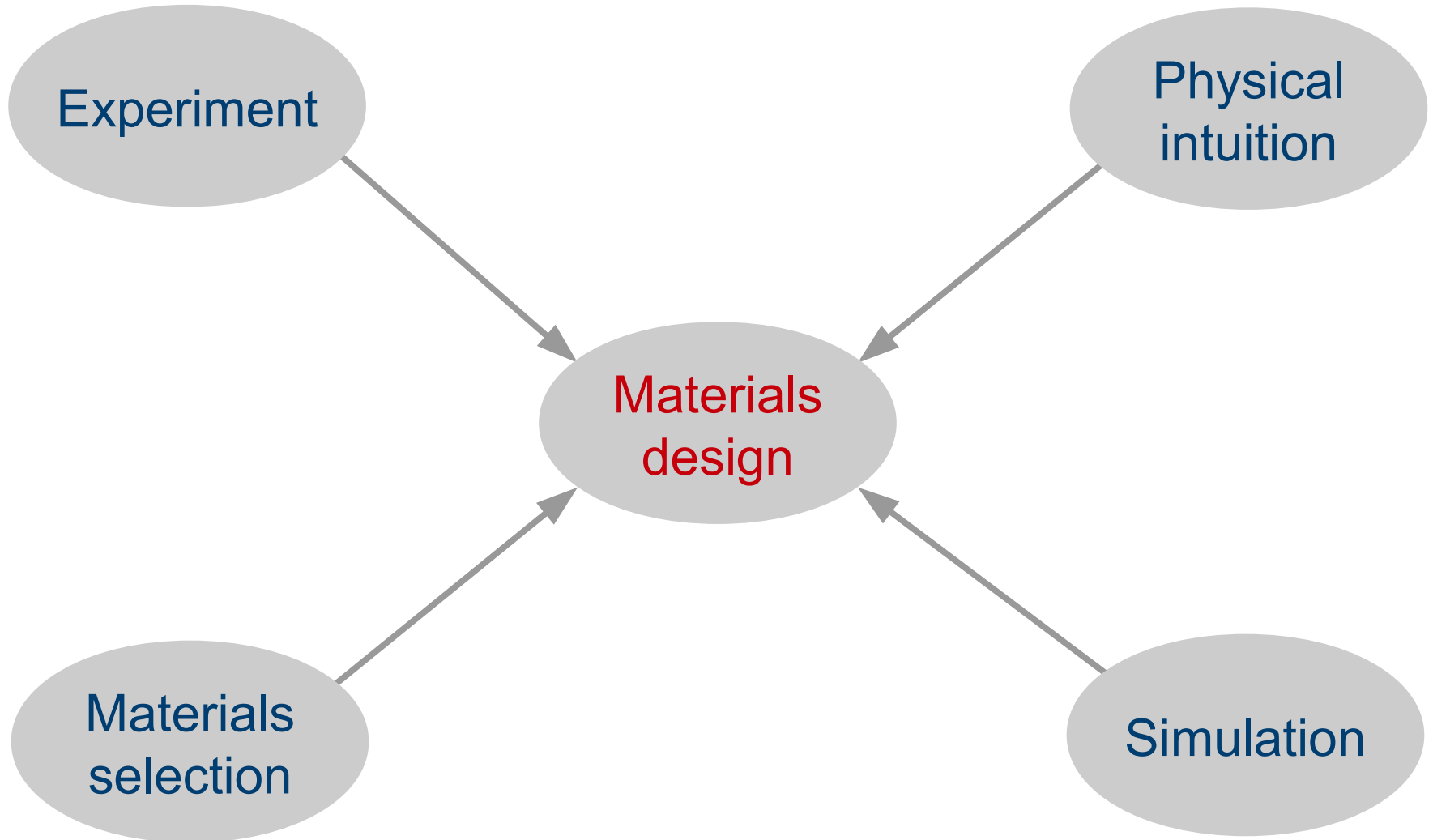UNIVERSITY OF CAMBRIDGE

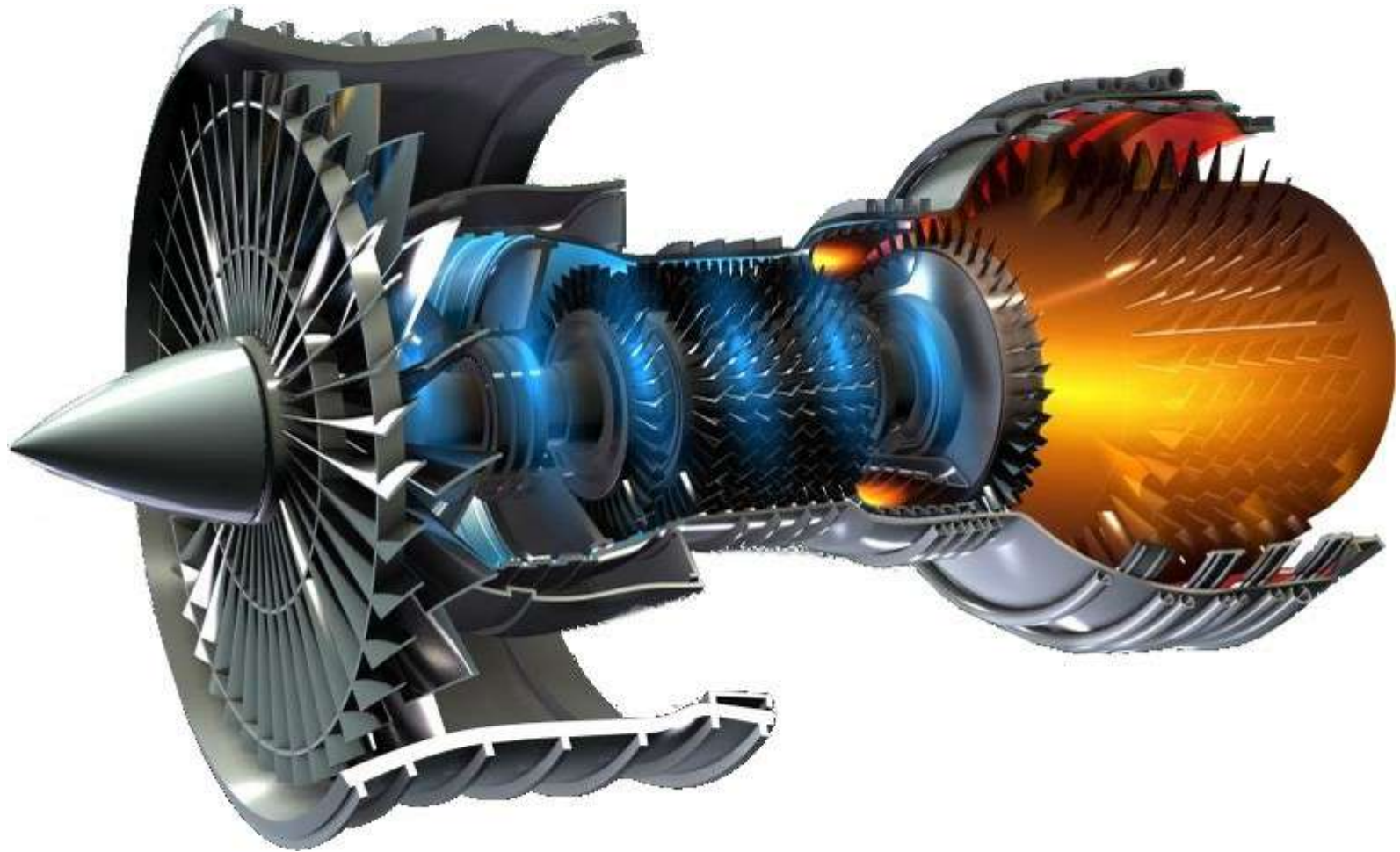# Materials discovery with artificial intelligence

Gareth Conduit
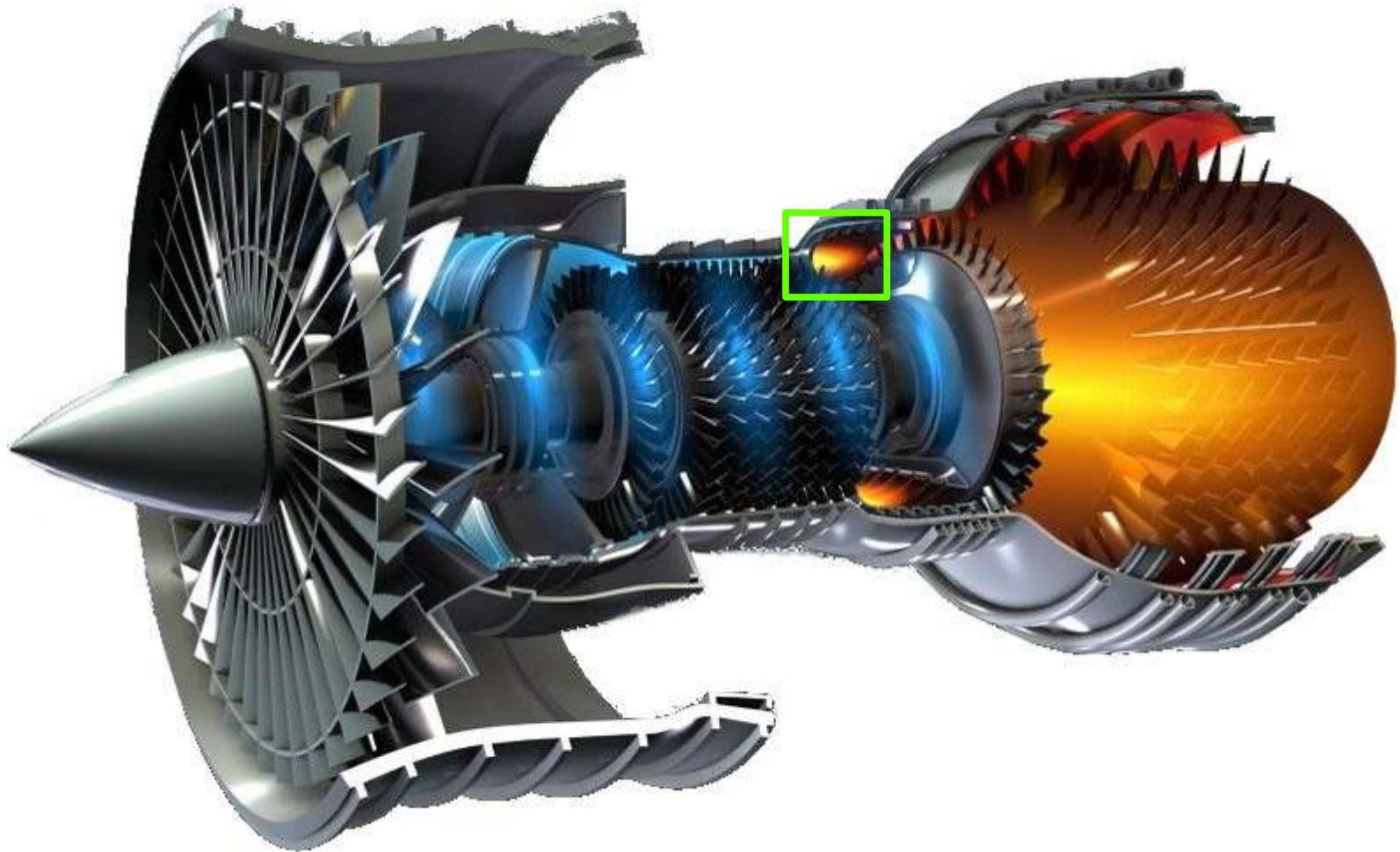
TCM Group, Department of Physics

Approaches to materials design

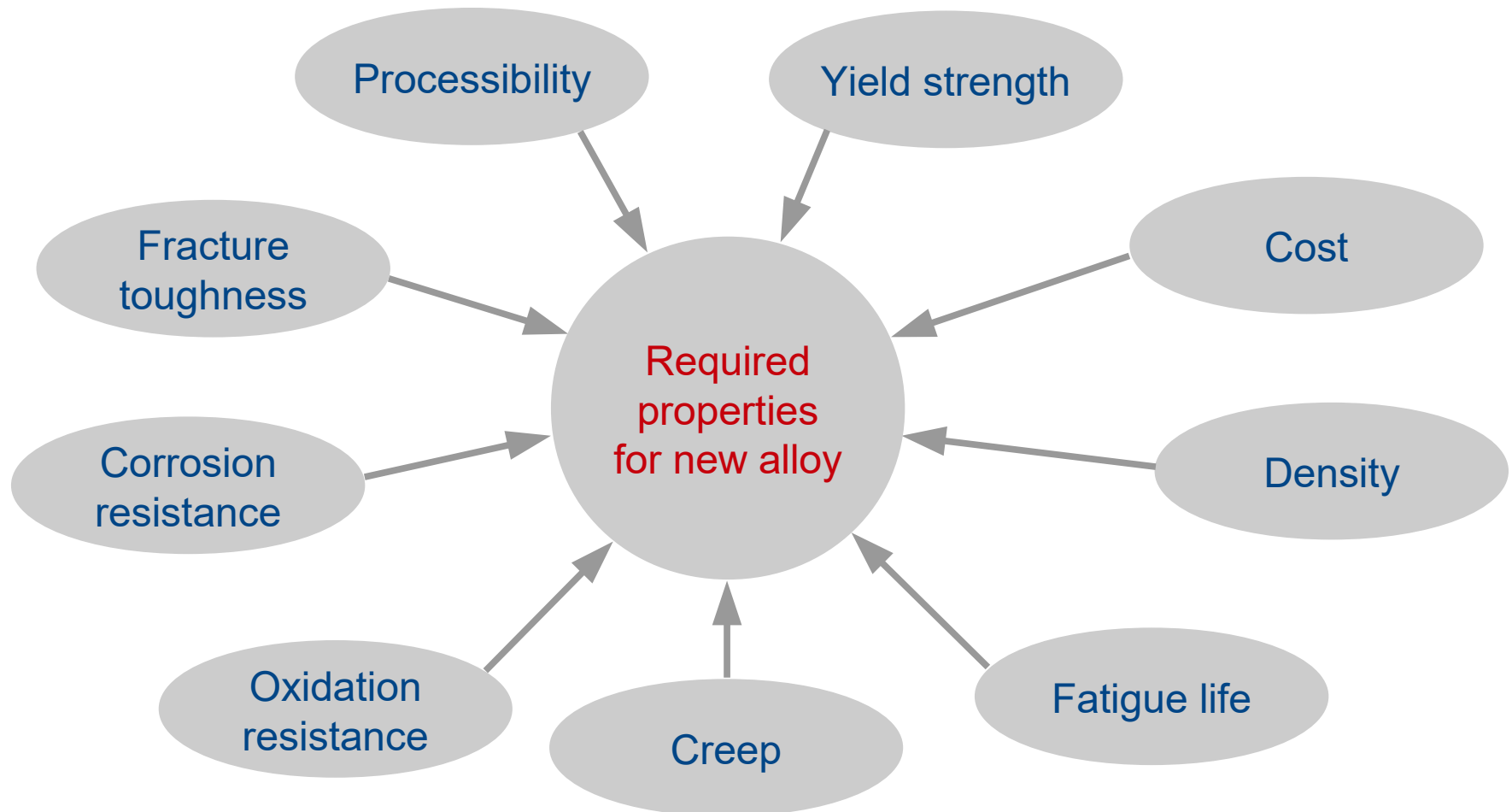# Schematic of a jet engine

Combustor liner

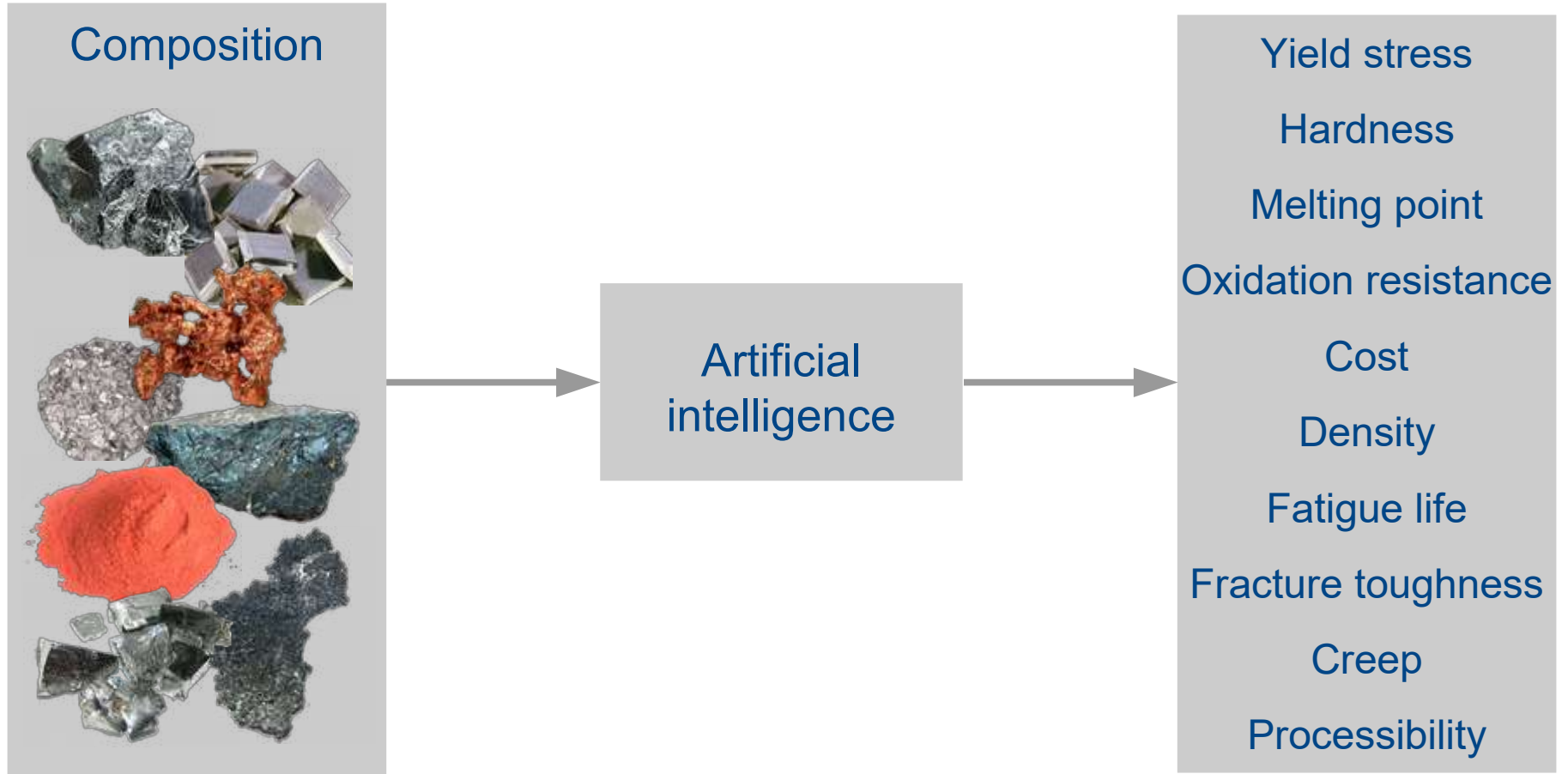# Designing a new alloy: what is required?
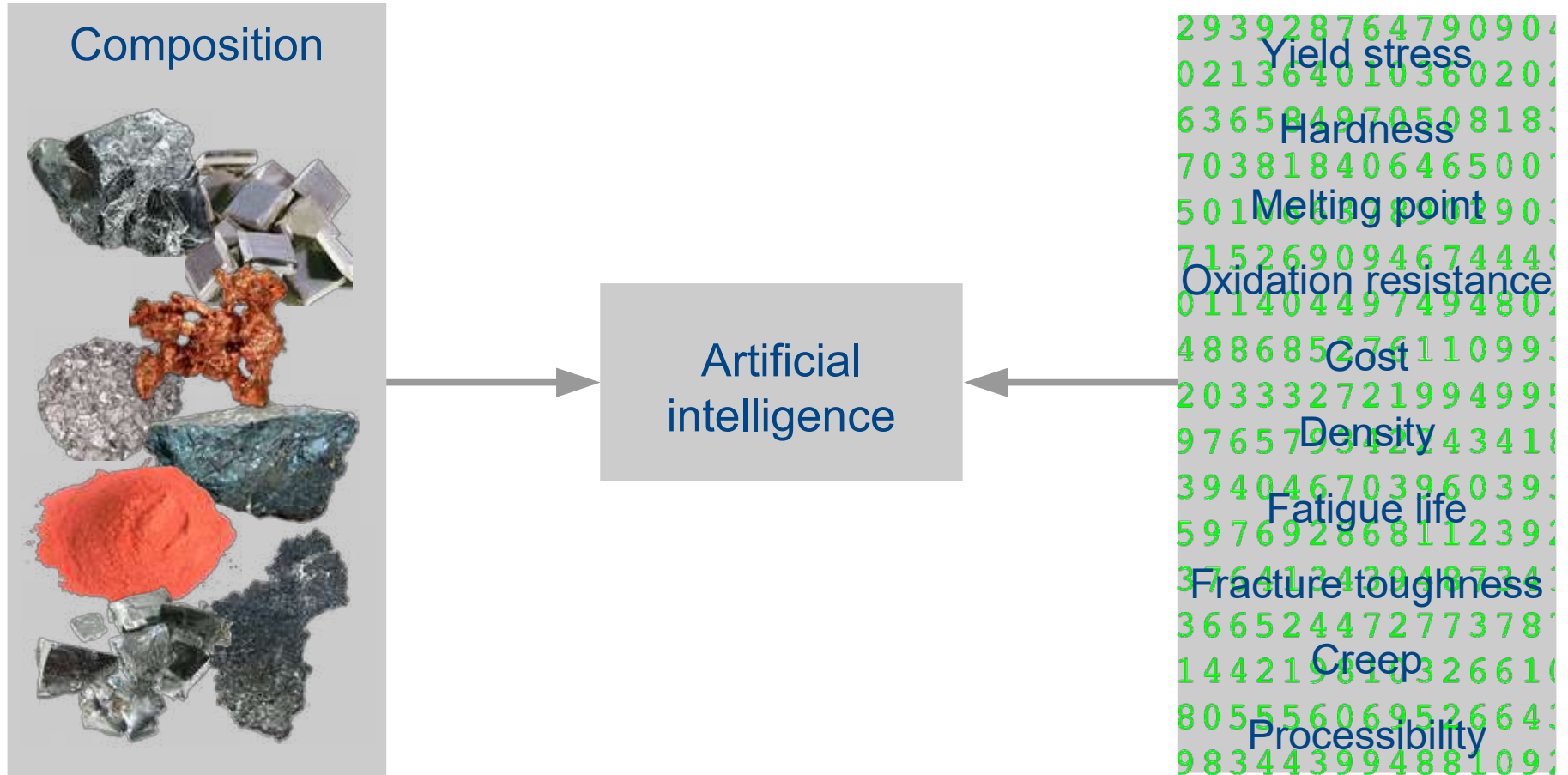
Multidimensional design space

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

Artificial intelligence

Composition

Artificial intelligence

Yield stress
Hardness
Melting point
Oxidation resistance
Cost
Density
Fatigue life
Fracture toughness
Creep
Processibility

Artificial intelligence

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Processibility
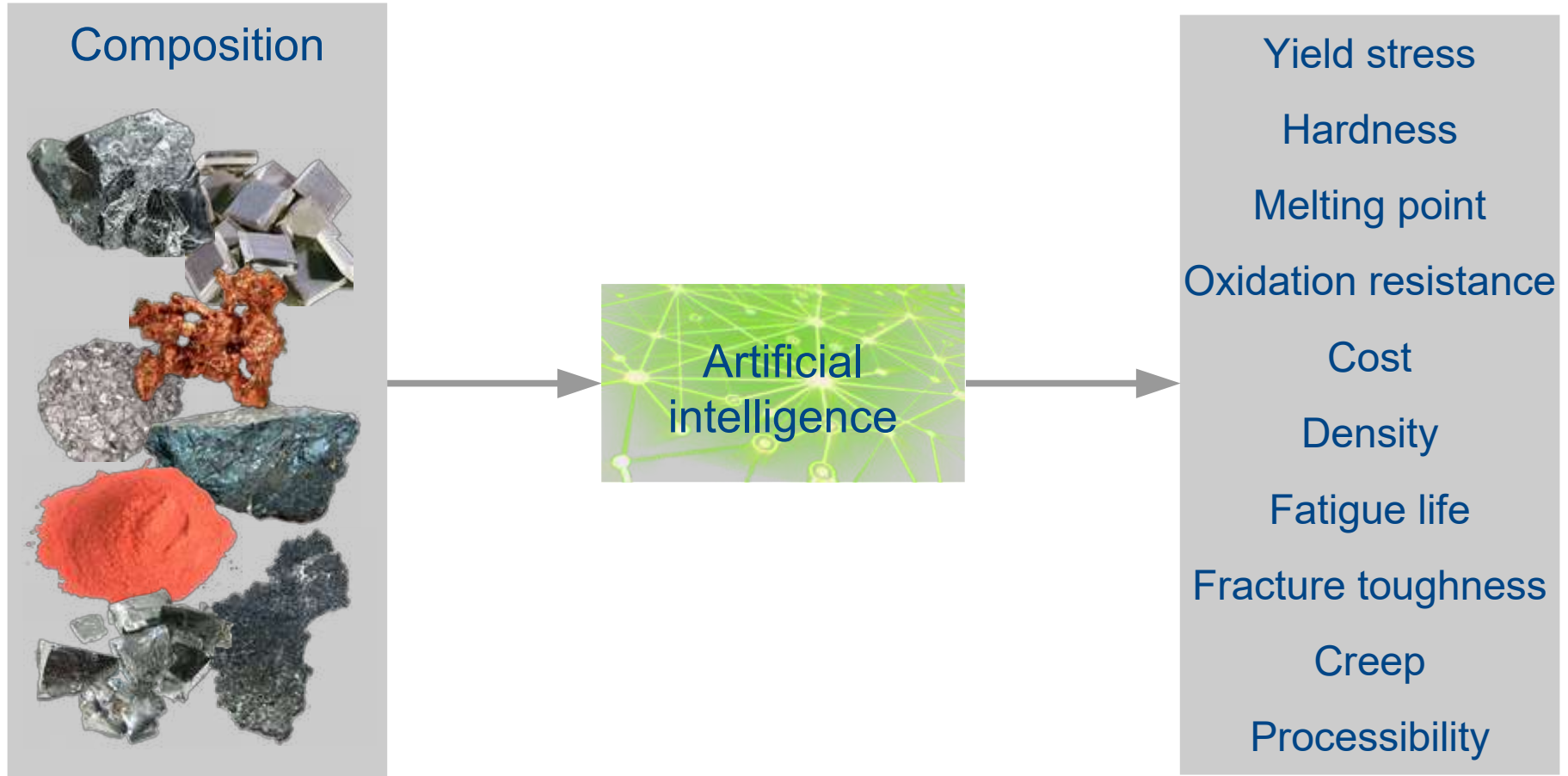
Proposed composition (wt. %)

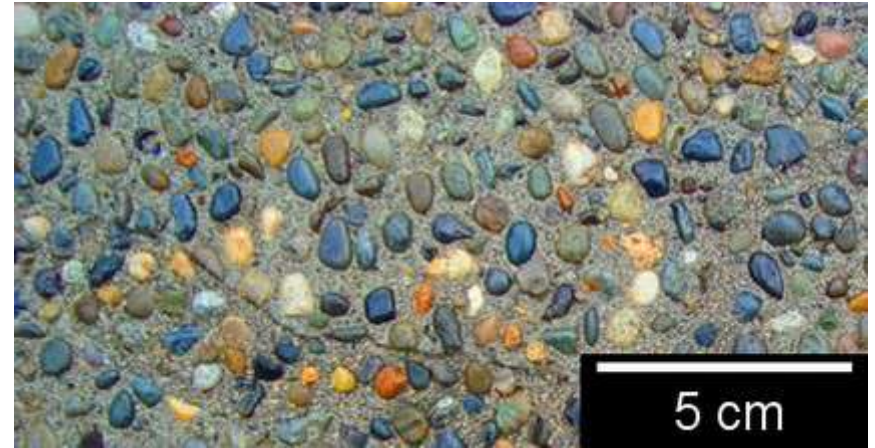|				
Mn	0.2		Cr	15.8
Co	20.0		Ti	3.0
Mo	0.5		Fe	3.9
W	0.5		Si	0.2
Ta	4.9		Zr	0.18
Nb	1.1		B	0.06
Al	2.4		C	0.02
Ni	Balance			
T	900ºC		*t*	30 hr

Microstructure

Microstructure
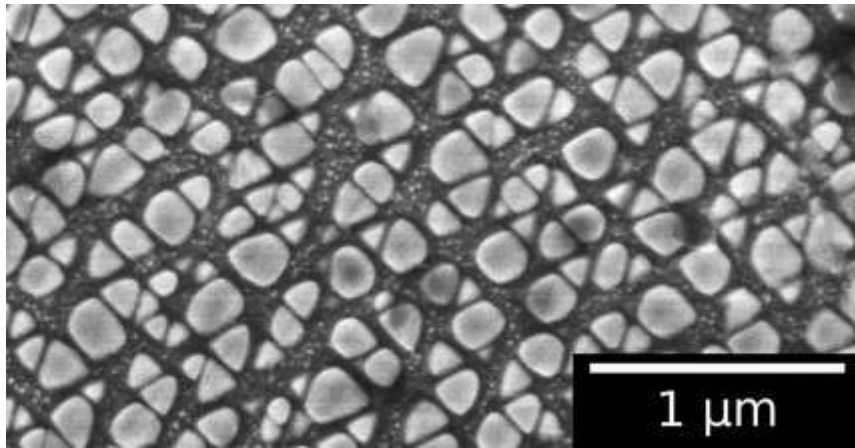
Proposed theory

Testing the yield stress

Proposed theory

RR1000

Testing the yield stress

Proposed expt
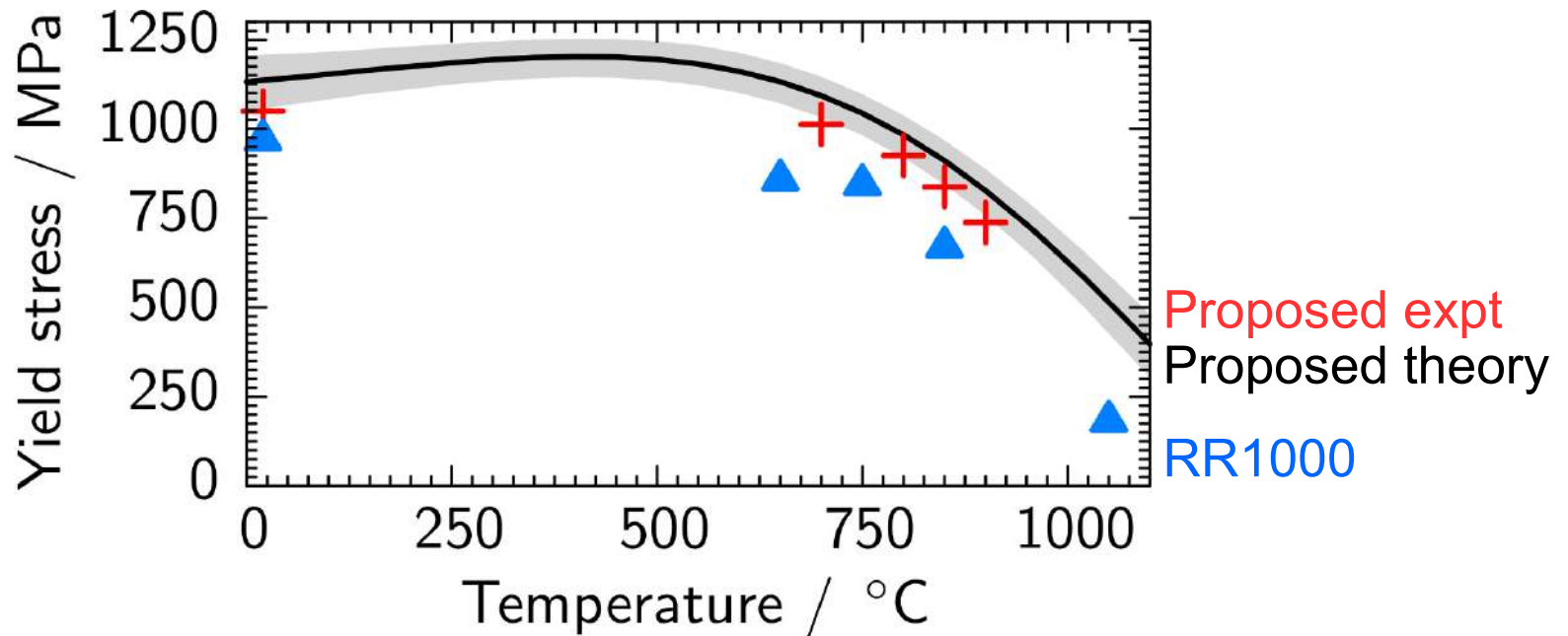Proposed theory
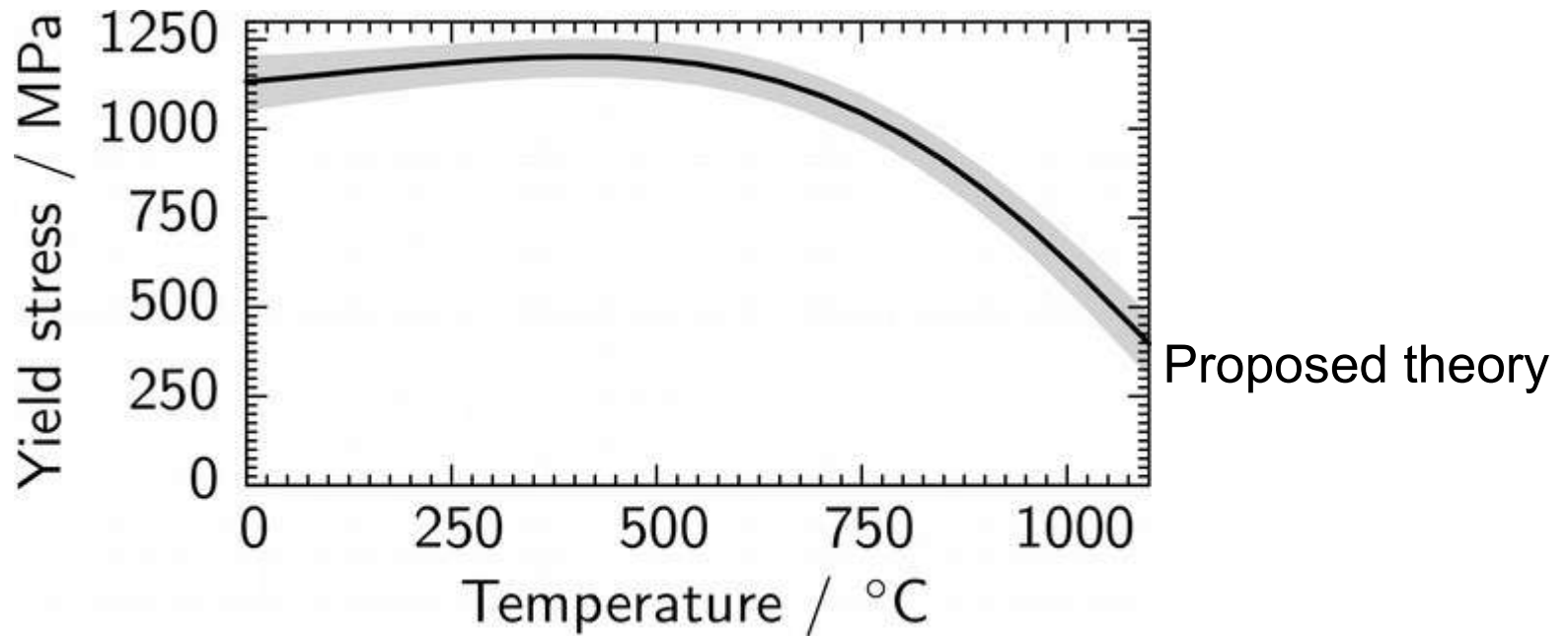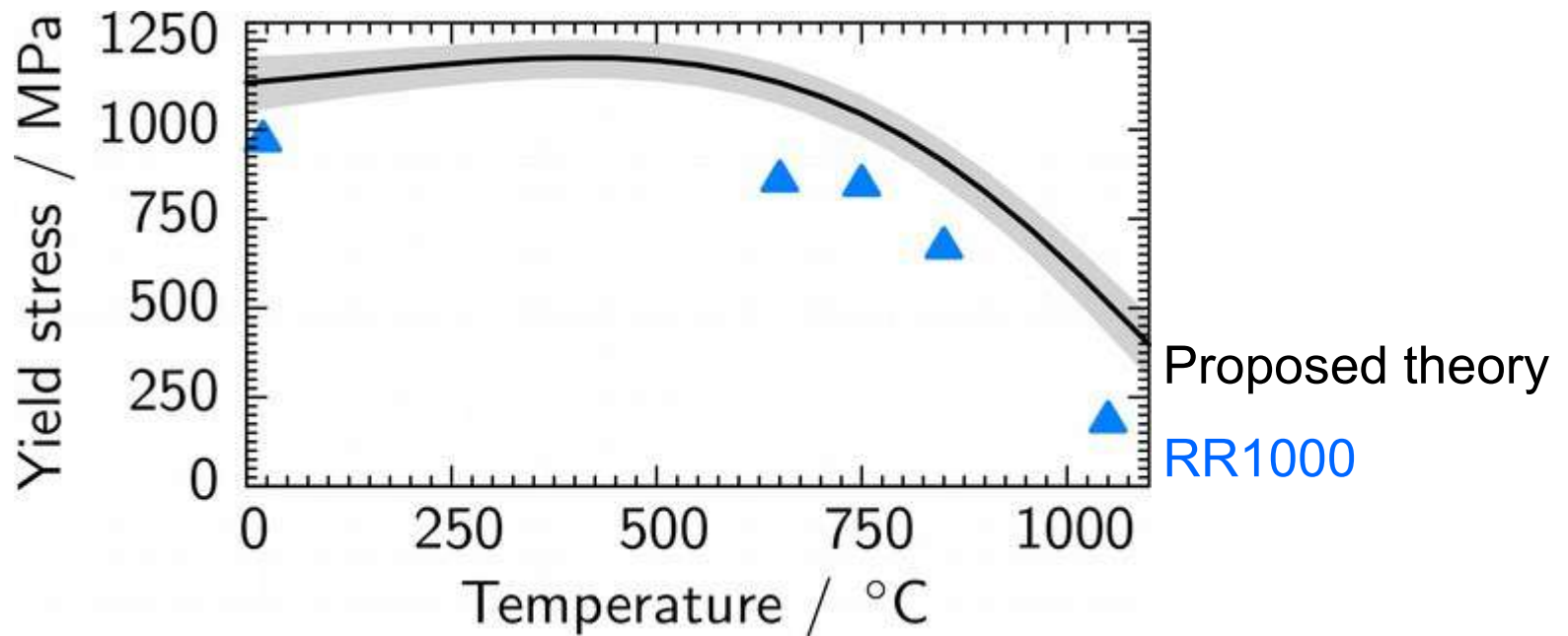
RR1000
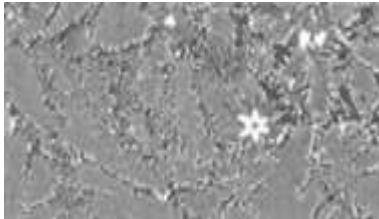
Testing the oxidation resistance
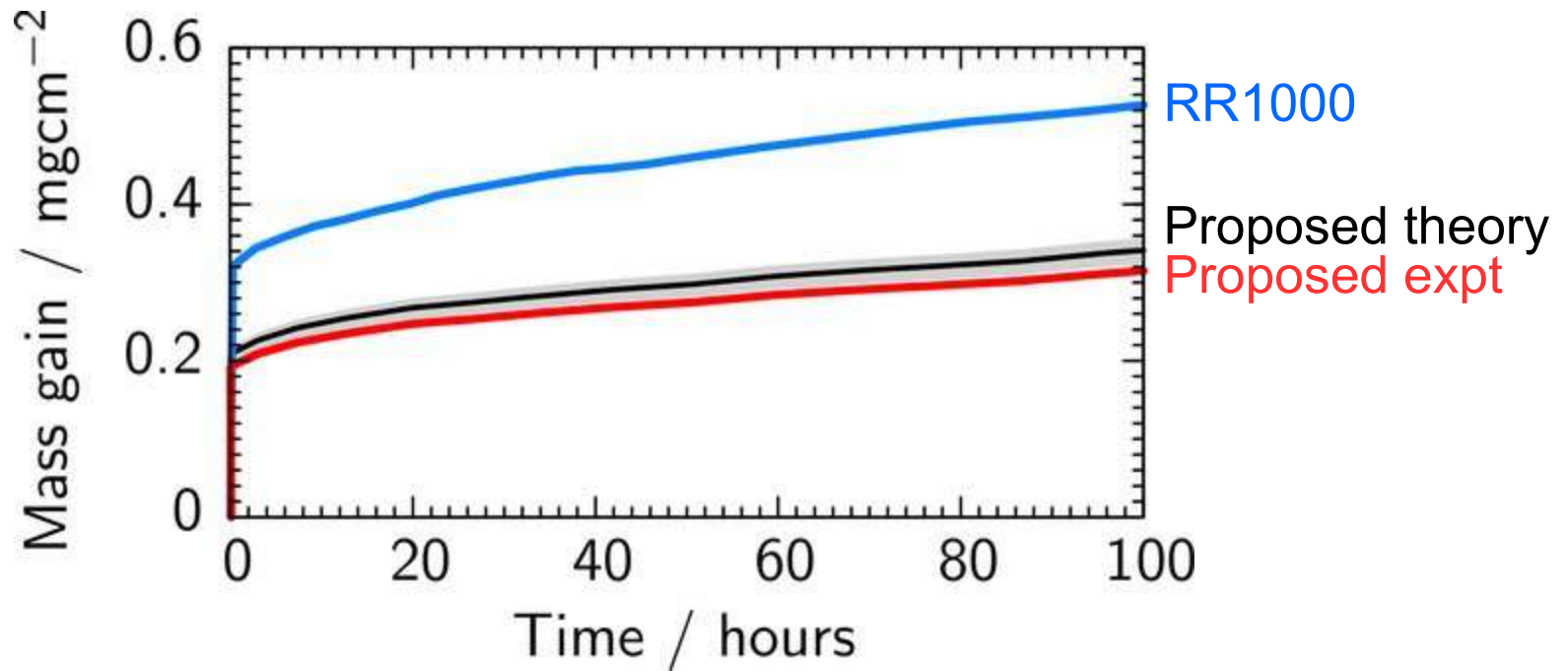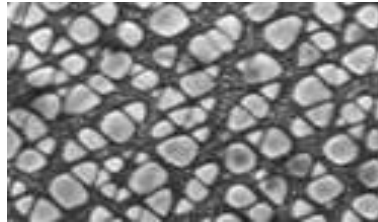
Alloys discovered

Cr-Cr$_2$Ta alloys
Intermetallics, 48, 62

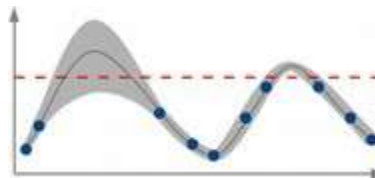**Combustor alloy**
GB1408536

RR1000 grain growth
Acta Materialia, 61, 3378

Discovery algorithm
EP14153898
US 2014/177578

Ni disc alloy
EP14157622
US 2013/0052077 A2
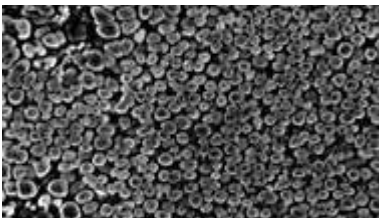
Mo-Hf forging alloy
EP14161255
US 2014/223465

Mo-Nb forging alloy
EP14161529
US 2014/224885

Materials databases
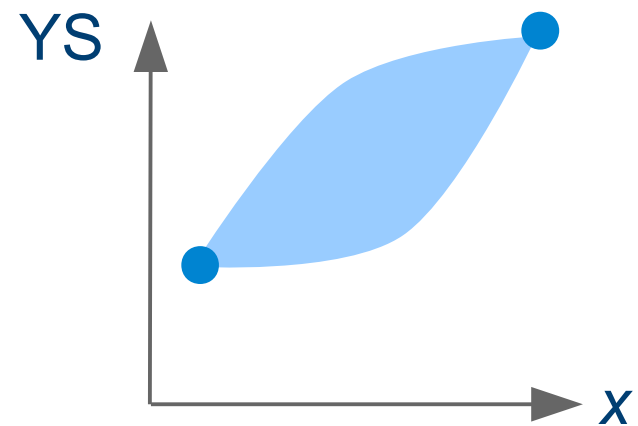
Ni	Al	W	Ti	Yield stress
✔	✔	✔	✔	✗
✔	✔	✔	✔	✗
✔	✔	✔	✔	✗
✔	✔	✔	✔	✗
✔	✔	✔	✔	✗
✔	✔	✔	✔	✗
✔	✔	✔	✔	✗
✔	✔	✔	✔	✗

Fragmented databases

Composition	UTS	Hardness	Yield stress
✔	✔	✔	✔
✔	✔	✘	✔
✔	✔	✘	✘
✔	✘	✔	✔
✔	✔	✘	✘
✔	✘	✘	✘
✔	✔	✔	✘
✔	✘	✘	✔

Fragmented databases

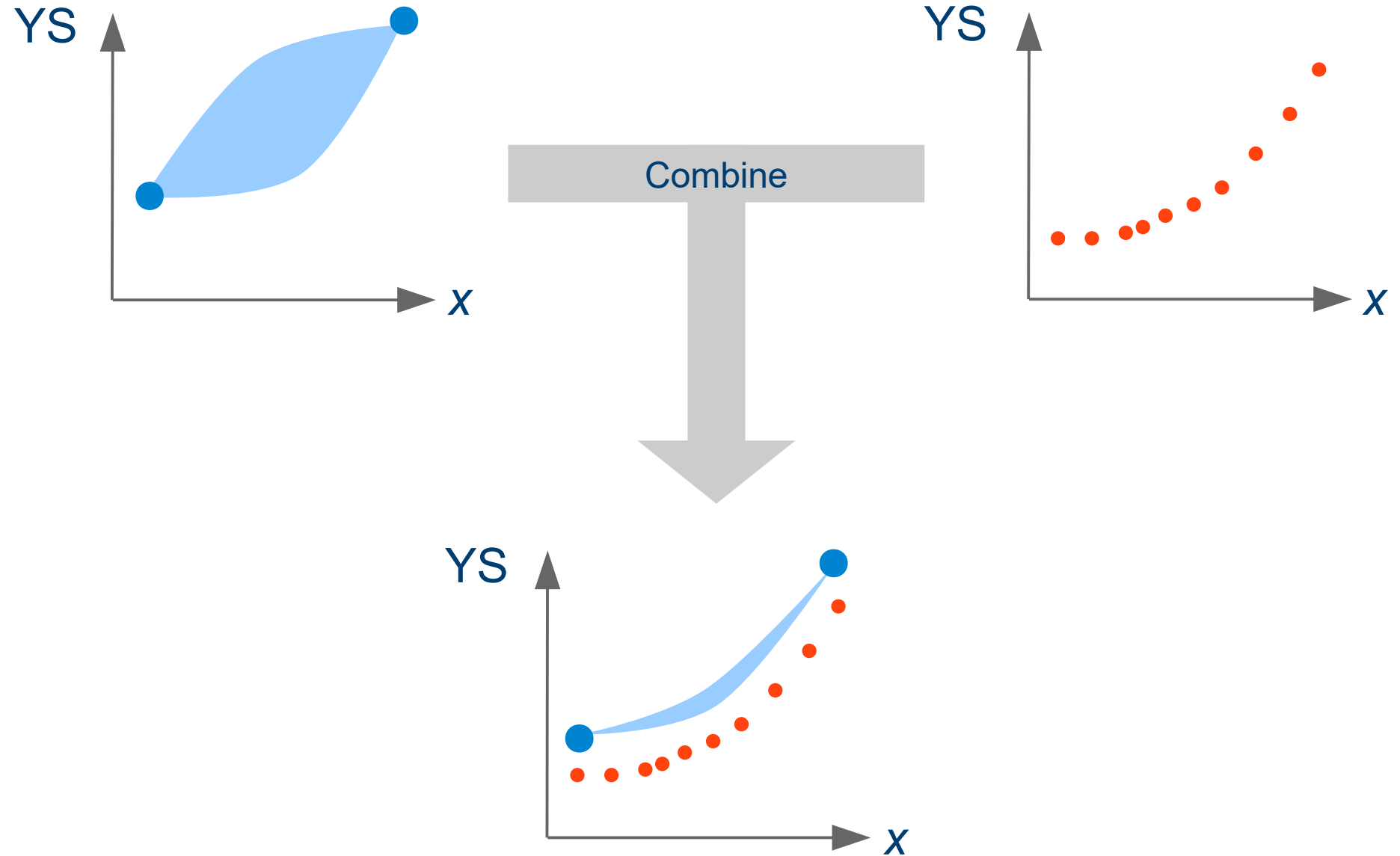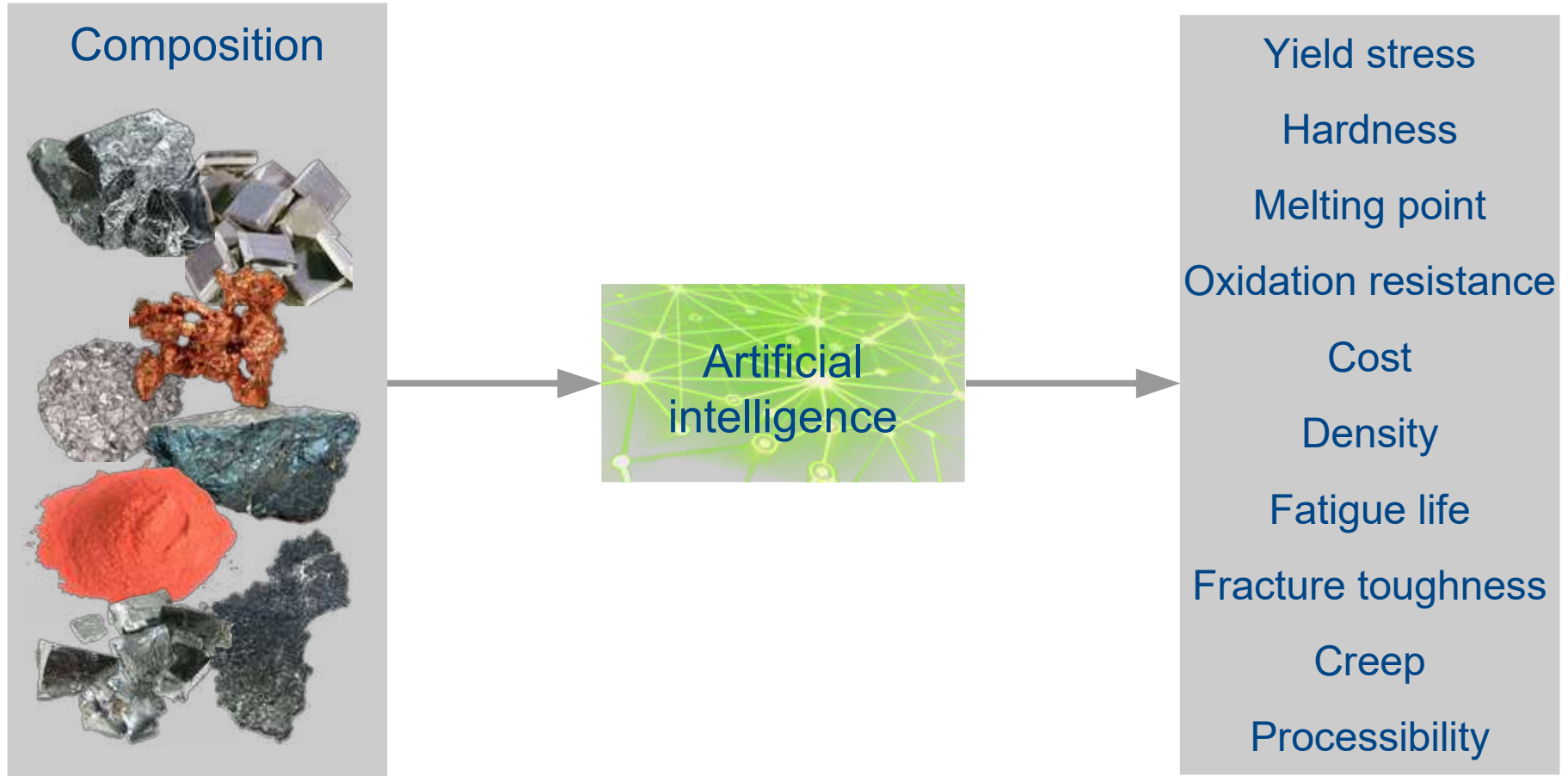| Composition	UTS	Hardness	Yield stress	Comp. YS
✓	✓	✓	✓	✓
✓	✓	✗	✓	✓
✓	✓	✗	✗	✓
✓	✗	✓	✓	✓
✓	✓	✗	✗	✓
✓	✗	✗	✗	✓
✓	✓	✓	✗	✓
✓	✗	✗	✓	✓

Merging simulation and experiment
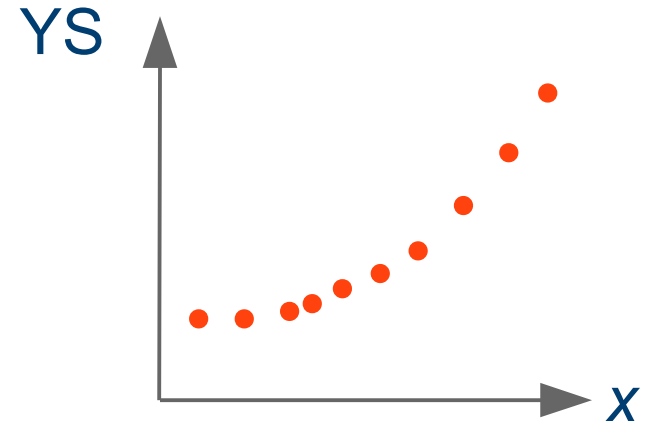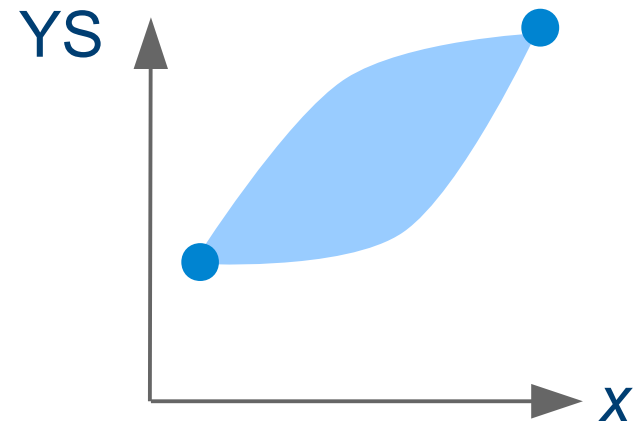
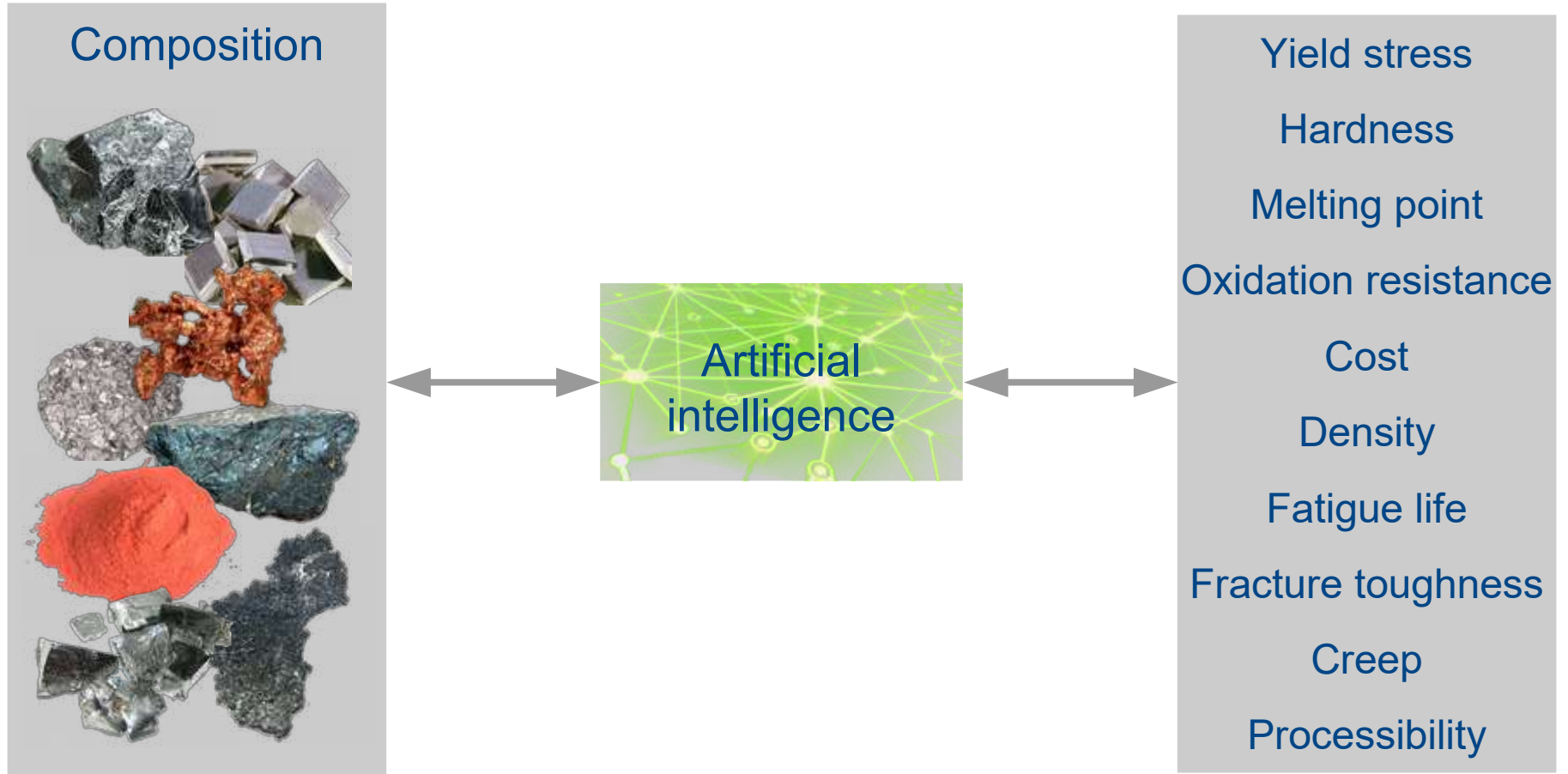# Merging simulation and experiment

Merging simulation and experiment

YS

Combine

YS

YS

Artificial intelligence

Composition

Artificial intelligence

Yield stress

Hardness

Melting point

Oxidation resistance

Cost

Density

Fatigue life

Fracture toughness

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Processibility

Artificial intelligence

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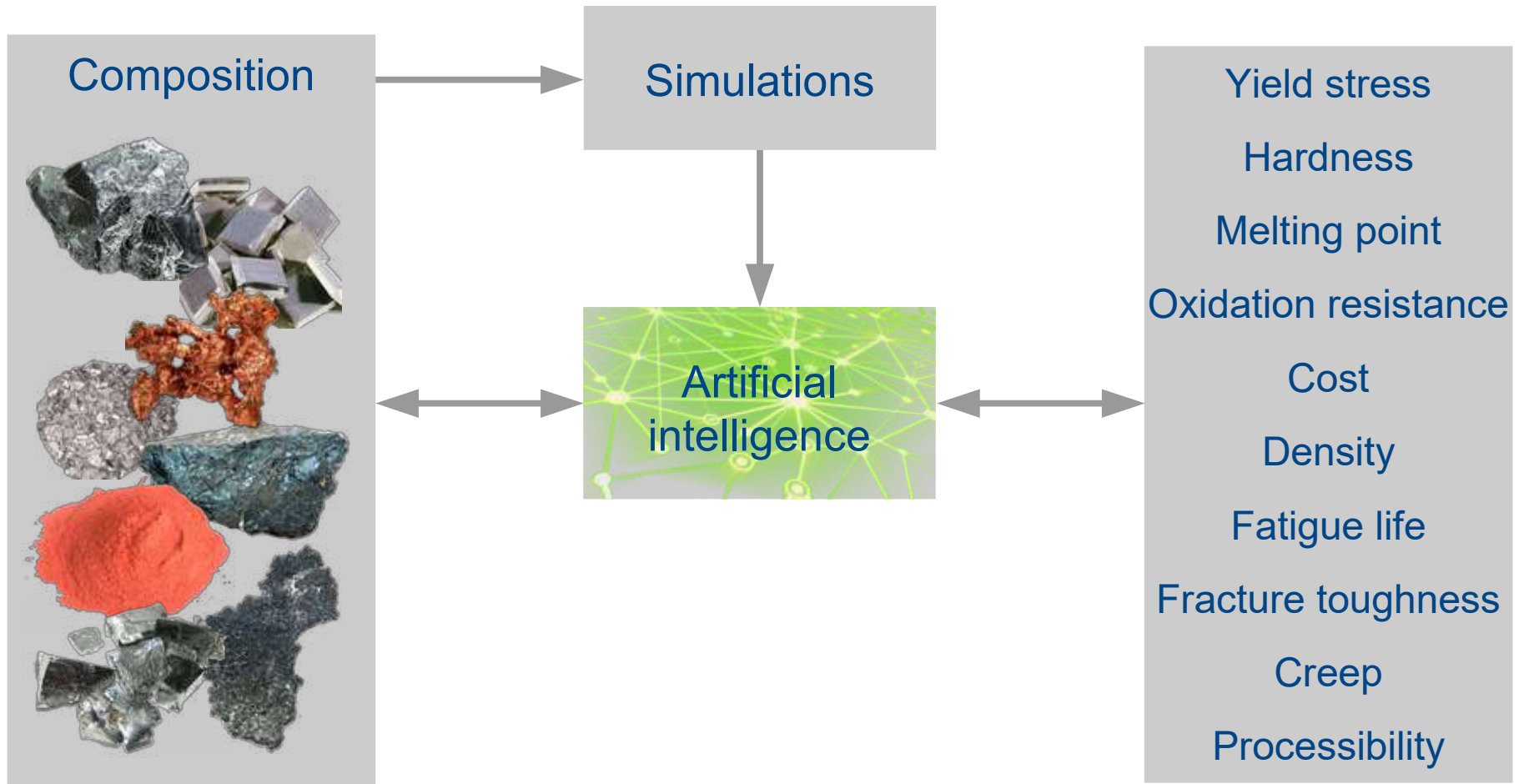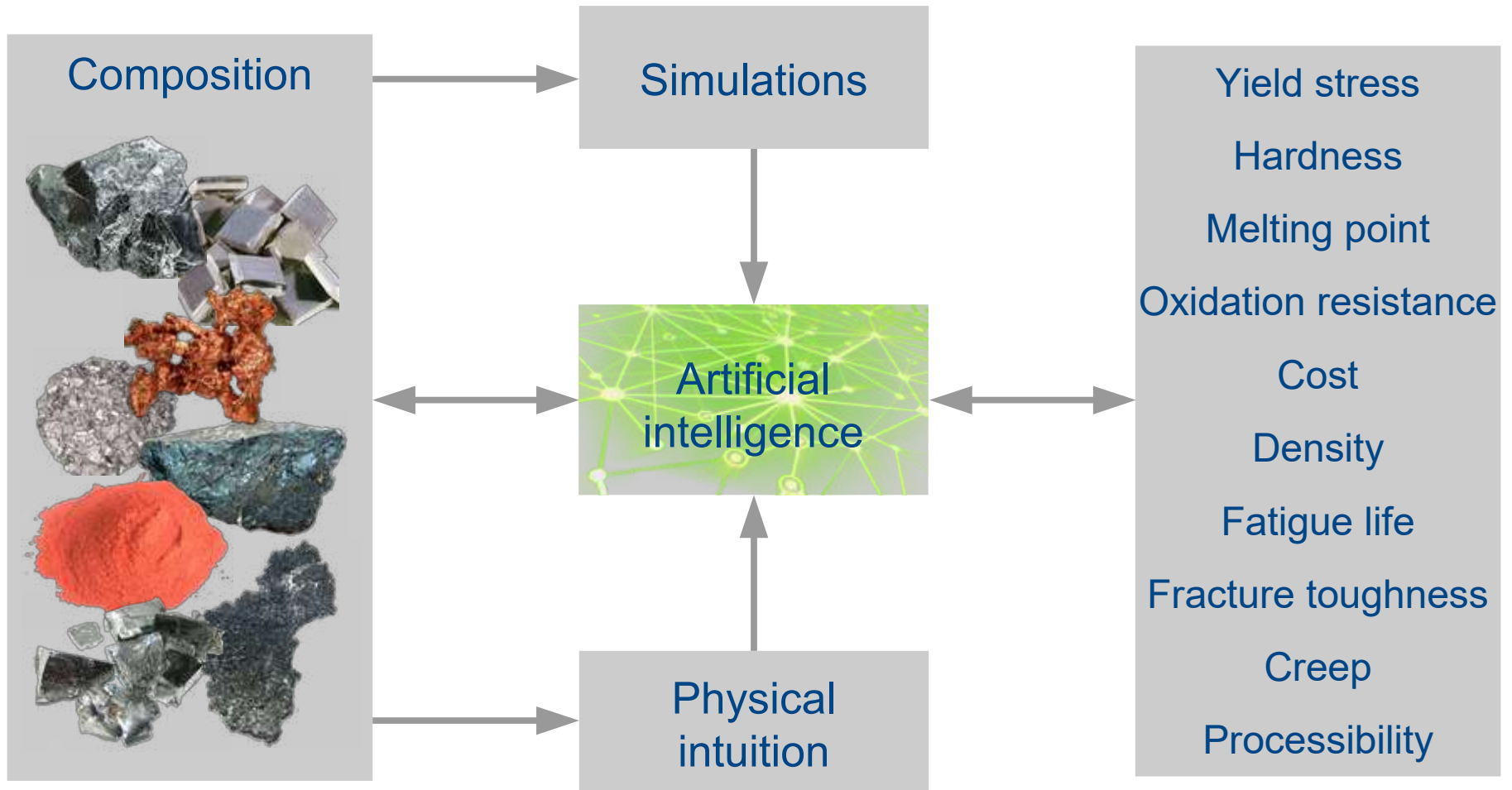
Artificial intelligence

Artificial intelligence

Exploiting material correlations

Alloy for direct laser deposition

3D printability ⟷ Weldability
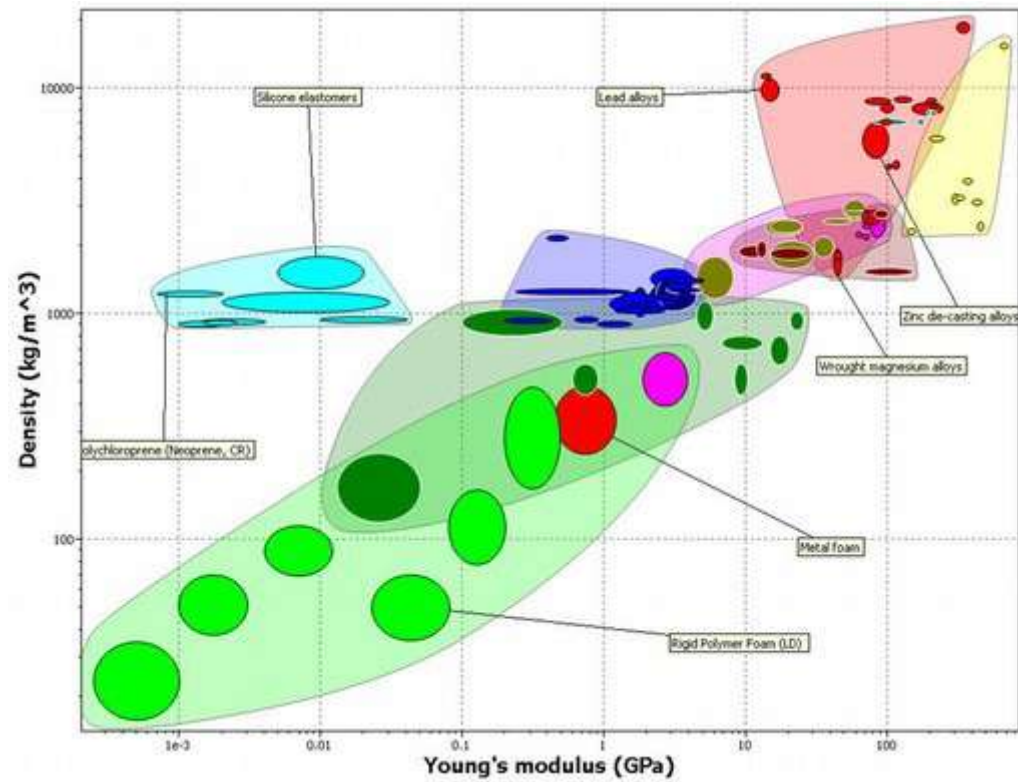
Exploiting material correlations

Alloy for direct laser deposition

3D printability	⟷	Weldability

Lithium cathode materials

Experiment	⟷	DFT

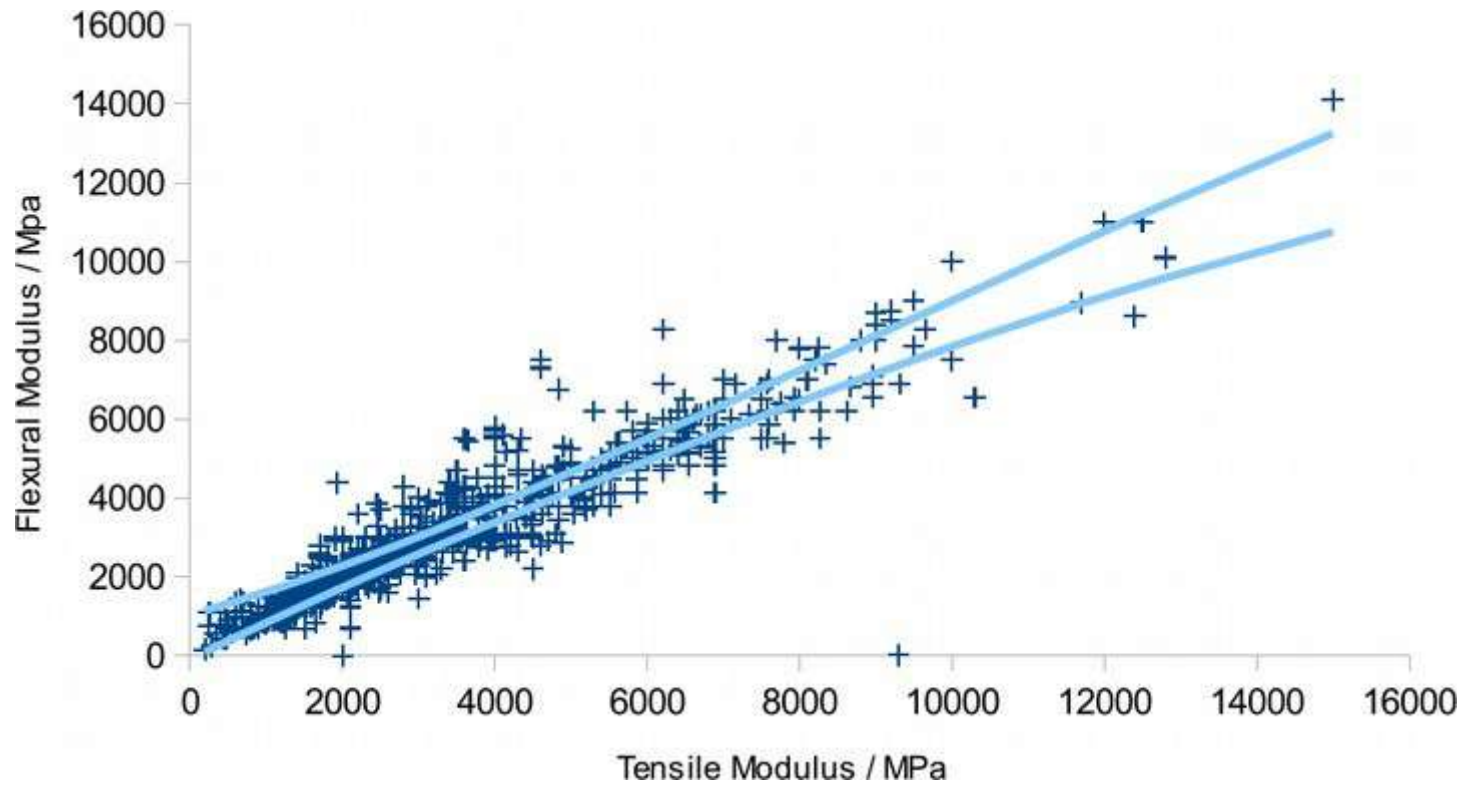# Database verification

Choice of basis set

Alloys

Composition
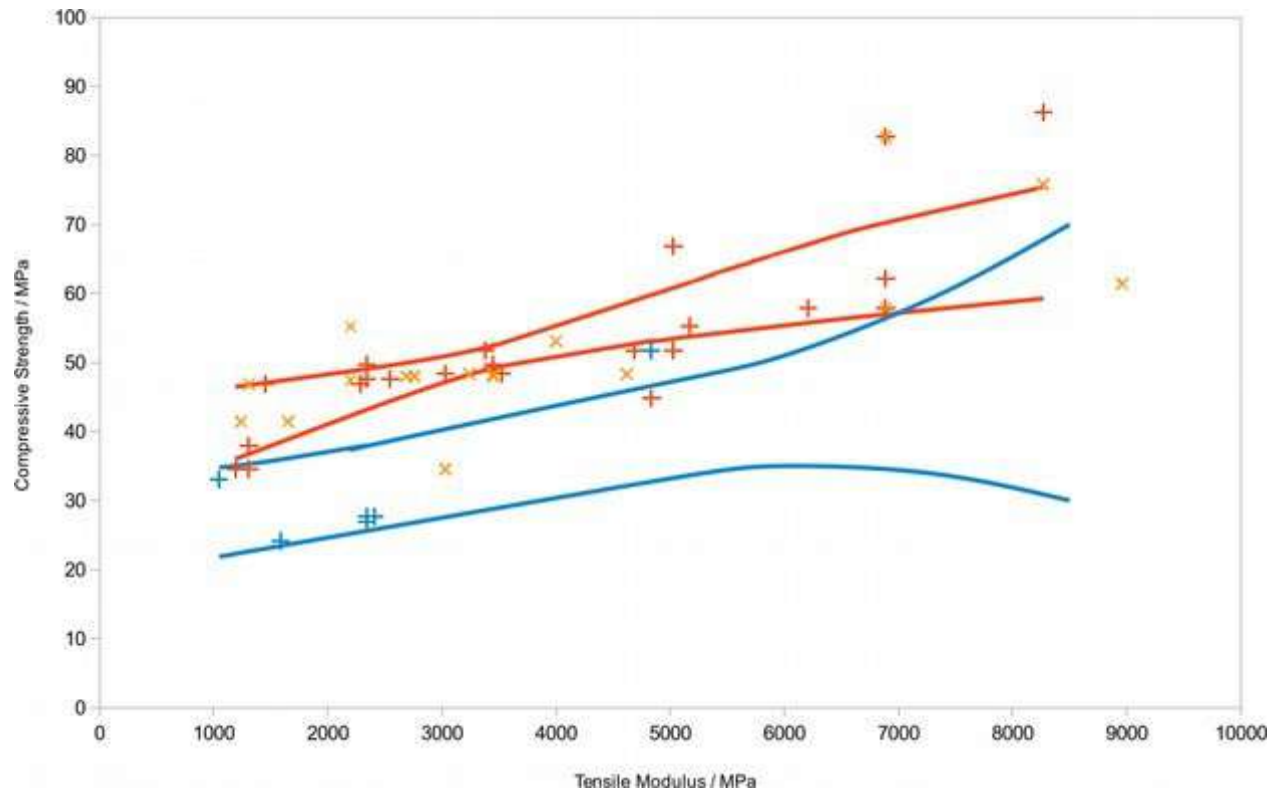Heat treatment

Polymers

Properties
Filler type and volume

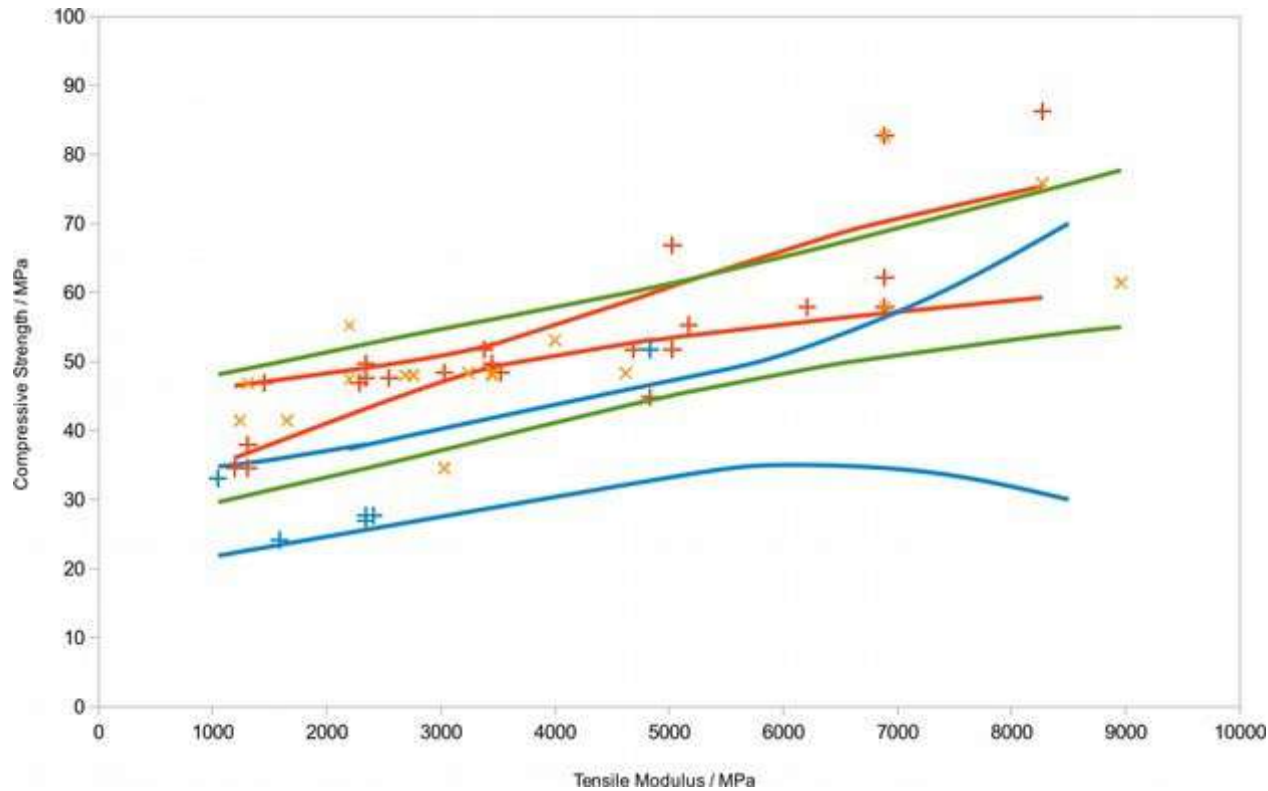# Polymers: flexural modulus vs tensile modulus

Polymers: compressive strength vs tensile modulus
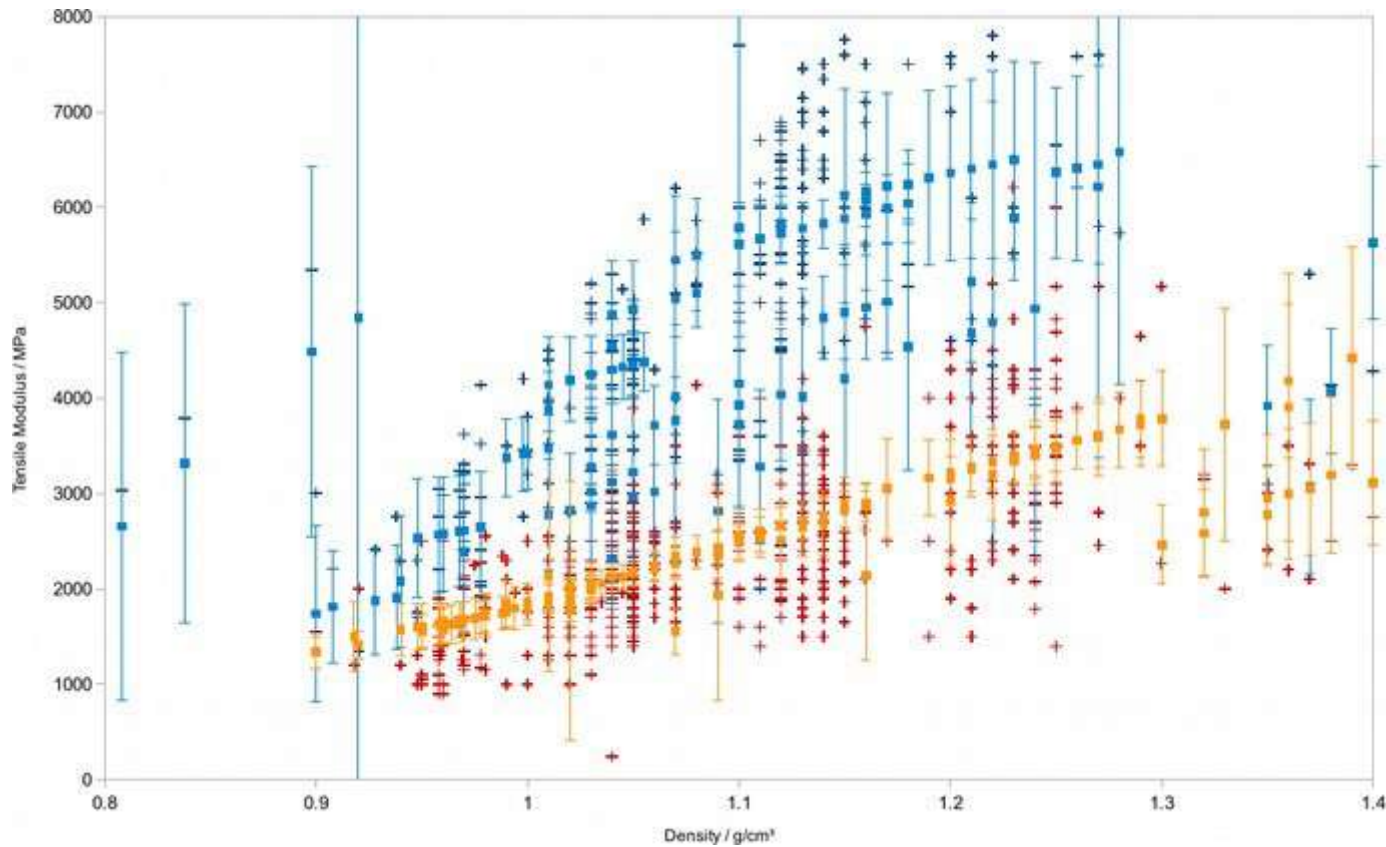

Homopolymer

Copolymer

Polymers: compressive strength vs tensile modulus

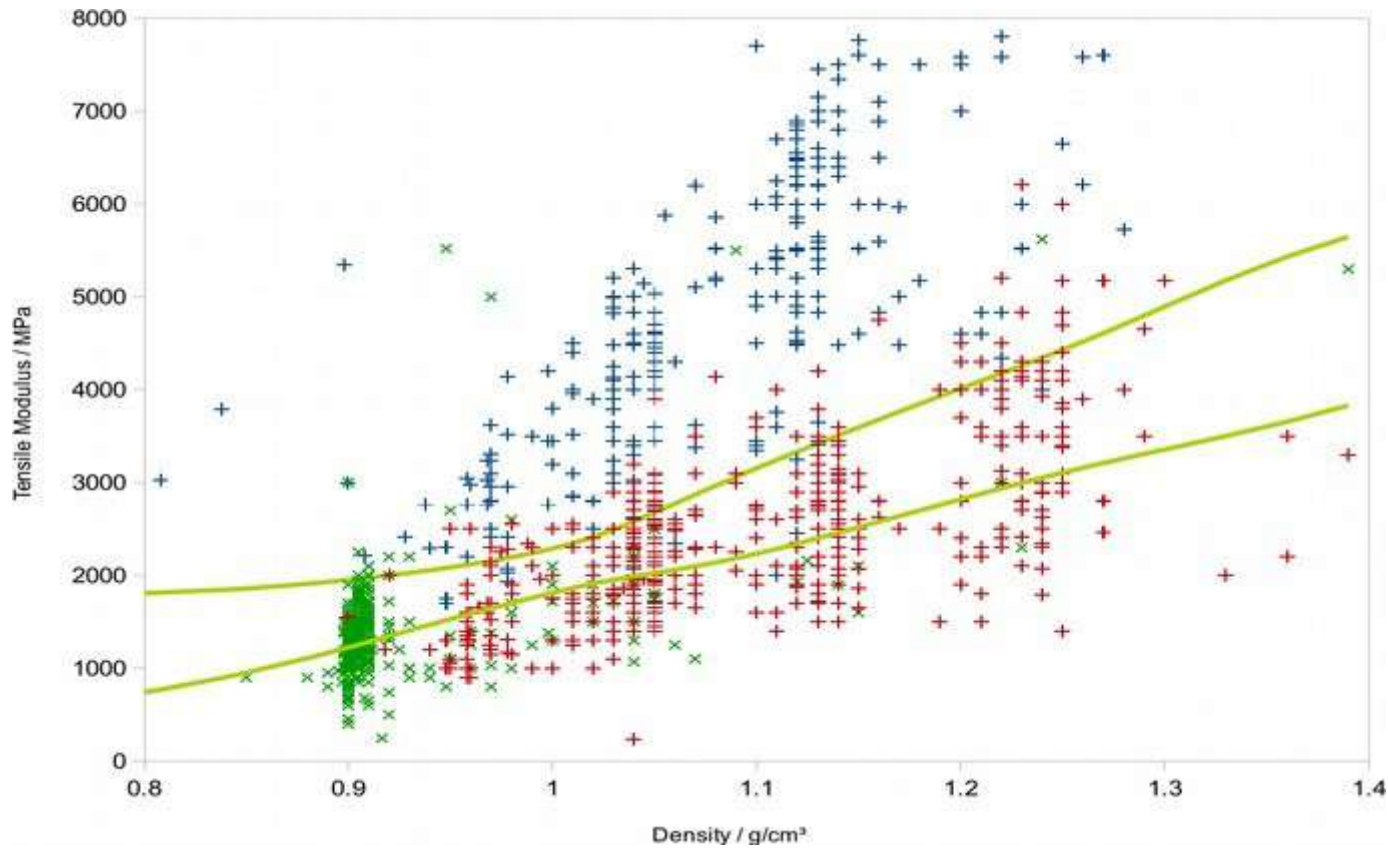Homopolymer
Unknown
Copolymer

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