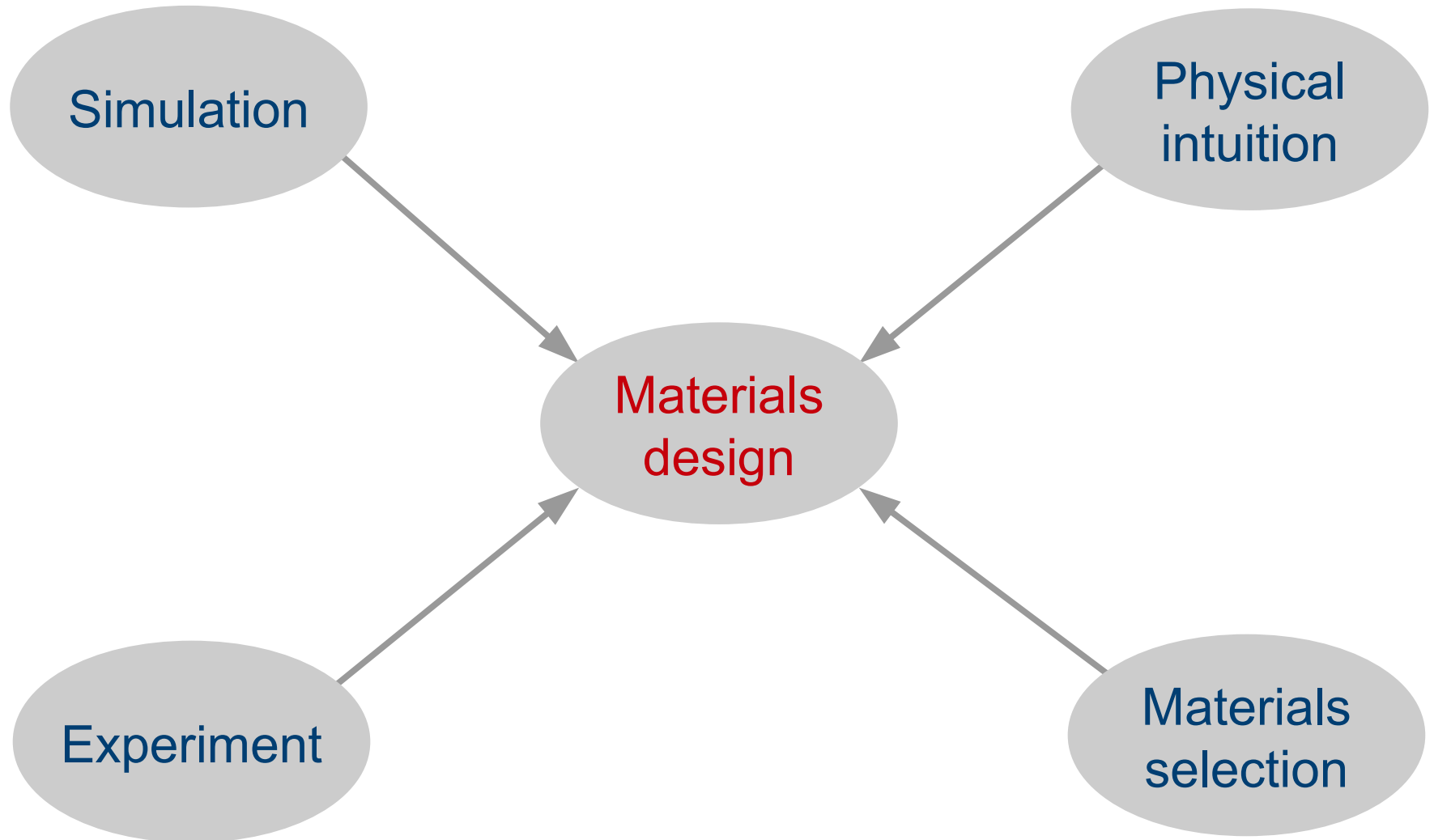


Materials discovery with artificial intelligence

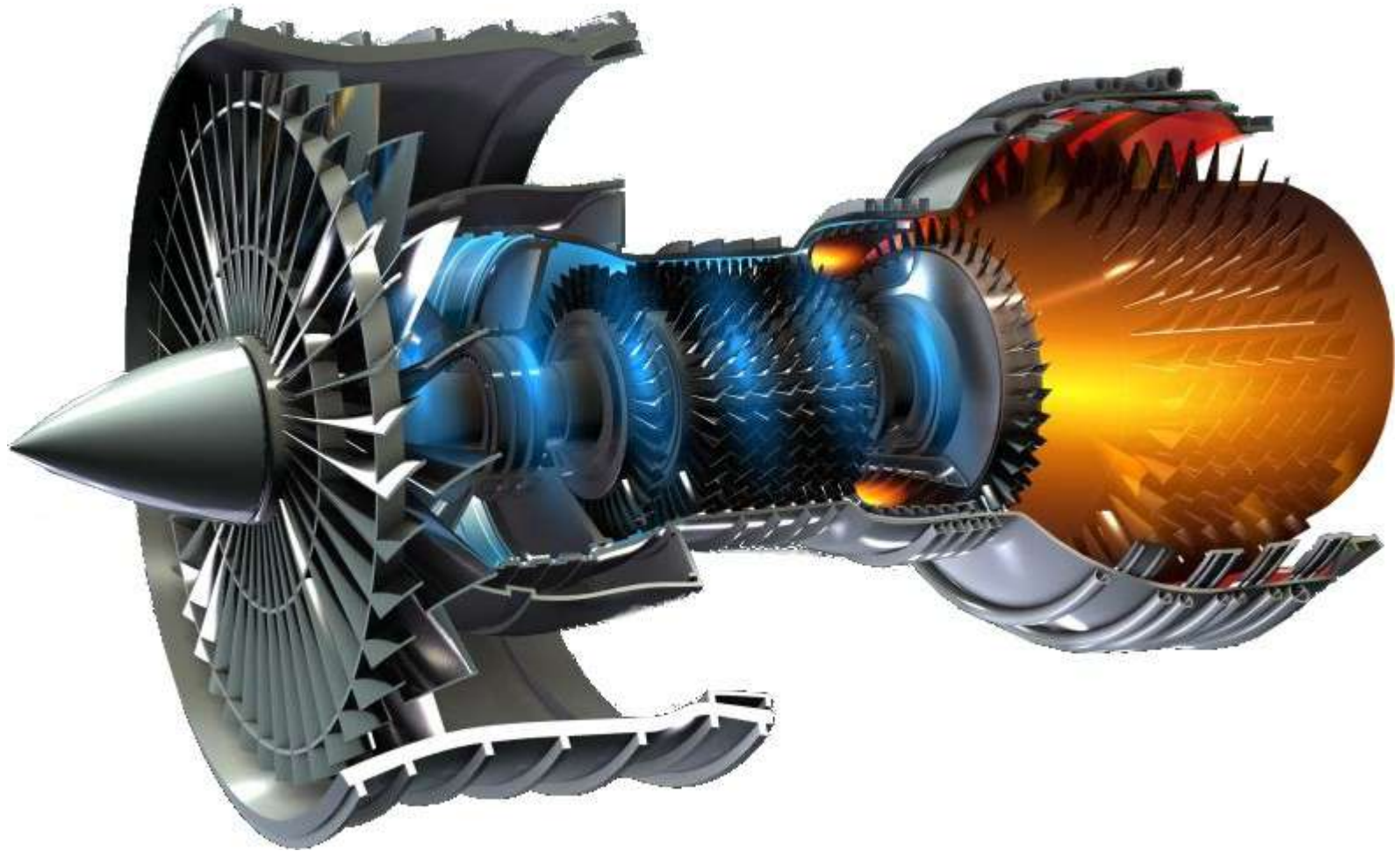
Gareth Conduit

TCM Group, Department of Physics

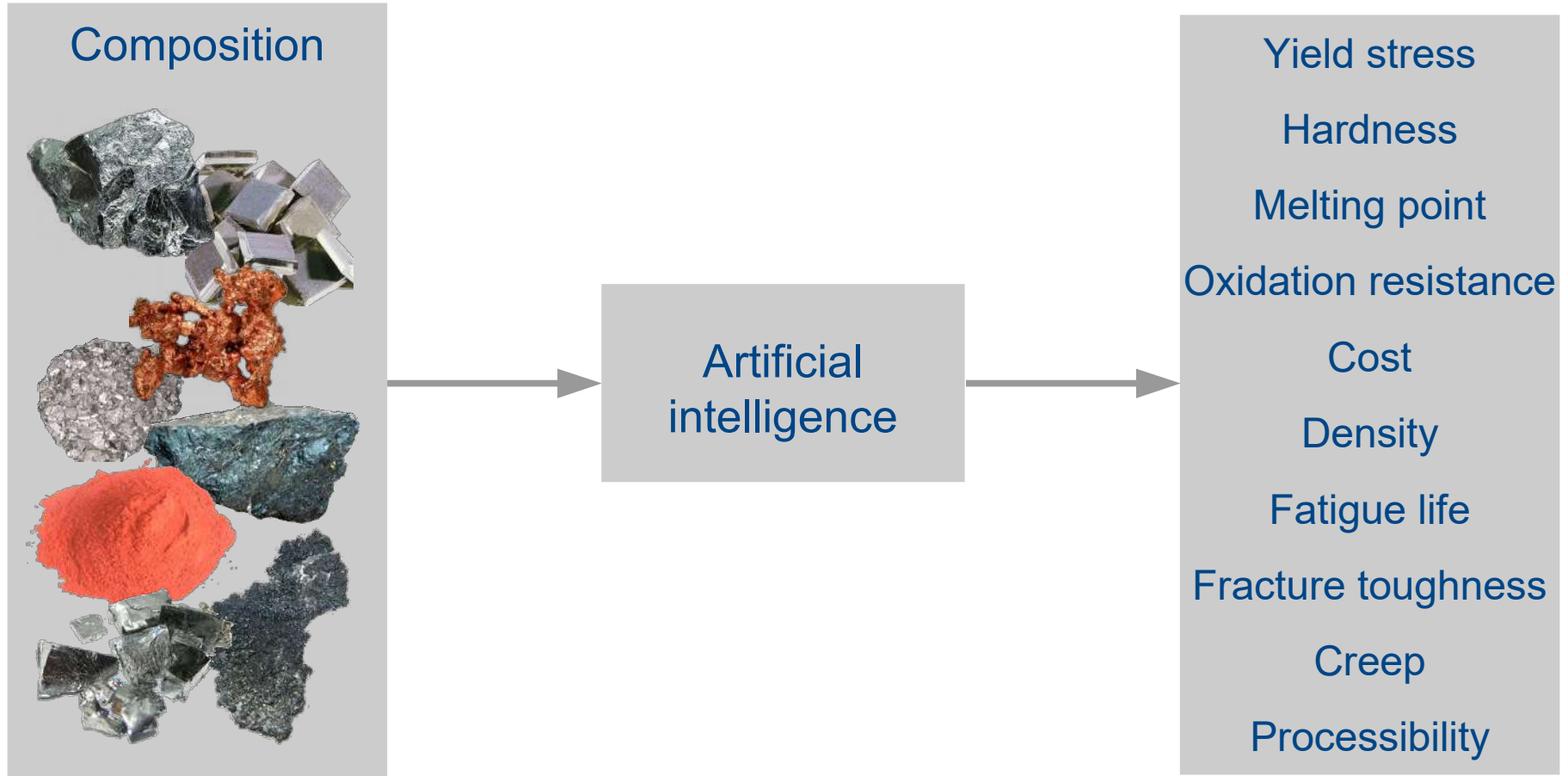
Approaches to materials design



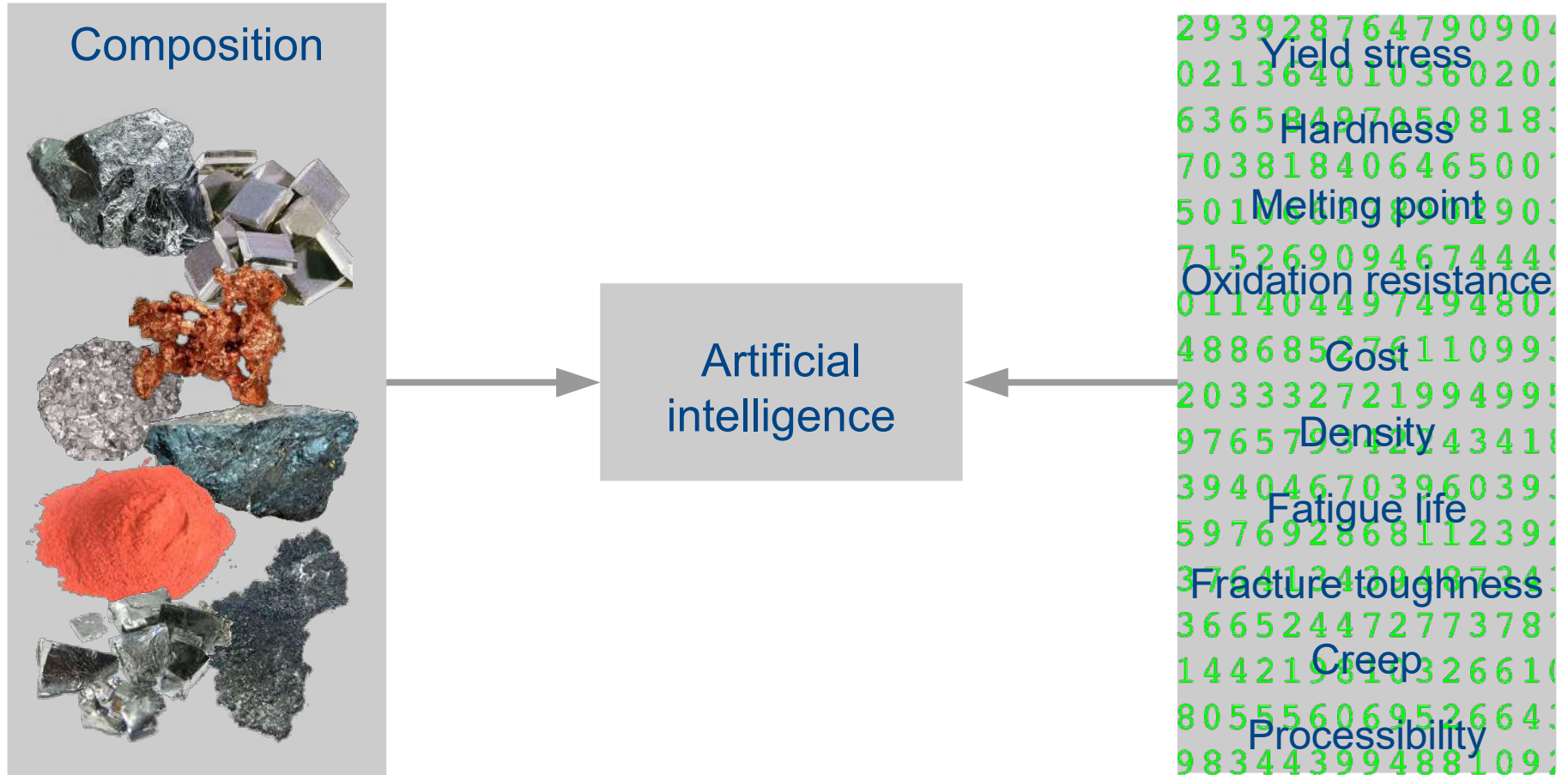
Schematic of a jet engine



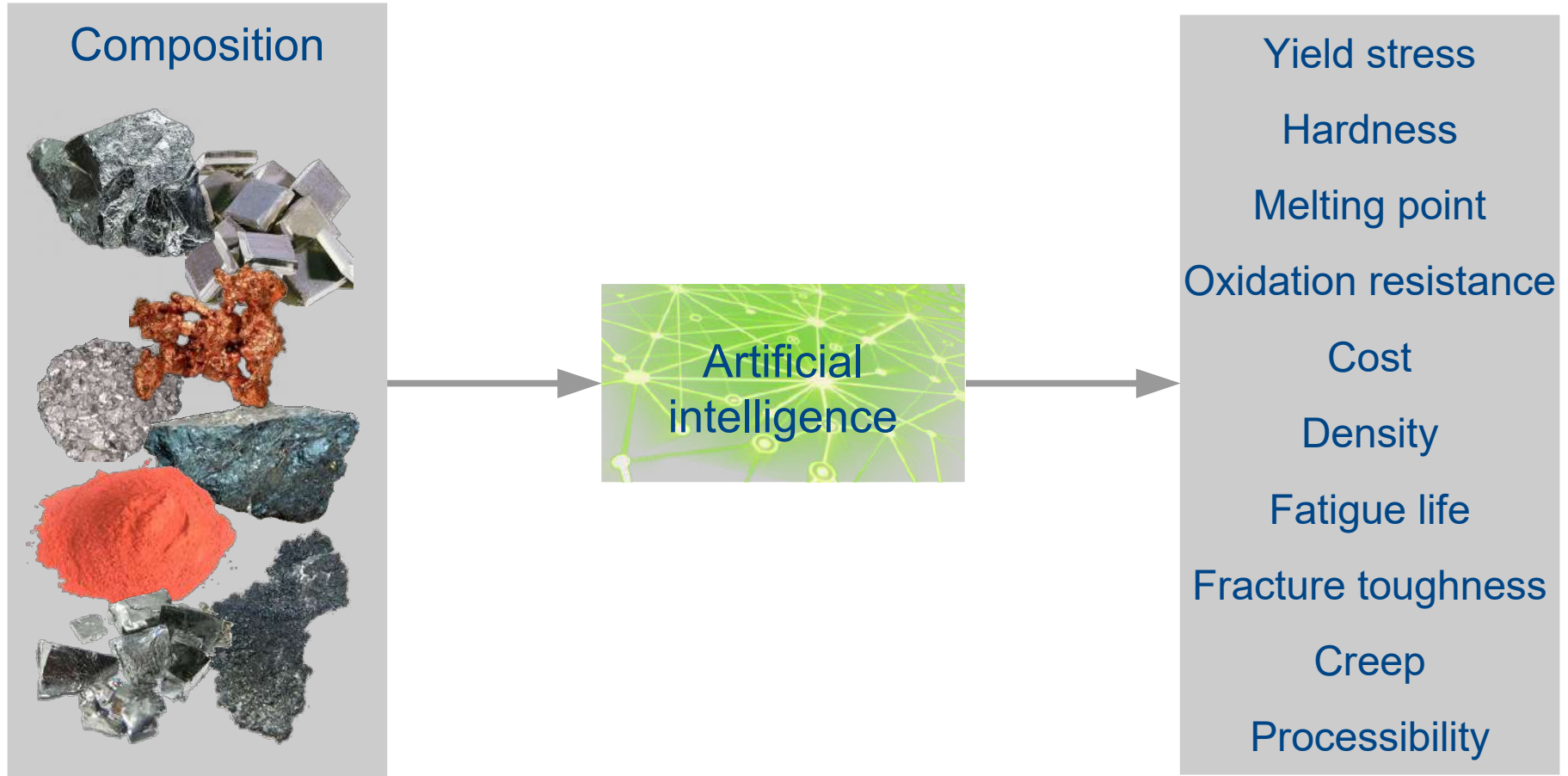
Artificial intelligence



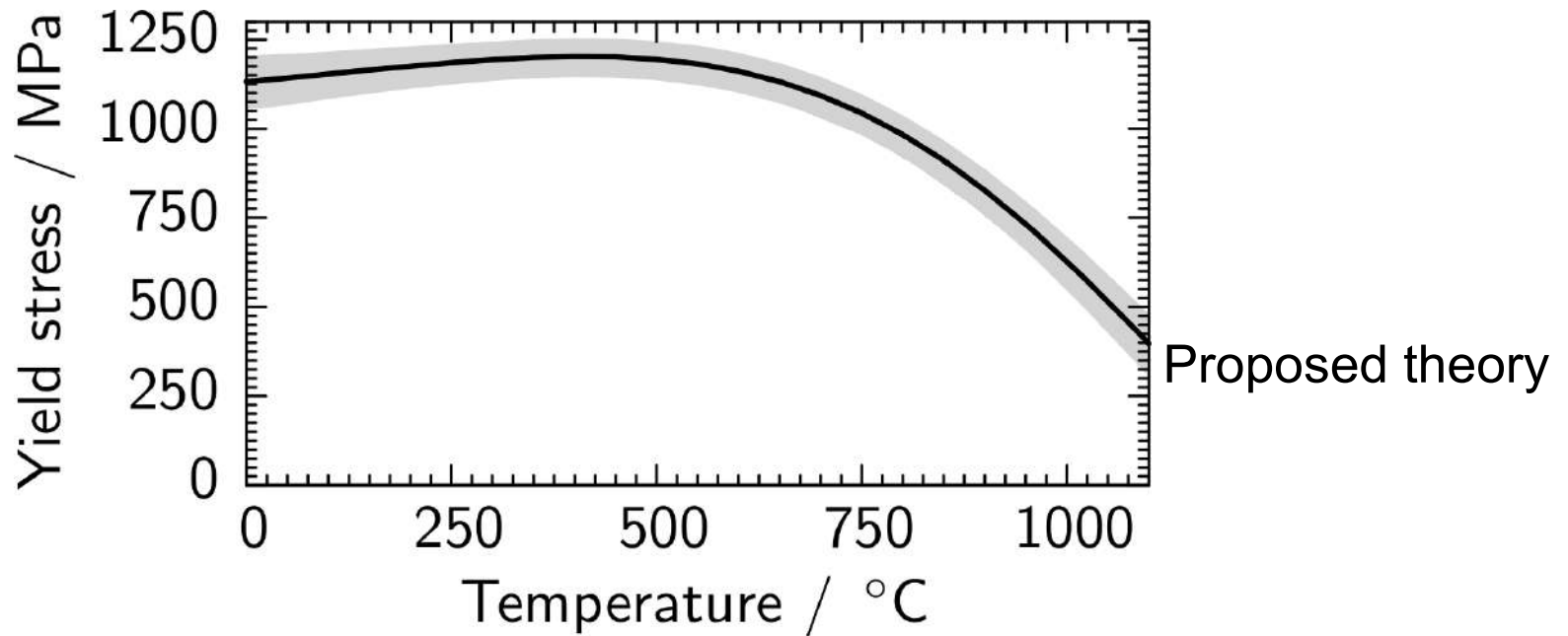
Artificial intelligence



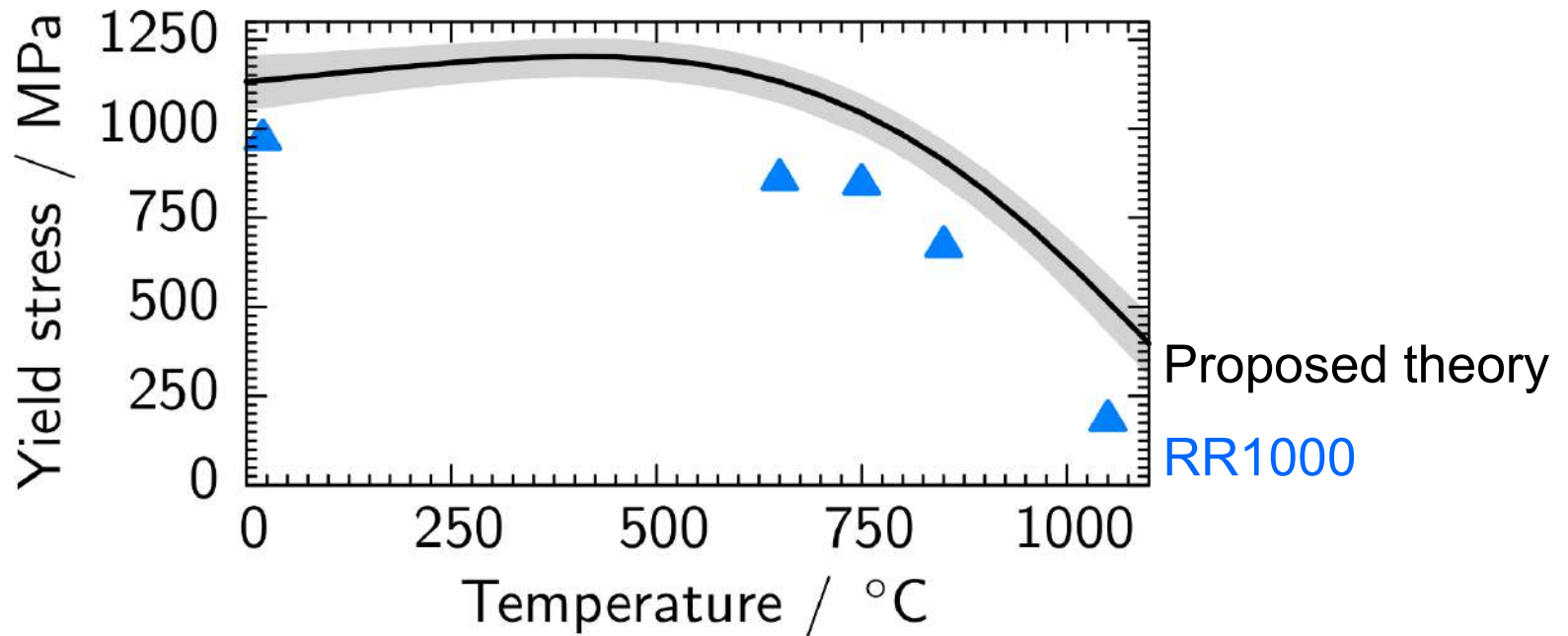
Artificial intelligence



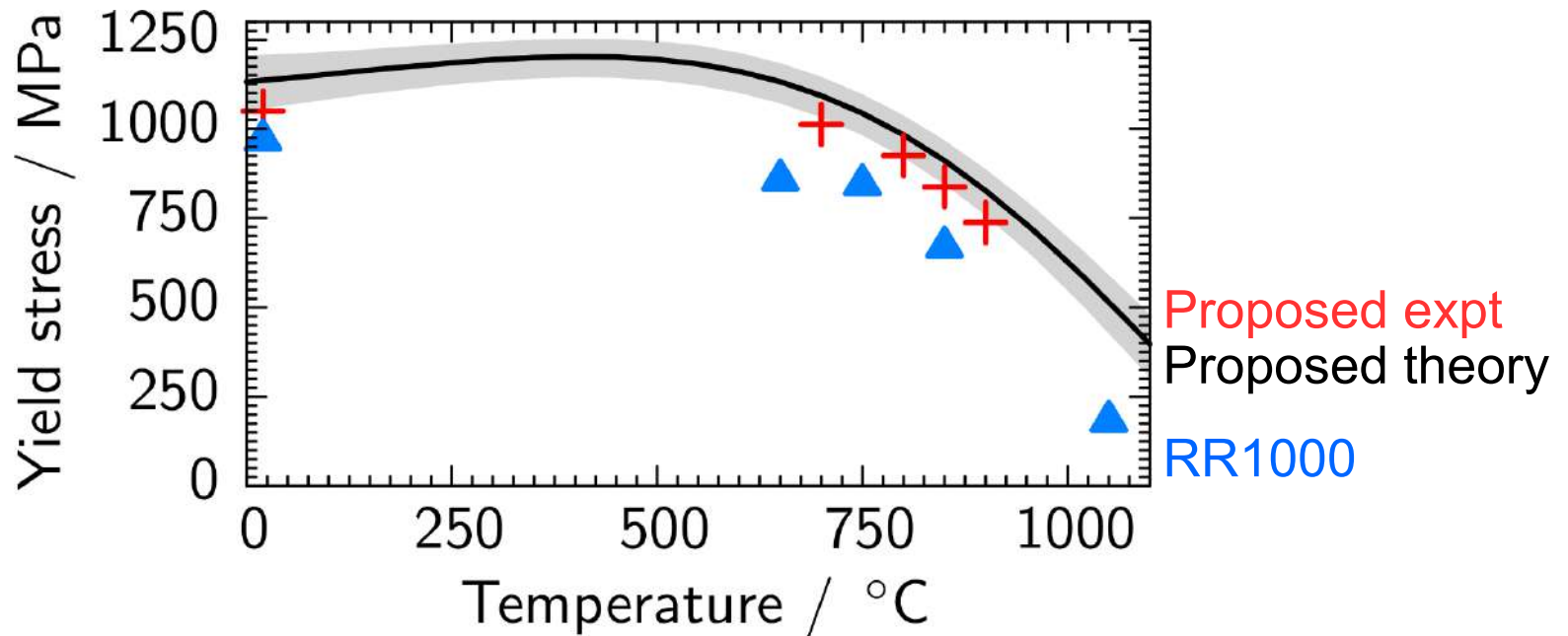
Testing the yield stress



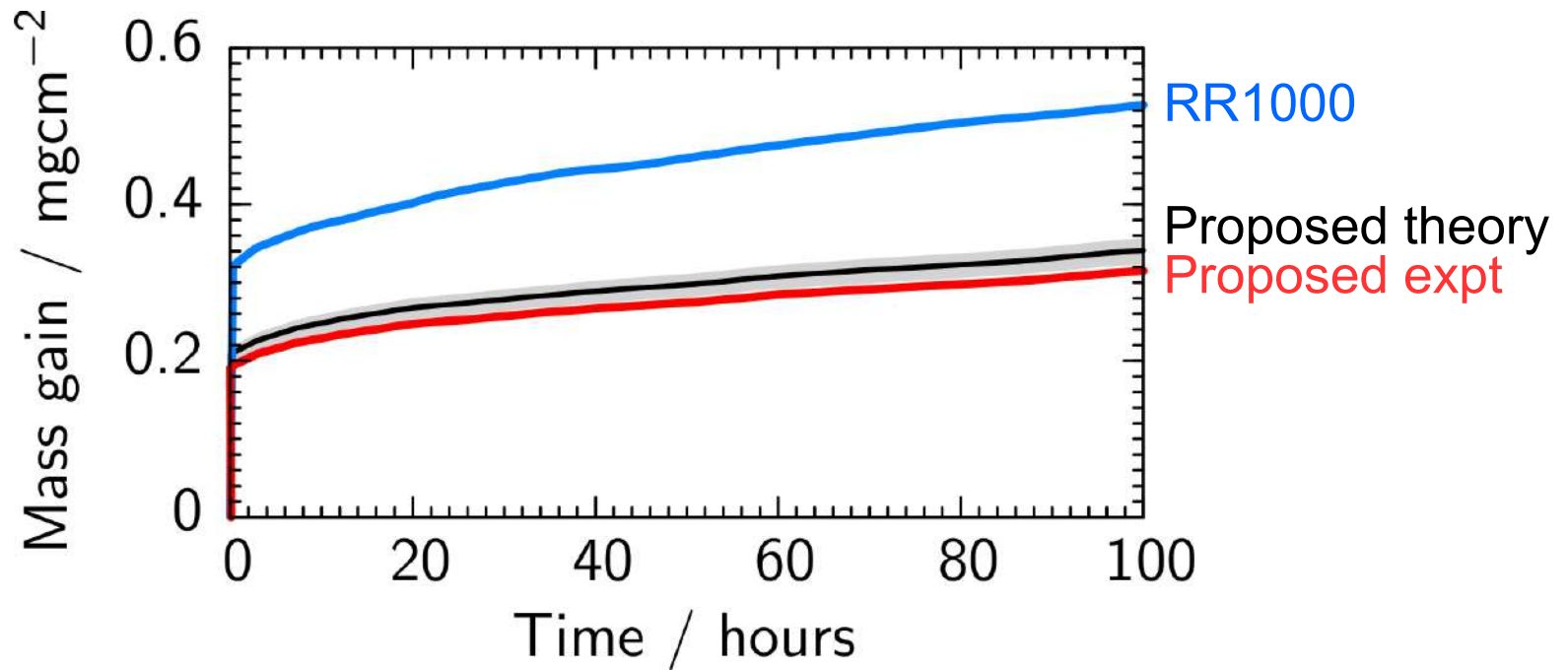
Testing the yield stress



Testing the yield stress



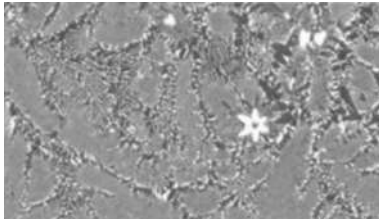
Testing the oxidation resistance



Alloys discovered

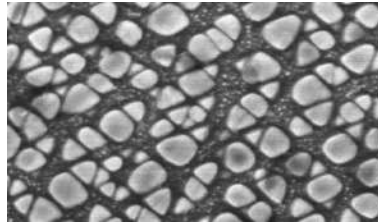
Cr-Cr₂Ta alloys

Intermetallics, 48, 62



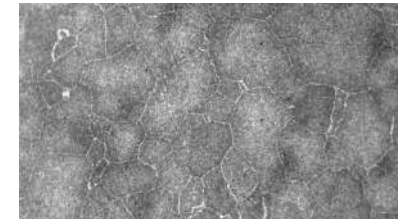
Combustor alloy

GB1408536



RR1000 grain growth

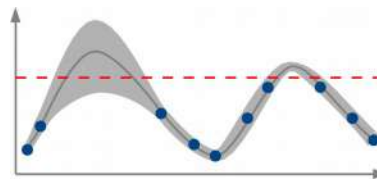
Acta Materialia, 61, 3378



Discovery algorithm

EP14153898

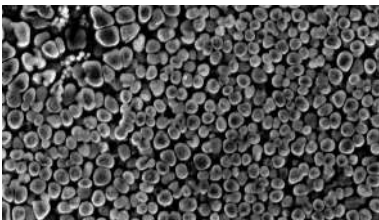
US 2014/177578



Ni disc alloy

EP14157622

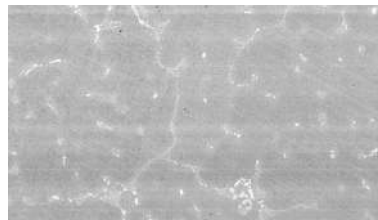
US 2013/0052077 A2



Mo-Hf forging alloy

EP14161255

US 2014/223465



Mo-Nb forging alloy

EP14161529

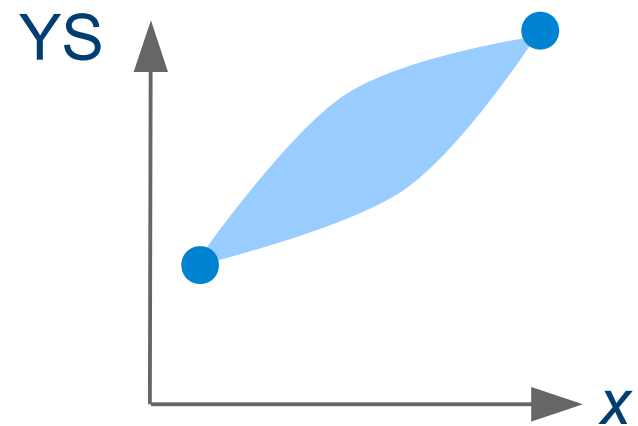
US 2014/224885



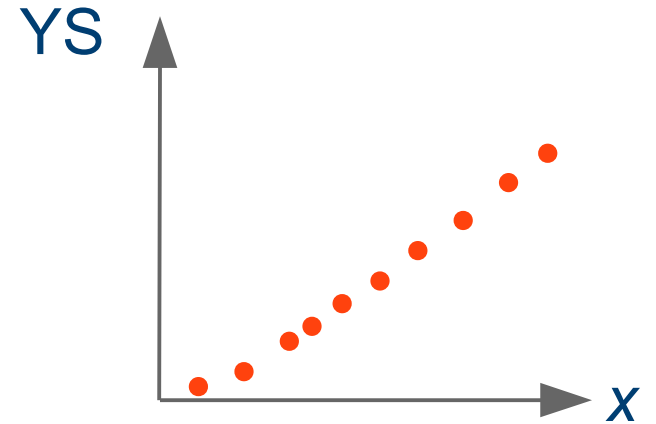
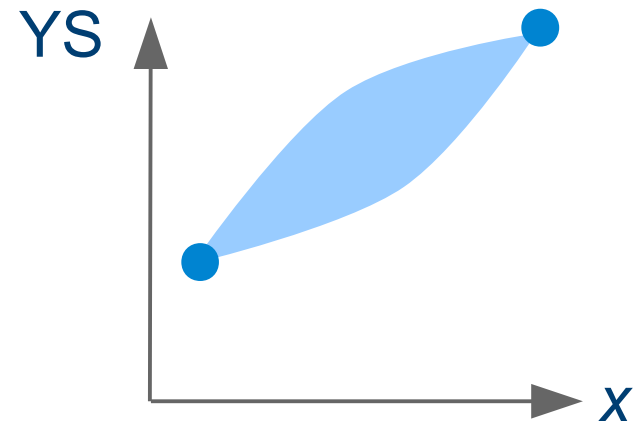
Fragmented databases

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

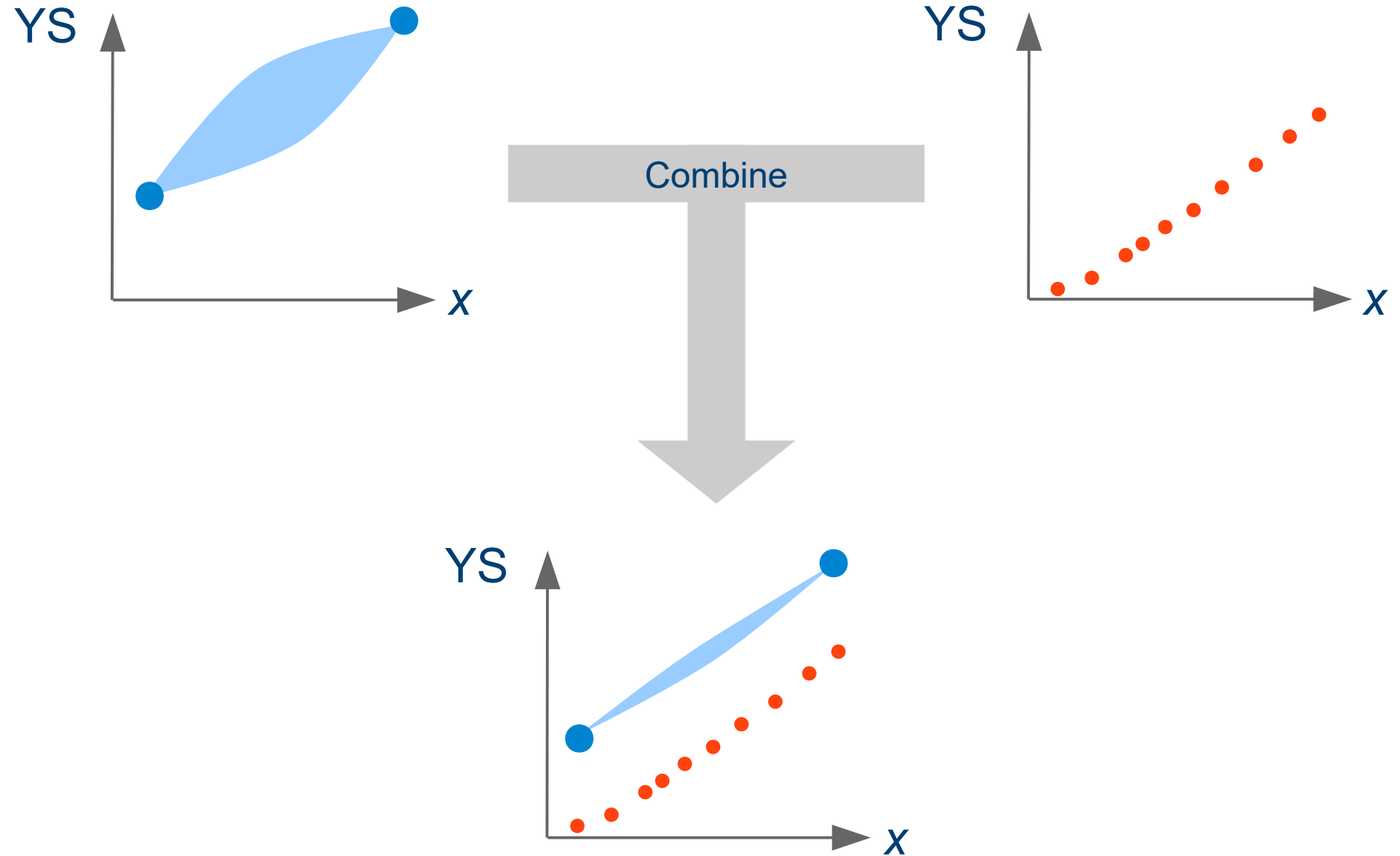
Merging simulation and experiment



Merging simulation and experiment



Merging simulation and experiment



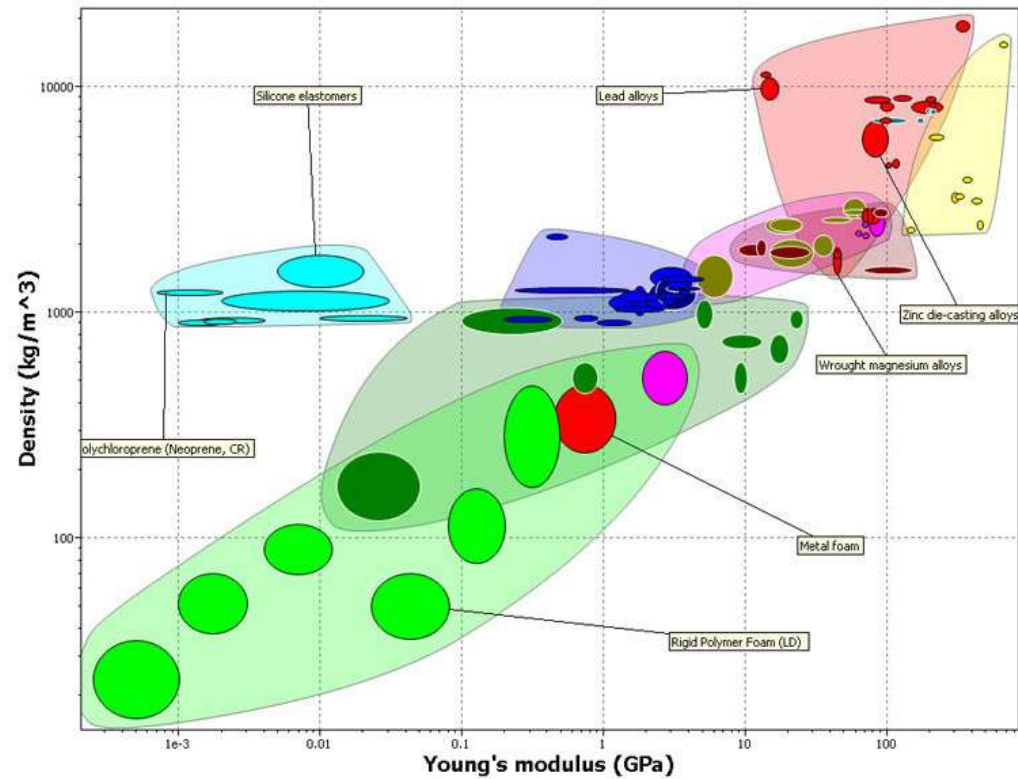
Exploiting material correlations



Lithium cathode materials

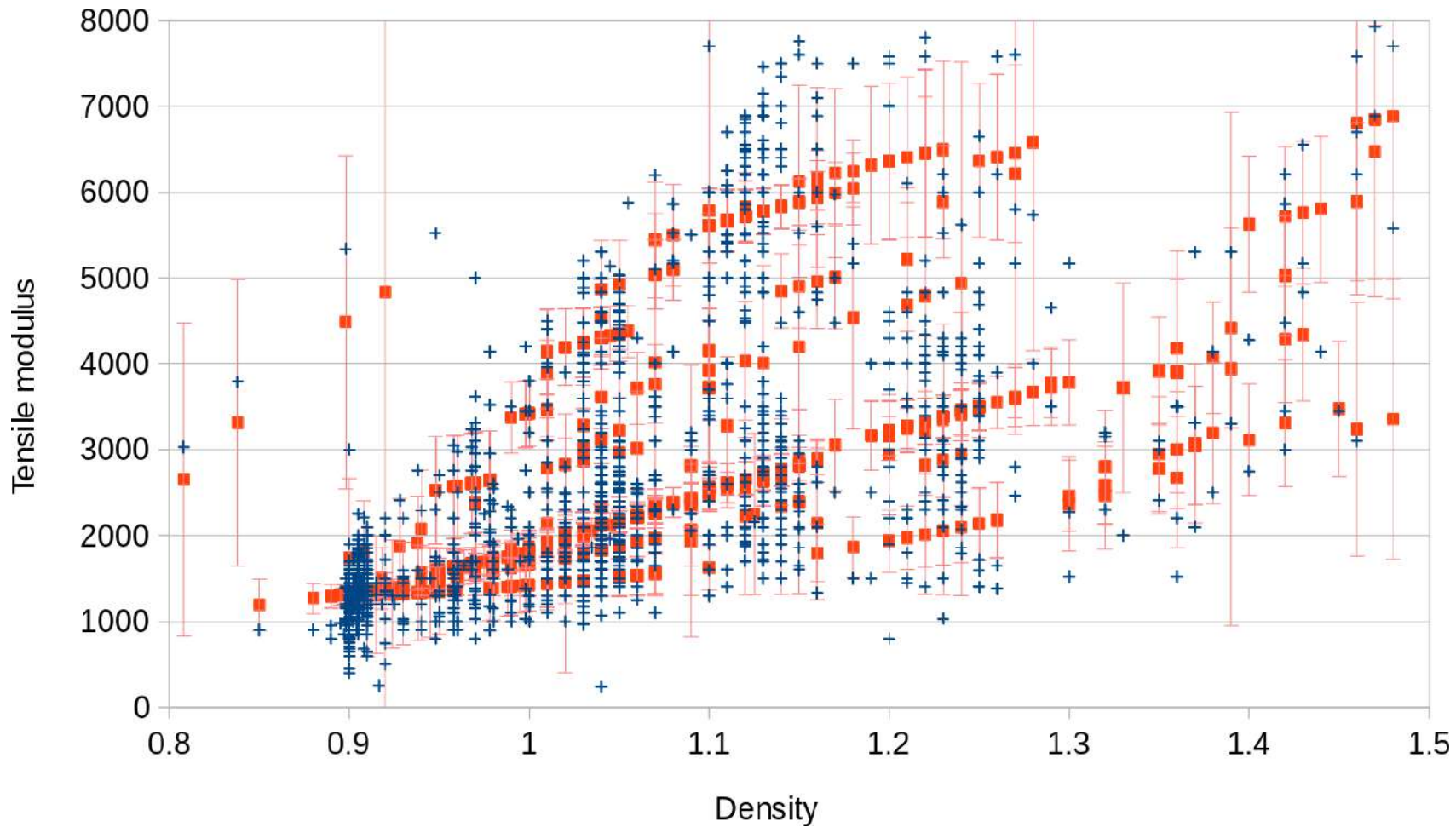


Database verification



Database contains $>10^7$ separate entries

Example: polymers



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