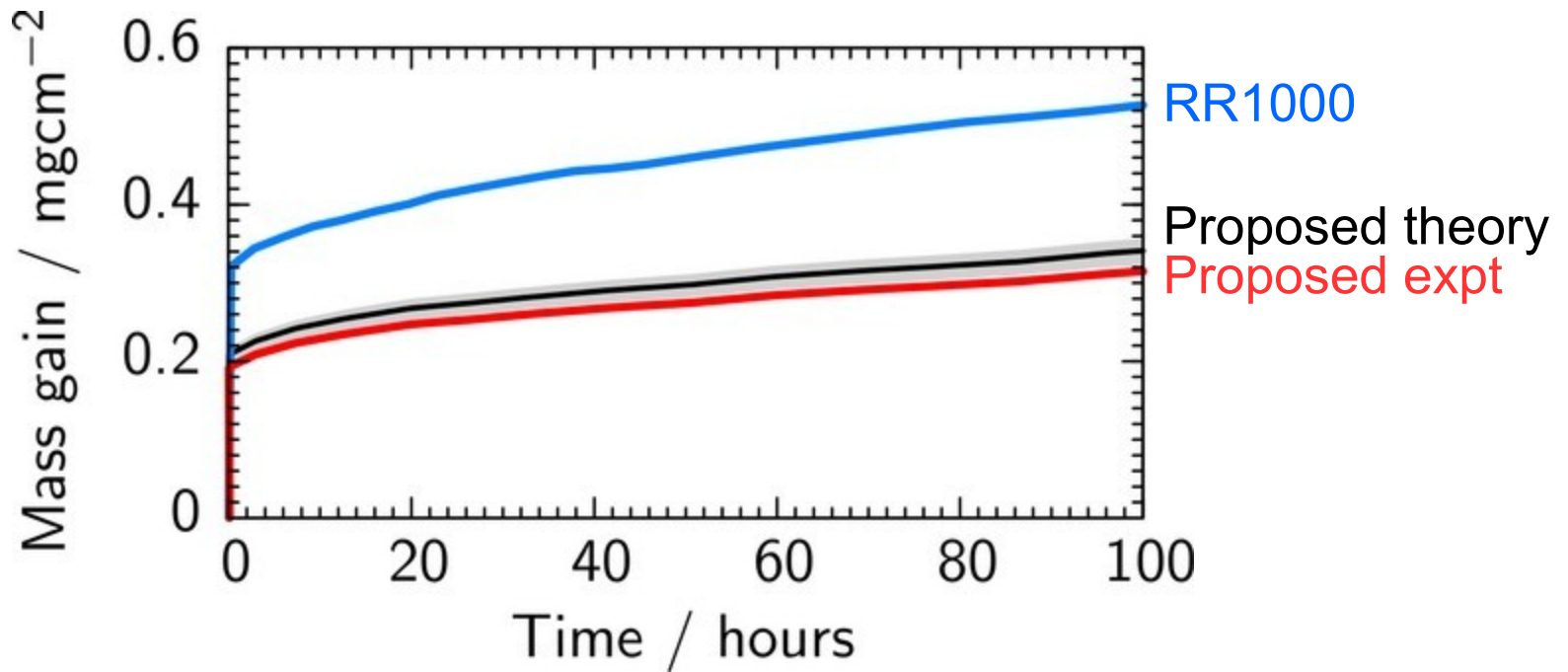
Testing the yield stress



Testing the yield stress



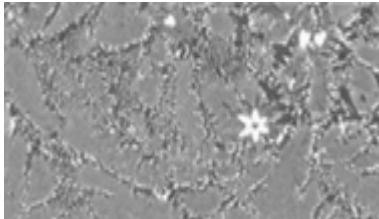
Testing the oxidation resistance



Alloys discovered

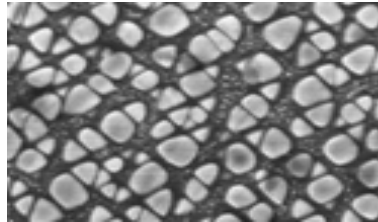
Cr-Cr₂Ta alloys

Intermetallics, 48, 62



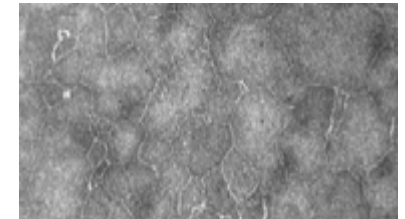
Combustor alloy

GB1408536



RR1000 grain growth

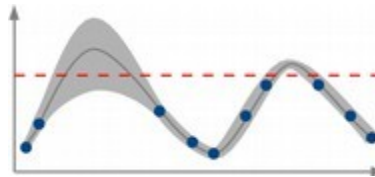
Acta Materialia, 61, 3378



Discovery algorithm

EP14153898

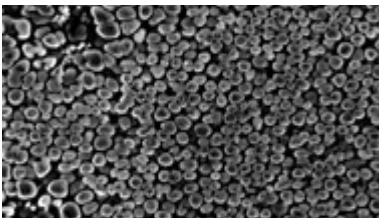
US 2014/177578



Ni disc alloy

EP14157622

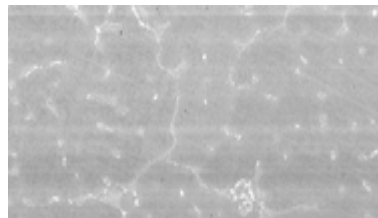
US 2013/0052077 A2



Mo-Hf forging alloy

EP14161255

US 2014/223465



Mo-Nb forging alloy

EP14161529

US 2014/224885



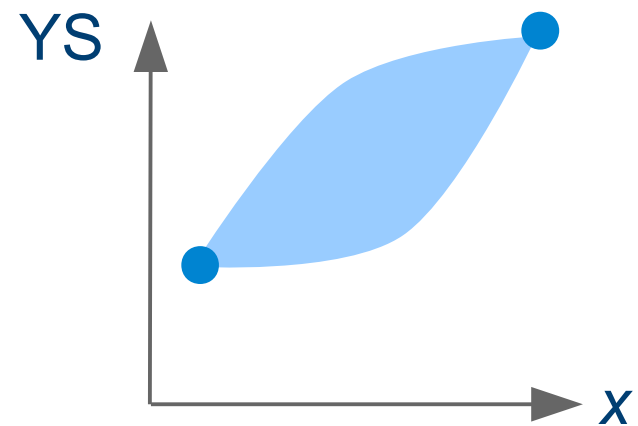
Fragmented databases

Composition	UTS	Hardness	Yield stress
✓	✓	✓	✓
✓	✓	✗	✓
✓	✓	✗	✗
✓	✗	✓	✓
✓	✓	✗	✗
✓	✗	✗	✗
✓	✓	✓	✗
✓	✗	✗	✓

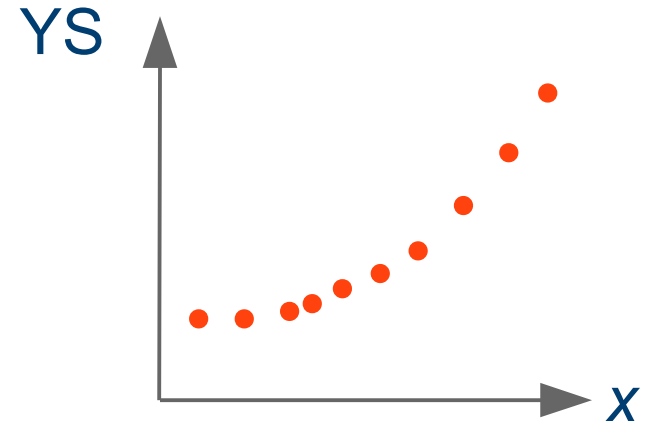
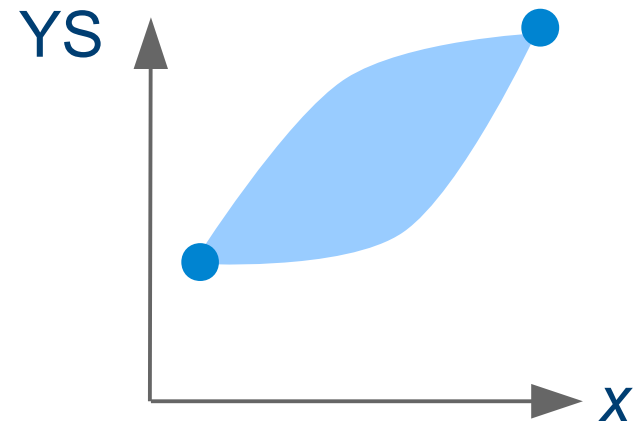
Fragmented databases

Composition	UTS	Hardness	Yield stress	Comp. YS
✓	✓	✓	✓	✓
✓	✓	✗	✓	✓
✓	✓	✗	✗	✓
✓	✗	✓	✓	✓
✓	✓	✗	✗	✓
✓	✗	✗	✗	✓
✓	✓	✓	✗	✓
✓	✗	✗	✓	✓

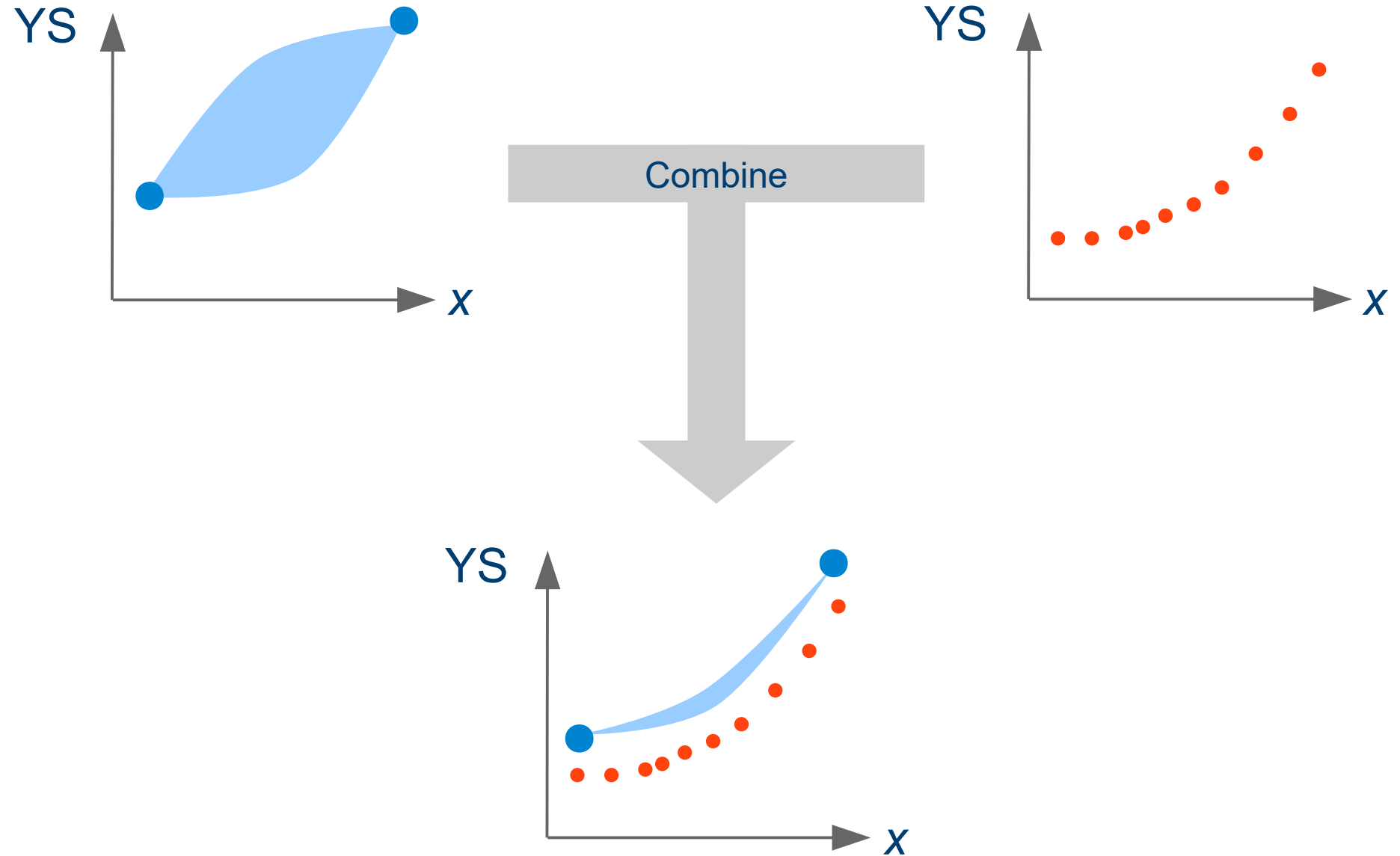
Merging simulation and experiment



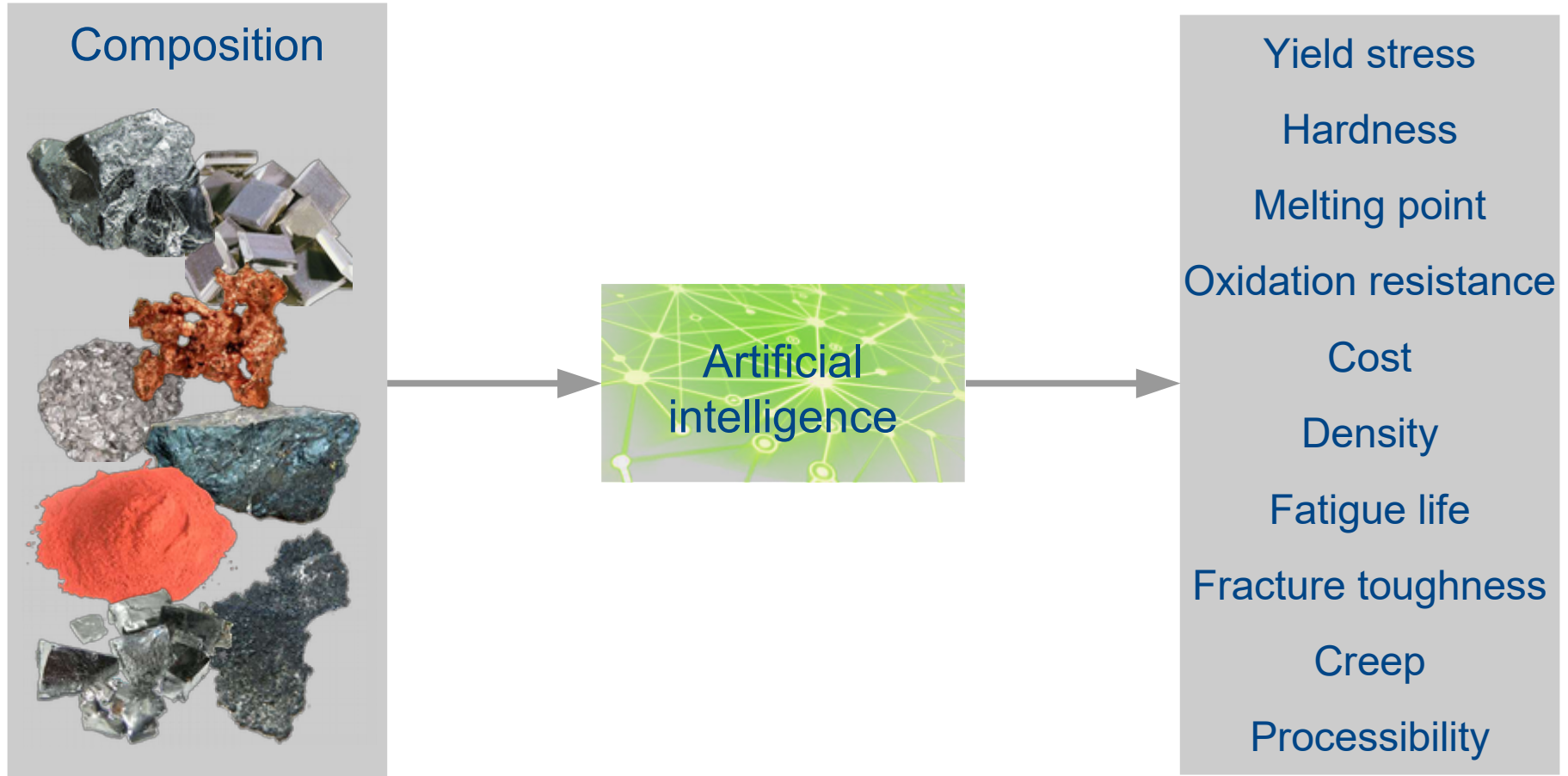
Merging simulation and experiment



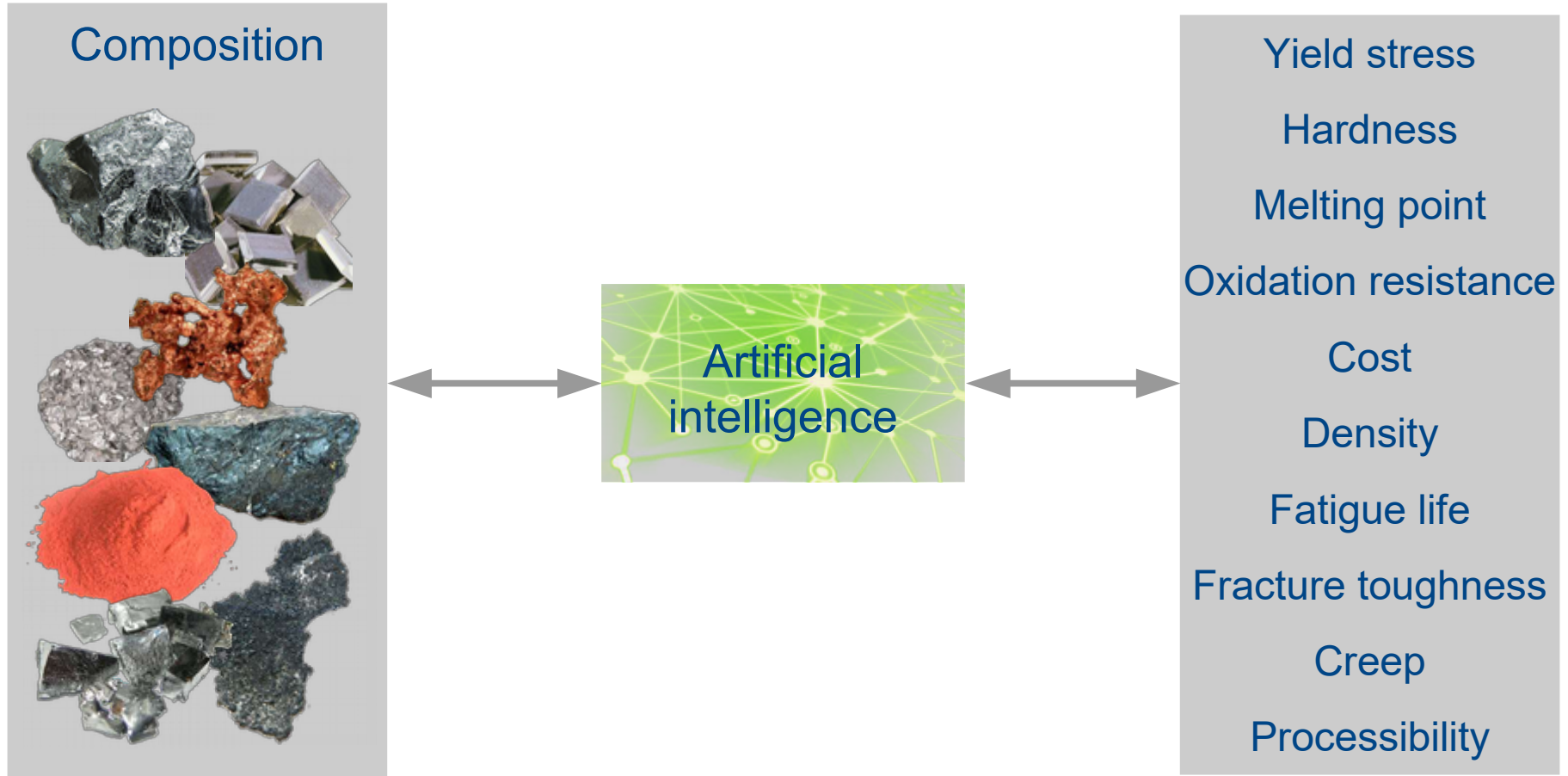
Merging simulation and experiment



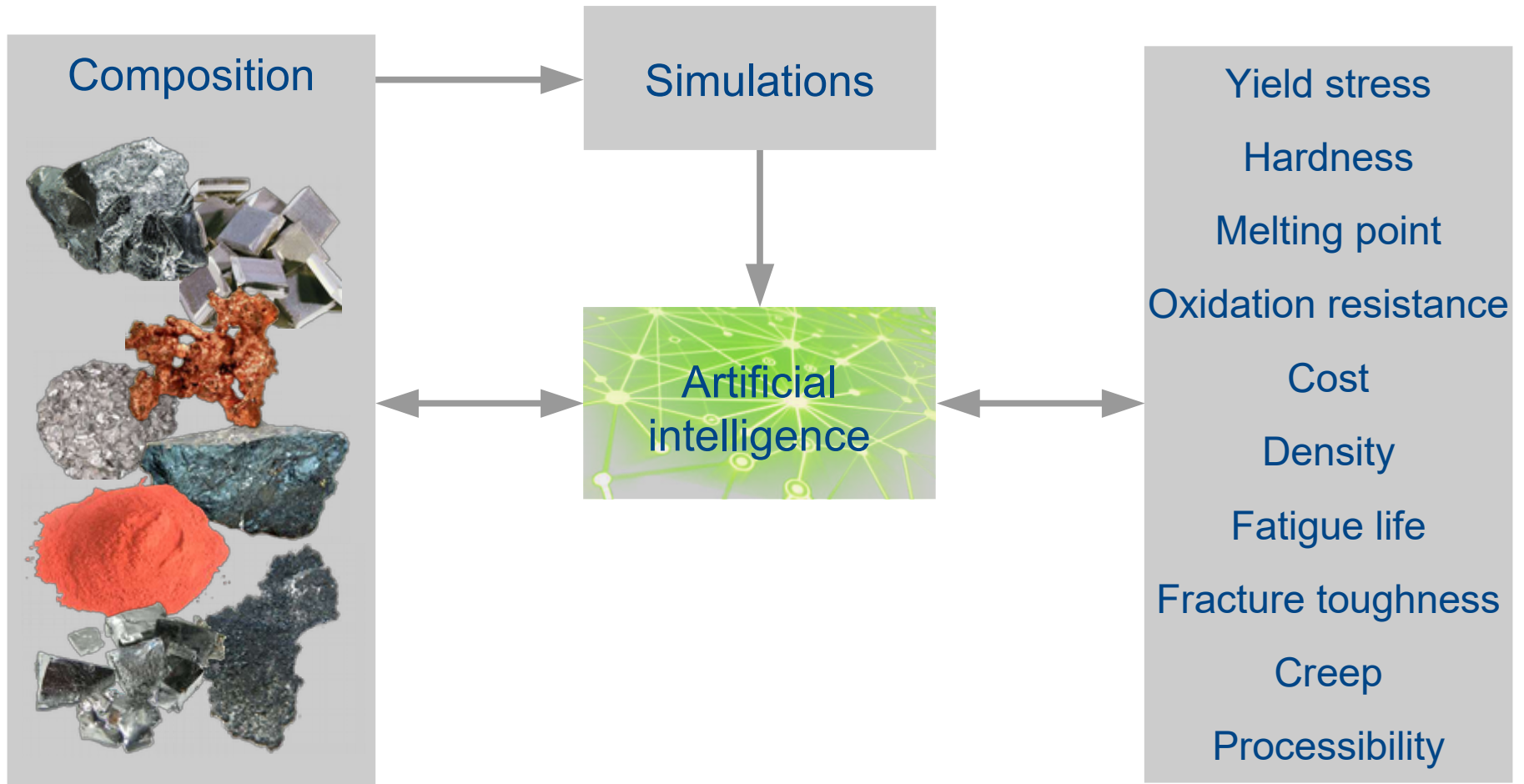
Artificial intelligence



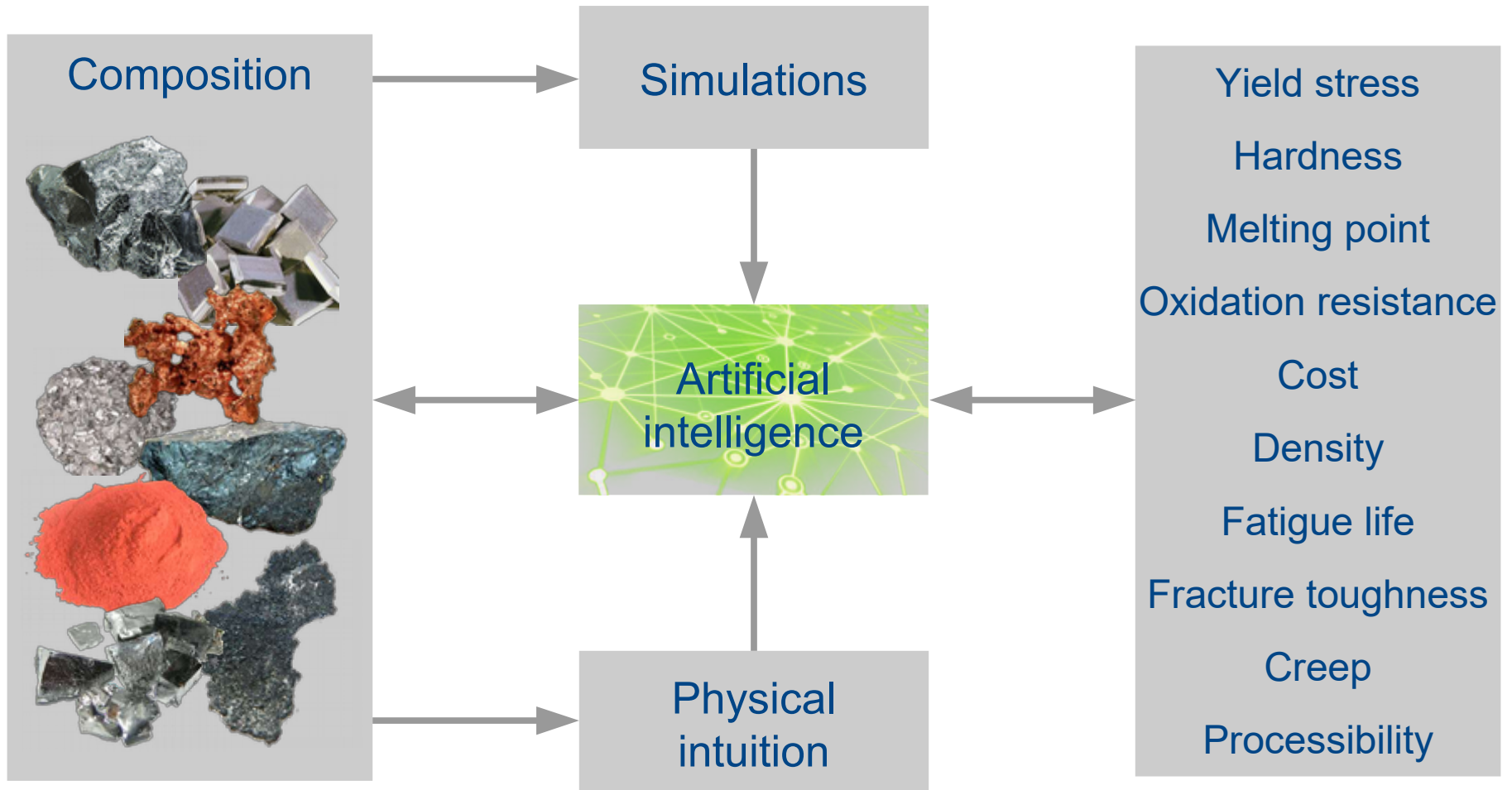
Artificial intelligence



Artificial intelligence



Artificial intelligence



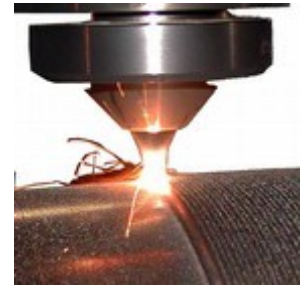
Exploiting material correlations

Alloy for direct laser deposition

3D printability

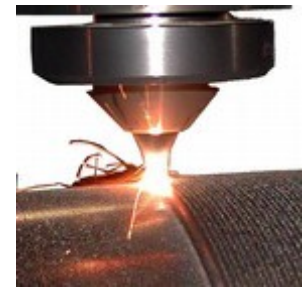


Weldability



Exploiting material correlations

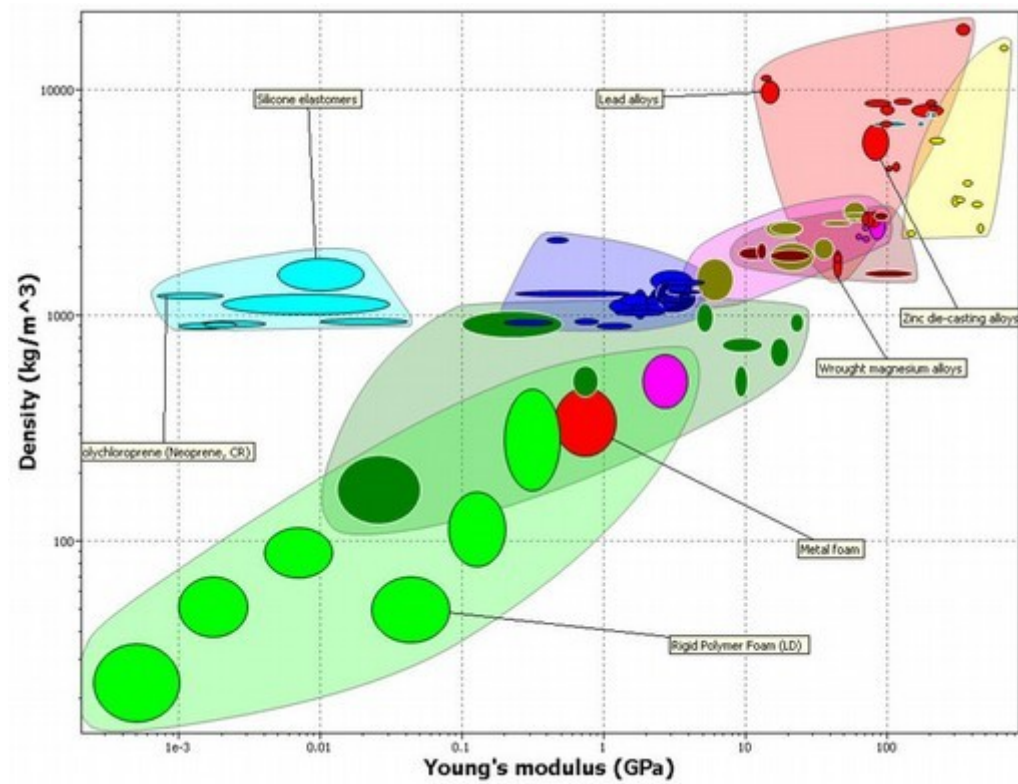
Alloy for direct laser deposition



Lithium cathode materials



Database verification



Choice of basis set



Alloys

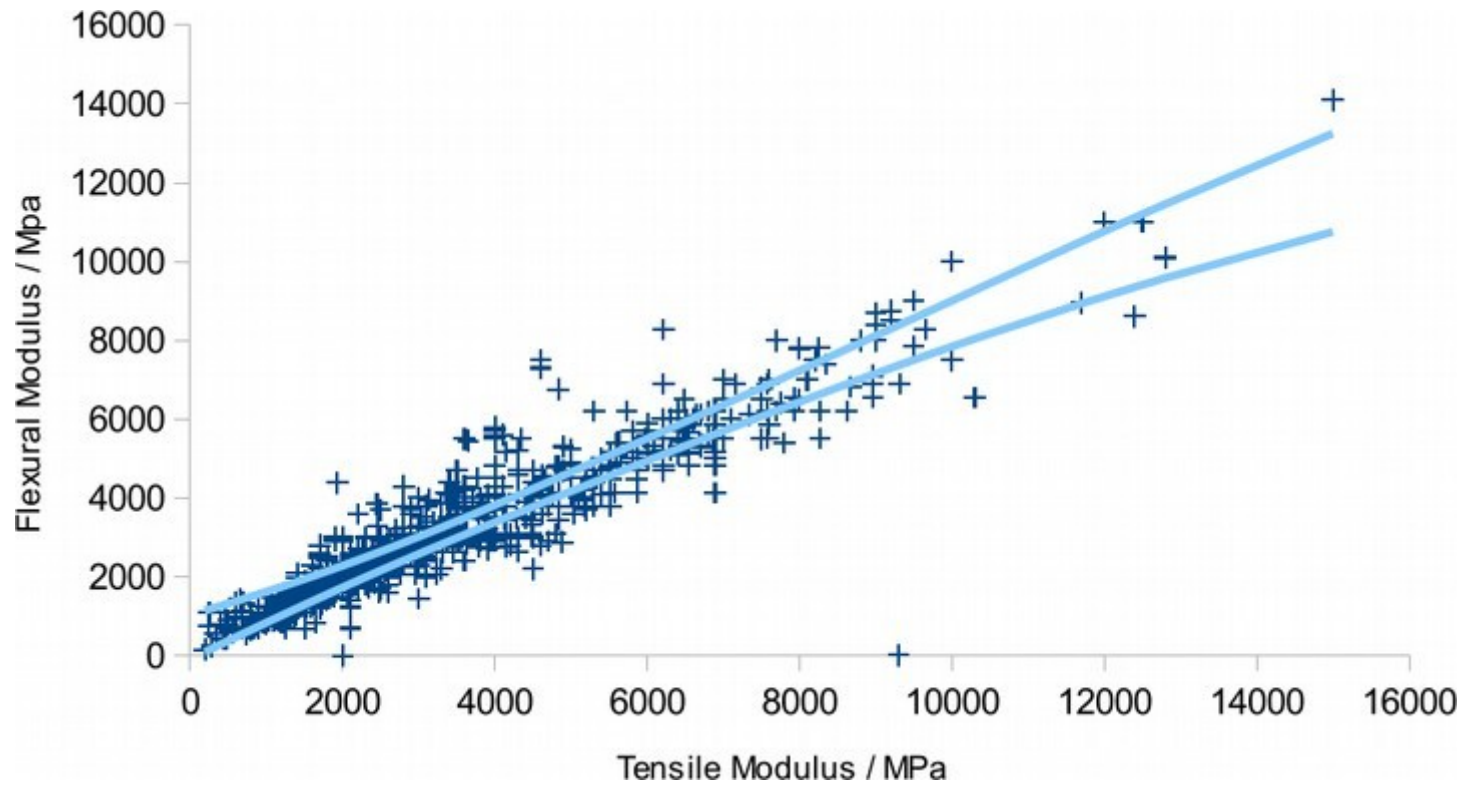
Composition
Heat treatment



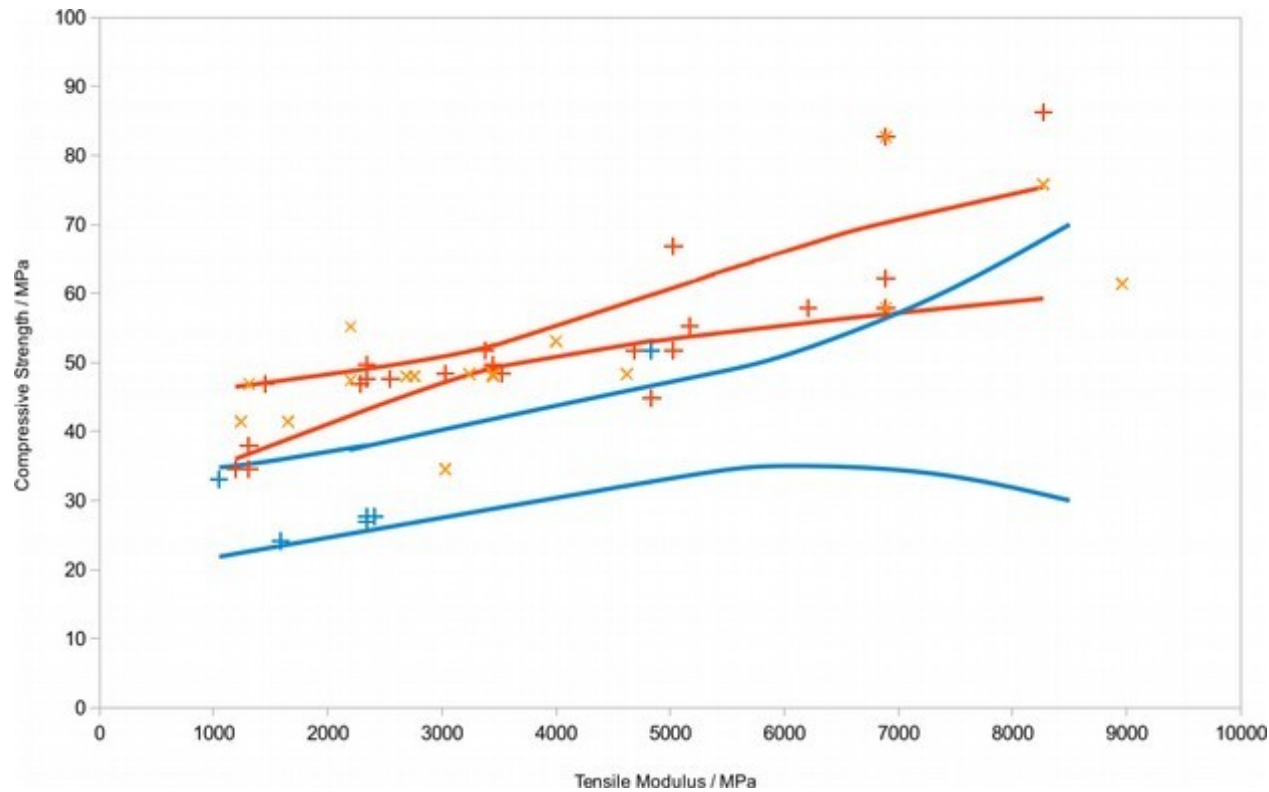
Polymers

Properties
Filler type and volume

Polymers: flexural modulus vs tensile modulus



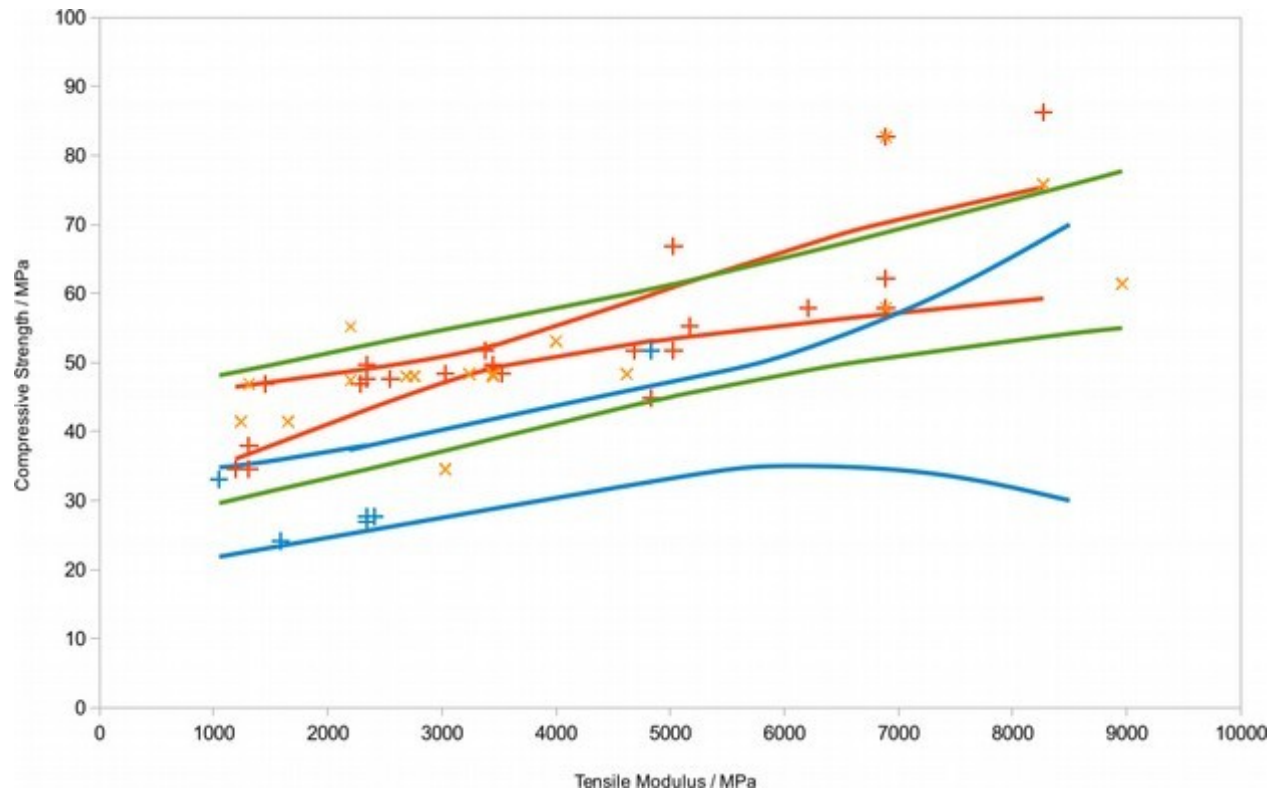
Polymers: compressive strength vs tensile modulus



Homopolymer

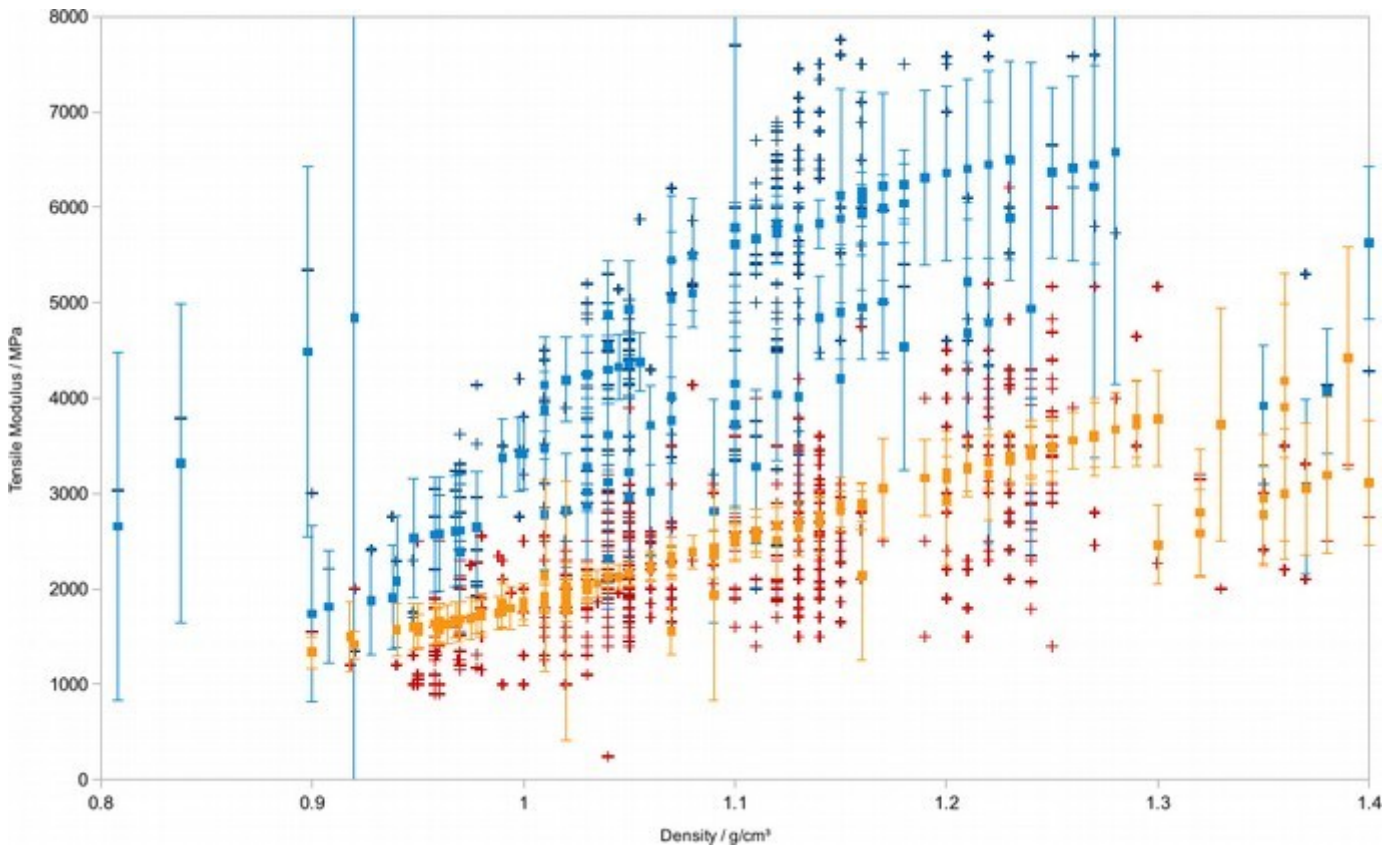
Copolymer

Polymers: compressive strength vs tensile modulus



Homopolymer
Unknown
Copolymer

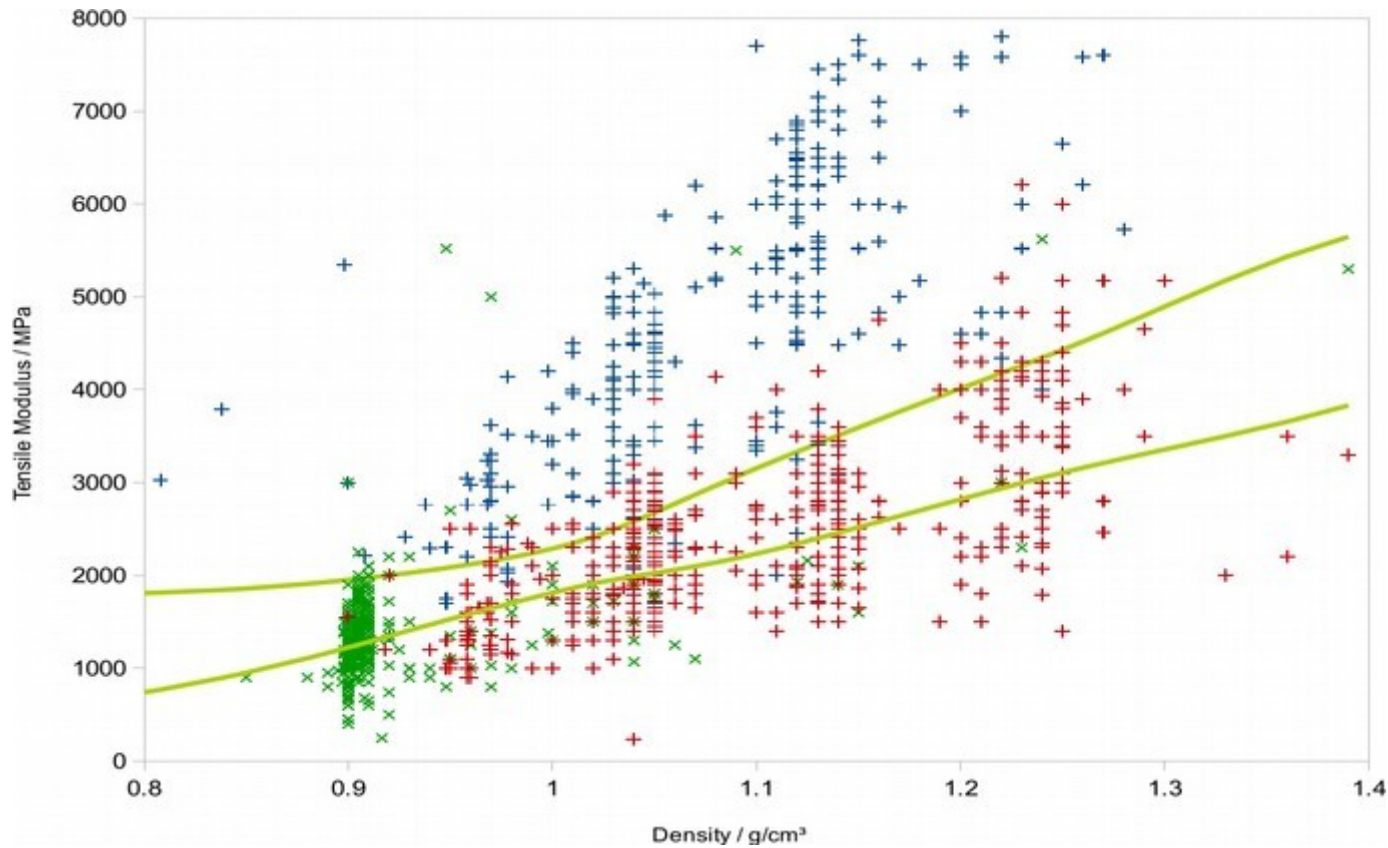
Polymers: tensile modulus vs density



Glass filler

Mineral filler

Polymers: tensile modulus vs density



Glass filler

Unknown

Mineral filler

Summary

Used artificial intelligence to discover materials

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

Merge simulations and experiments into holistic design tool

Materials database verification and analysis