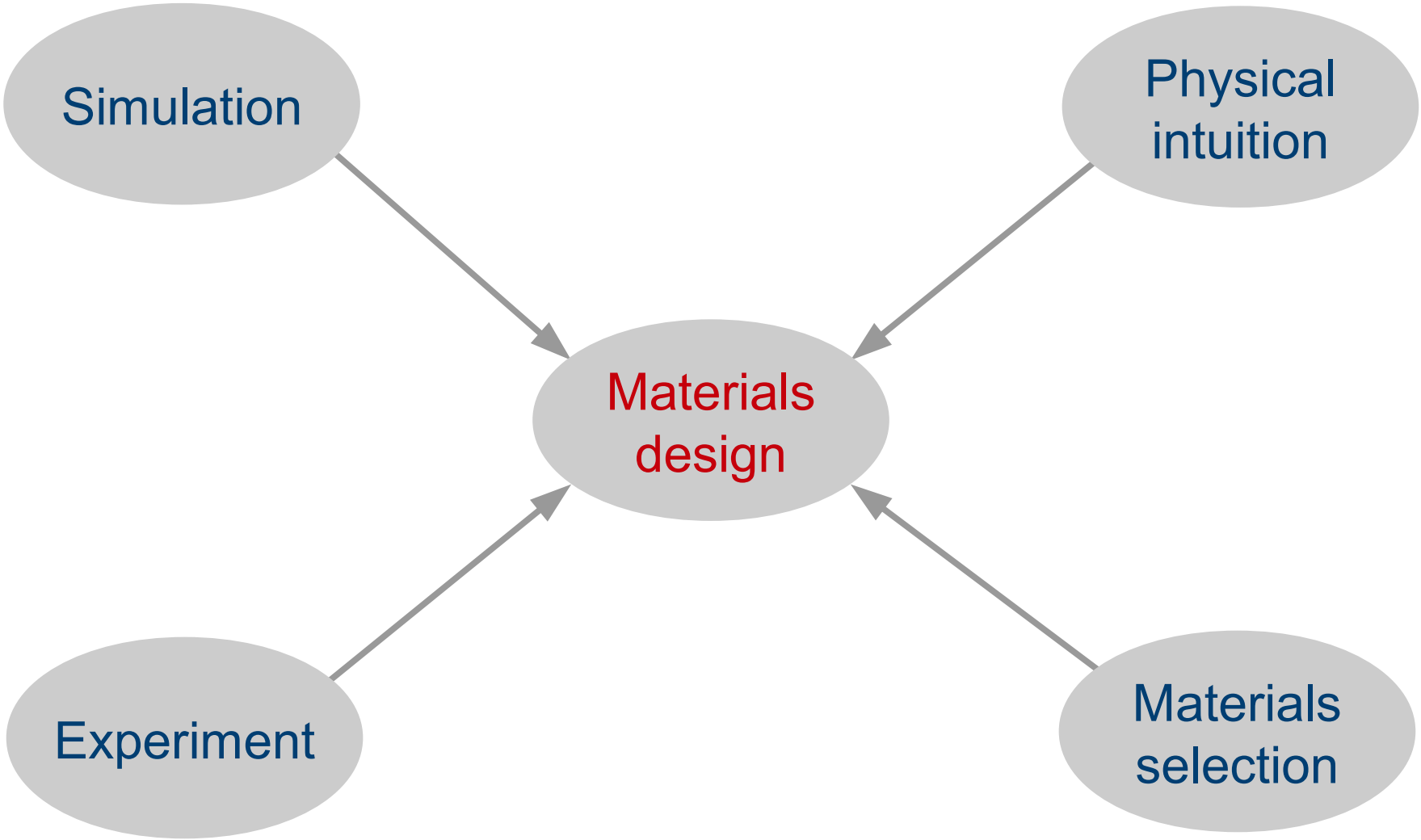
UNIVERSITY OF CAMBRIDGE

Materials discovery with artificial intelligence

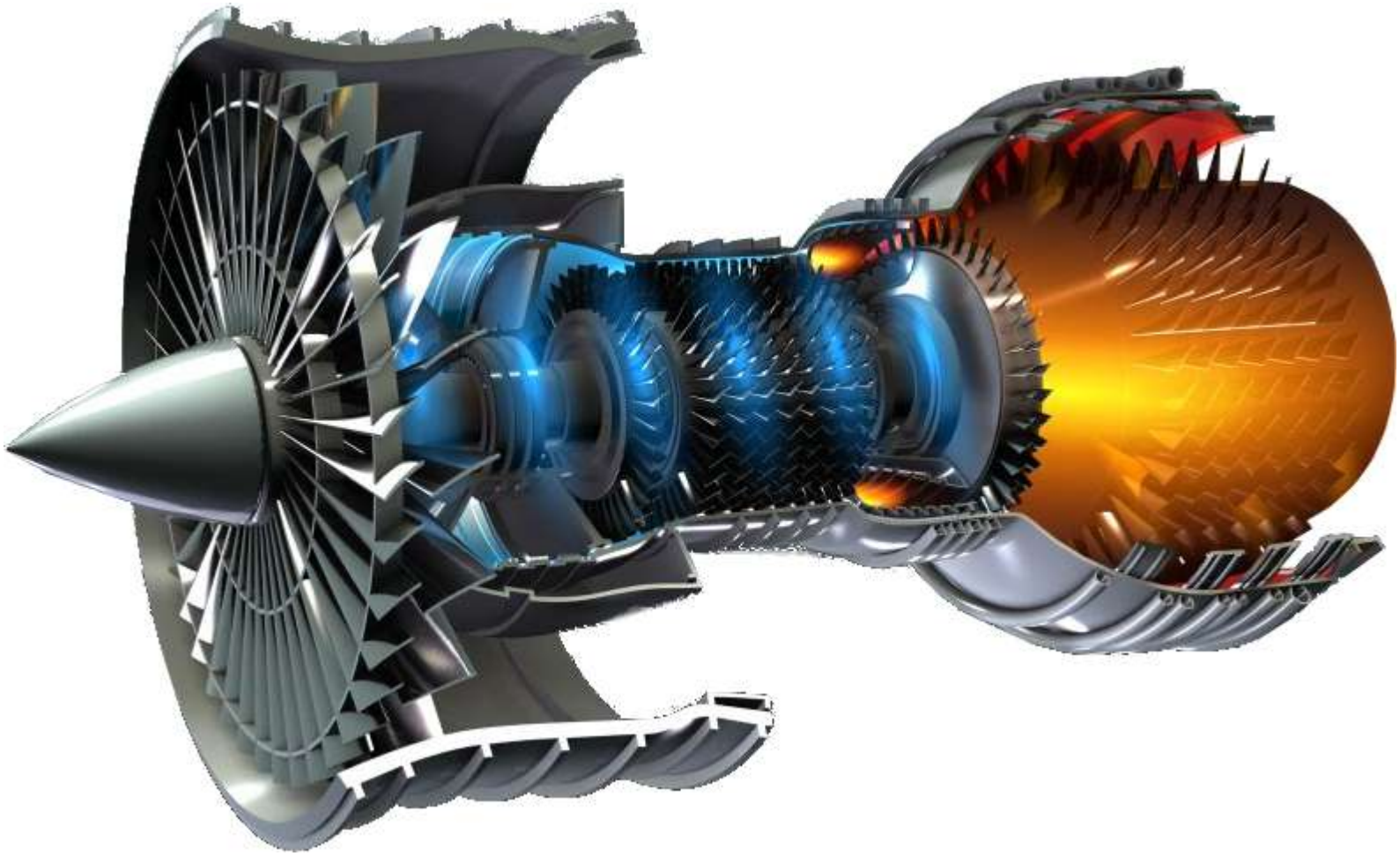
Gareth Conduit

TCM Group, Department of Physics

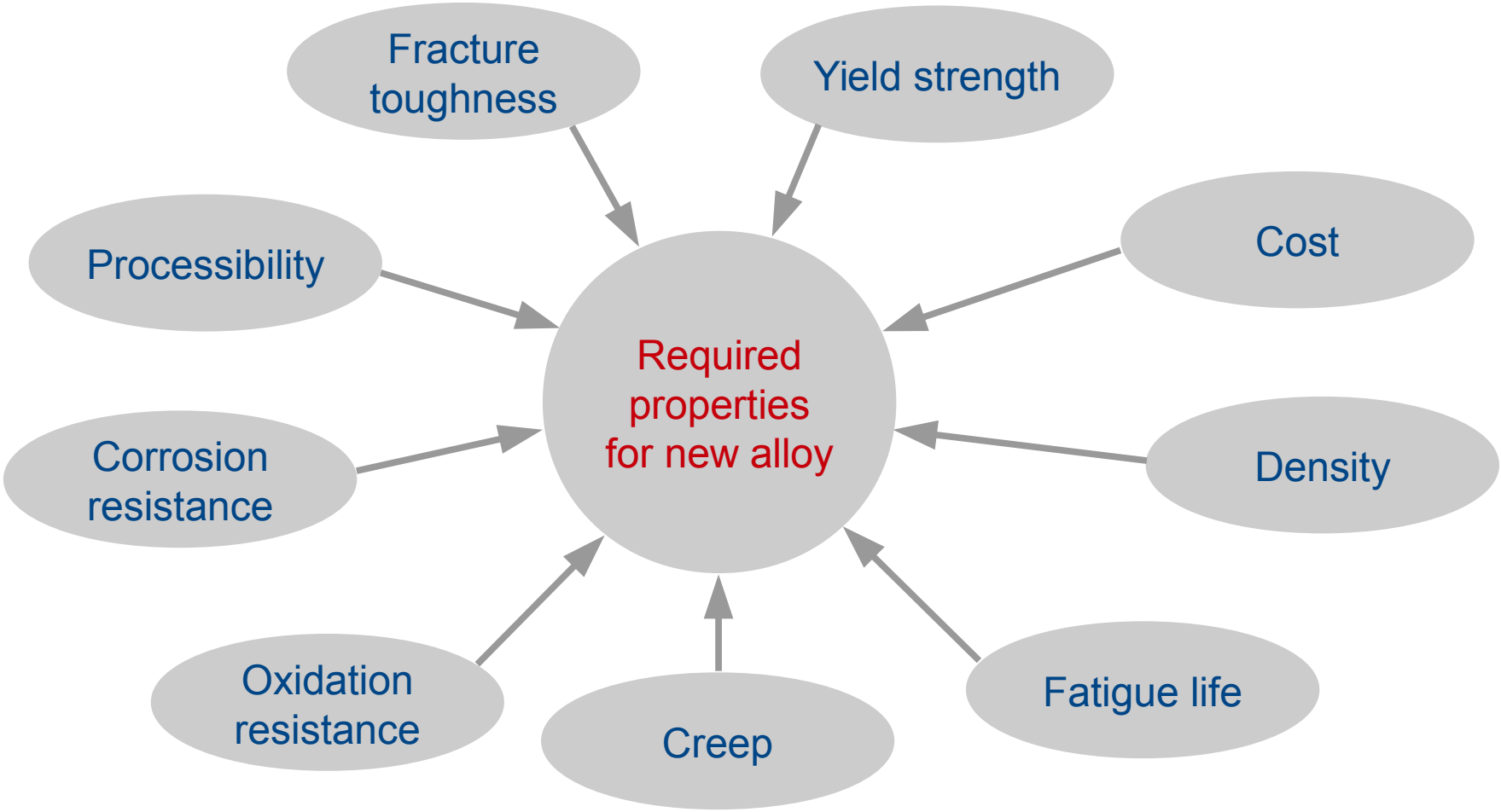
Approaches to materials design



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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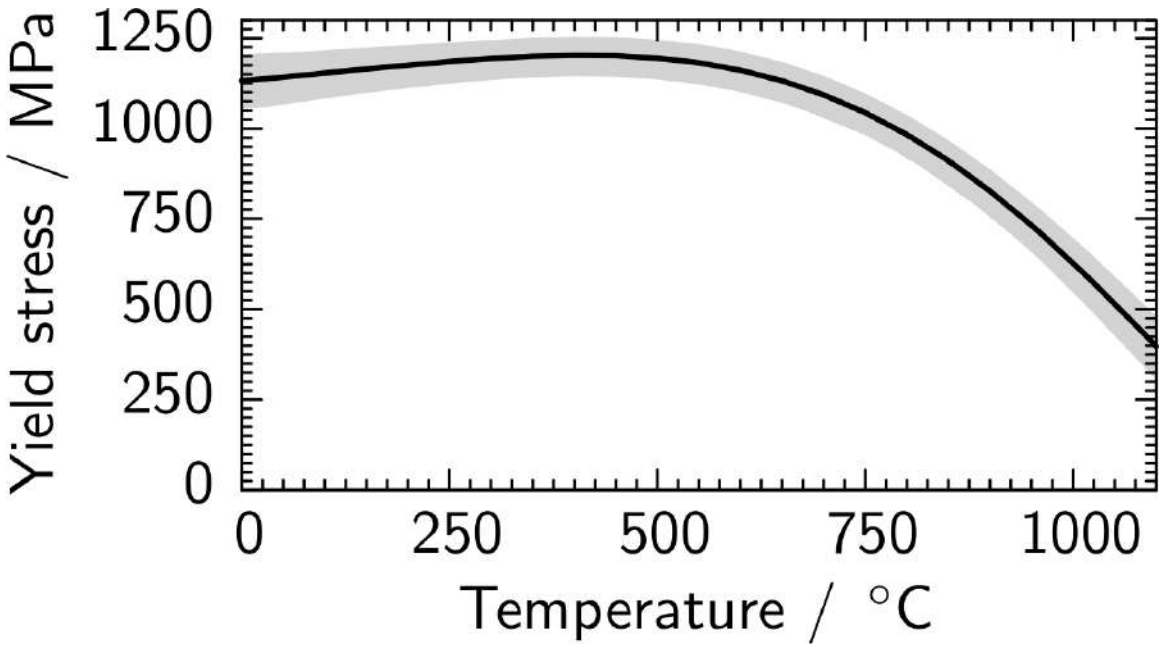
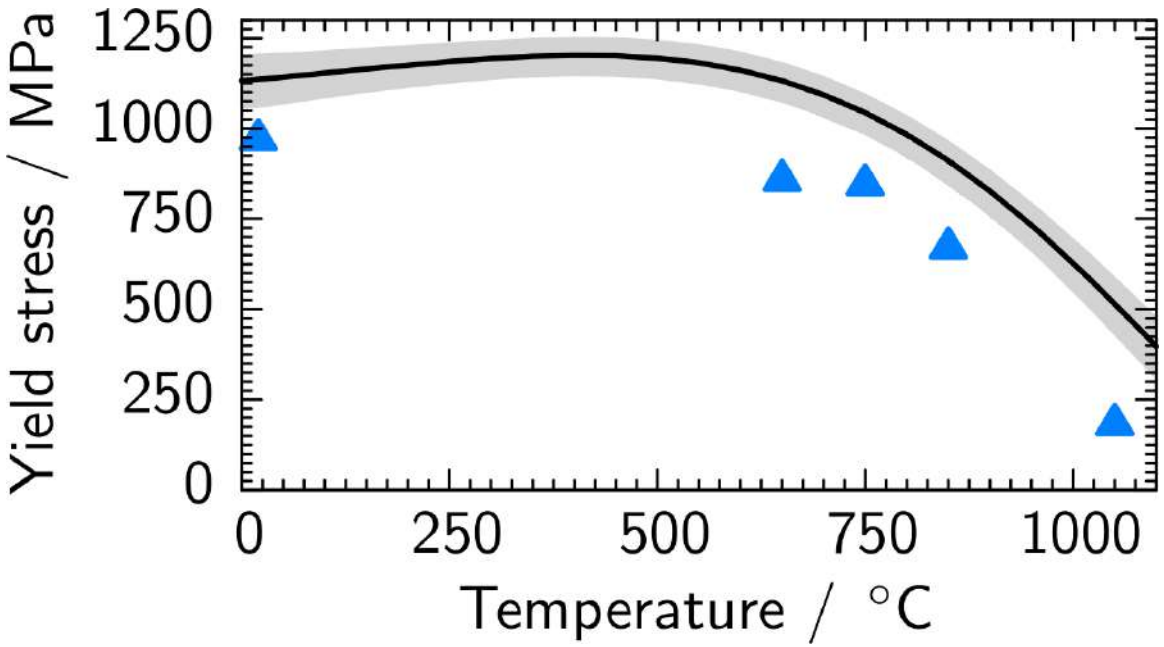
Testing the yield stress



Proposed theory

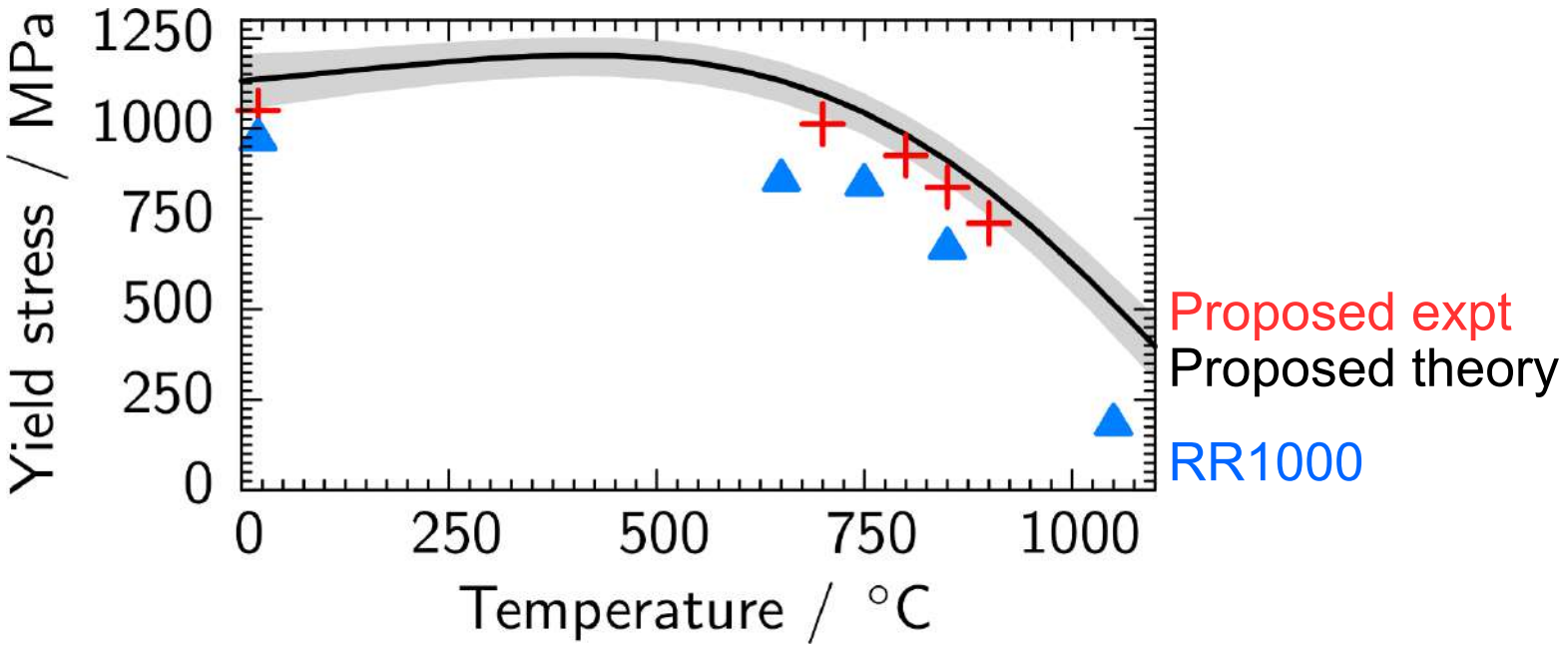
Testing the yield stress



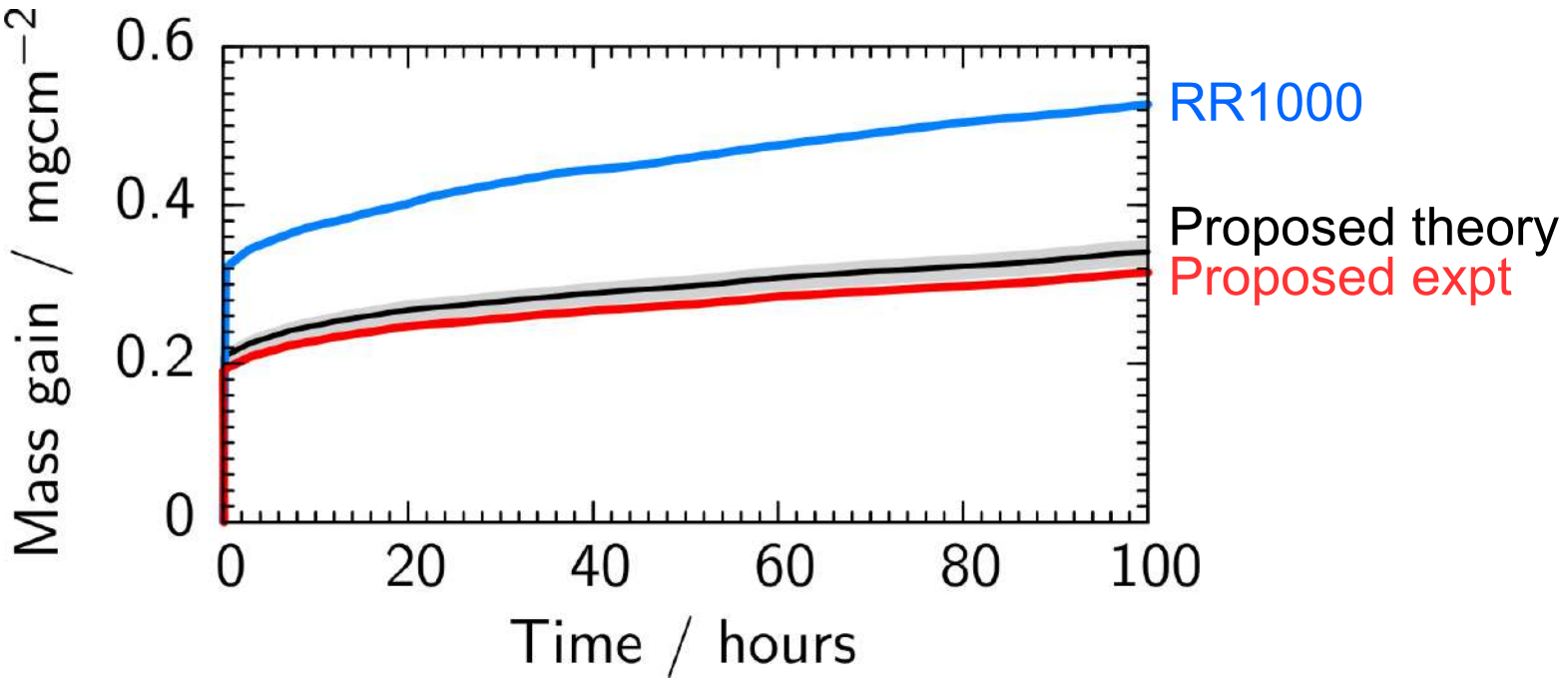
Proposed theory

RR1000

Testing the yield stress

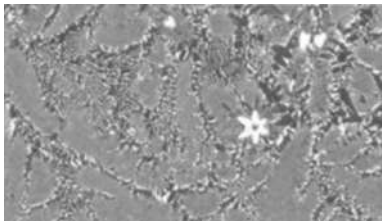


Testing the oxidation resistance

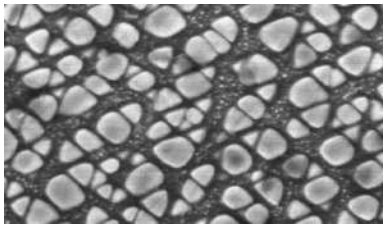


Alloys discovered

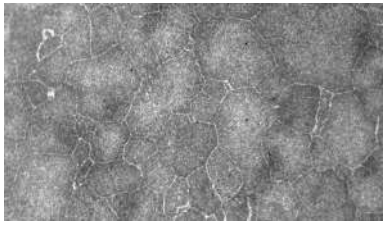
Cr-Cr_2Ta alloys
Intermetallics, 48, 62



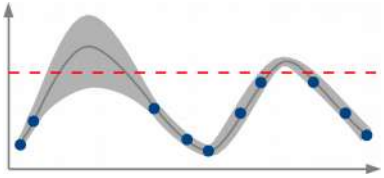
Combustor alloy
GB1408536



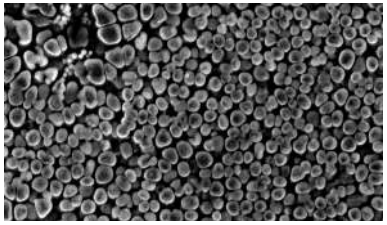
RR1000 grain growth
Acta Materialia, 61, 3378



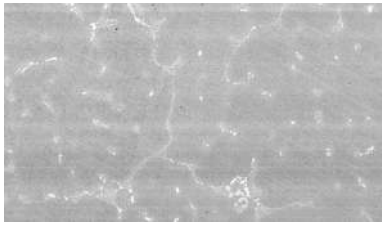
Discovery algorithm
EP14153898
US 2014/177578



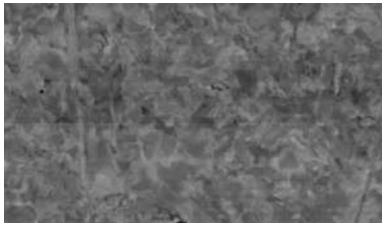
Ni disc alloy
EP14157622
US 2013/0052077 A2



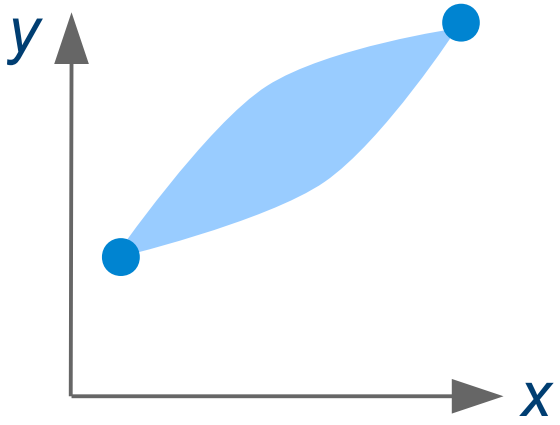
Mo-Hf forging alloy
EP14161255
US 2014/223465



Mo-Nb forging alloy
EP14161529
US 2014/224885



Merging simulation and experiment



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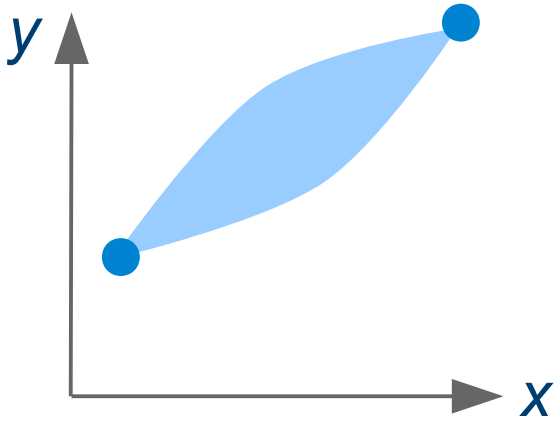

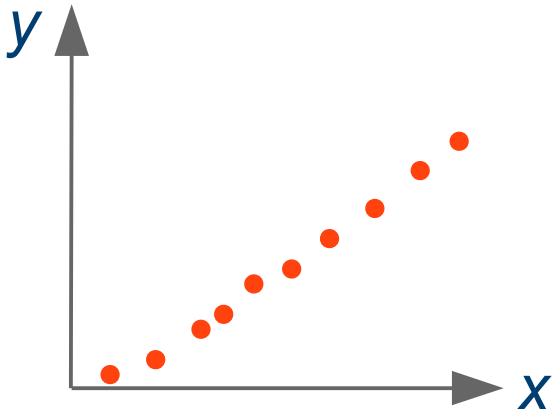

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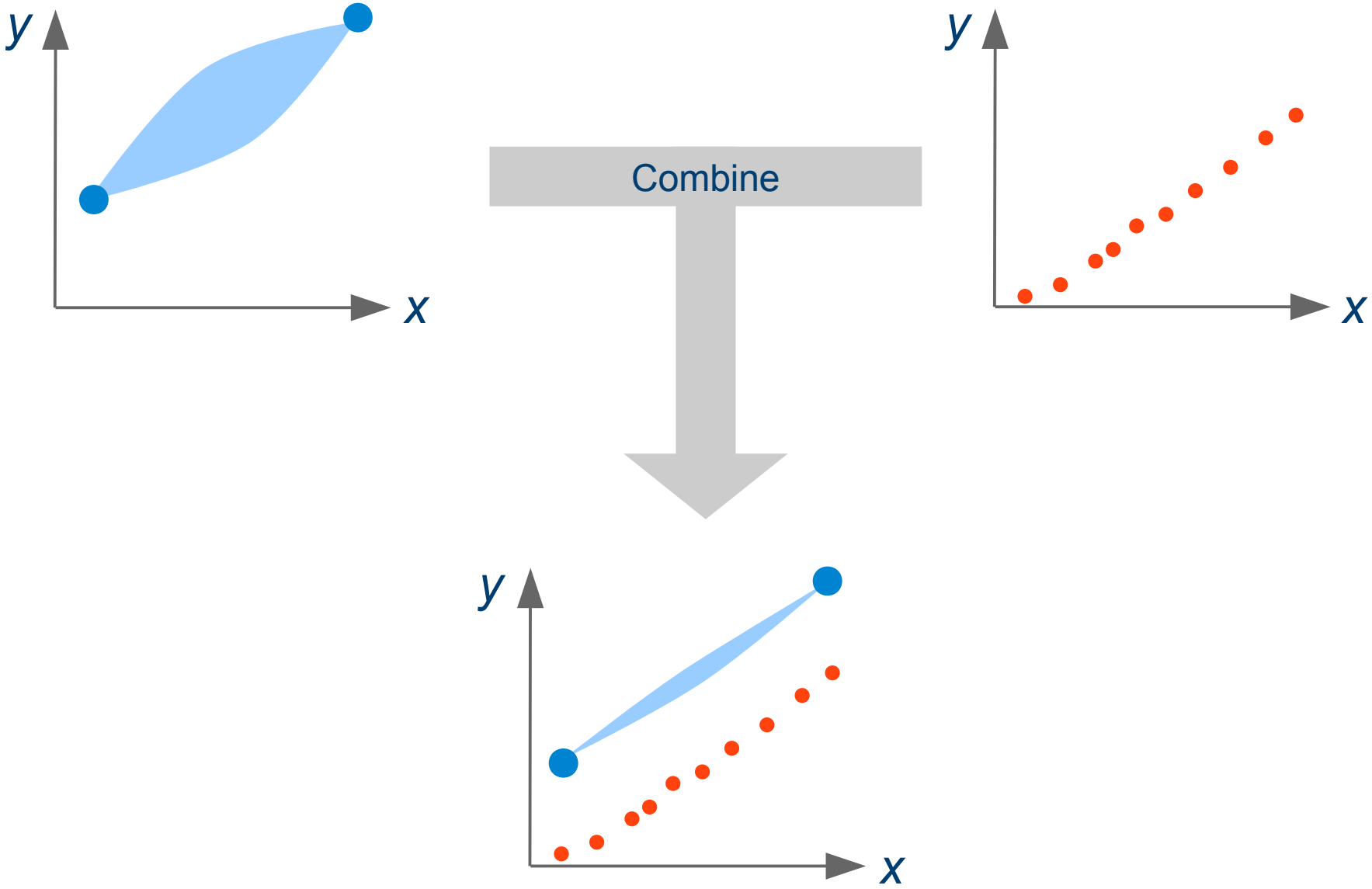

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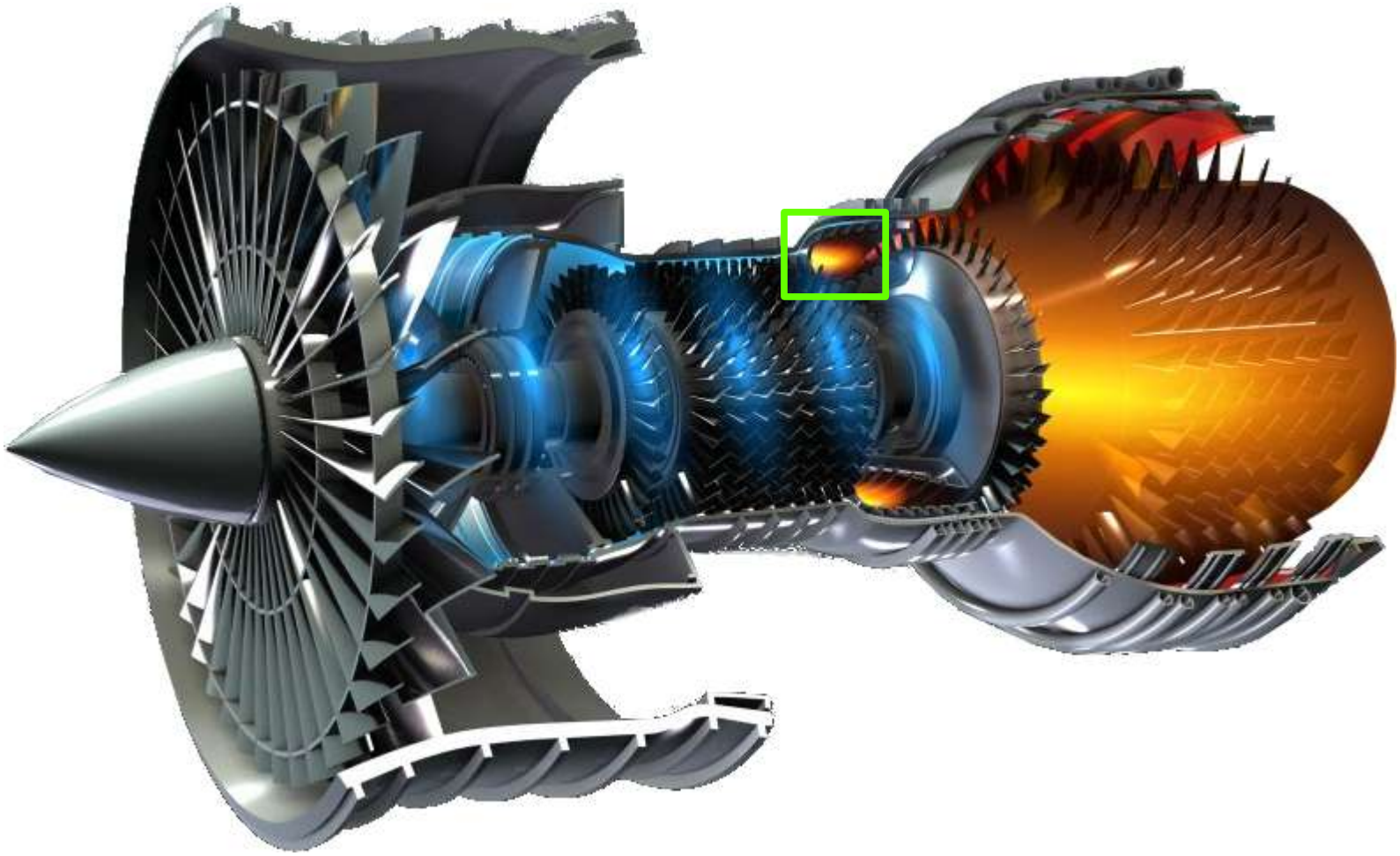
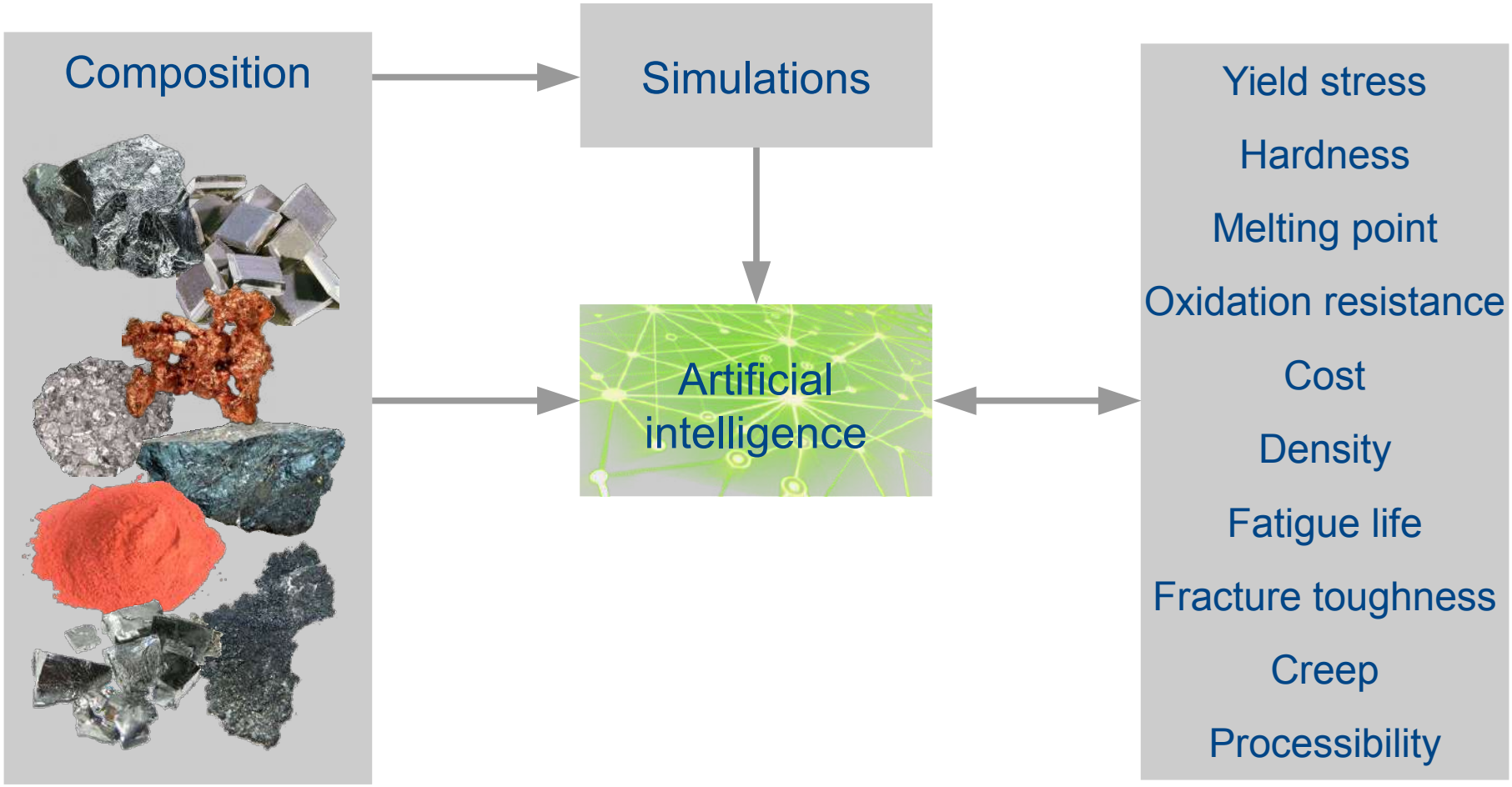
Exploiting material correlations

Alloy for direct laser deposition

Combustor liner



Artificial intelligence

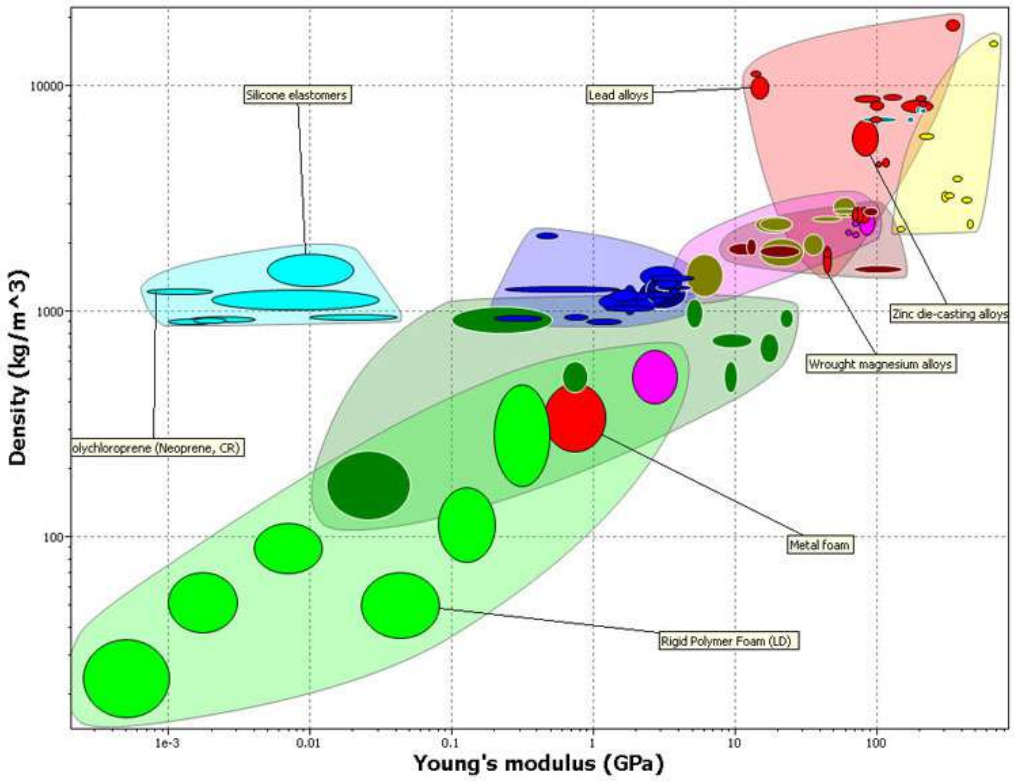


Exploiting material correlations

Alloy for direct laser deposition

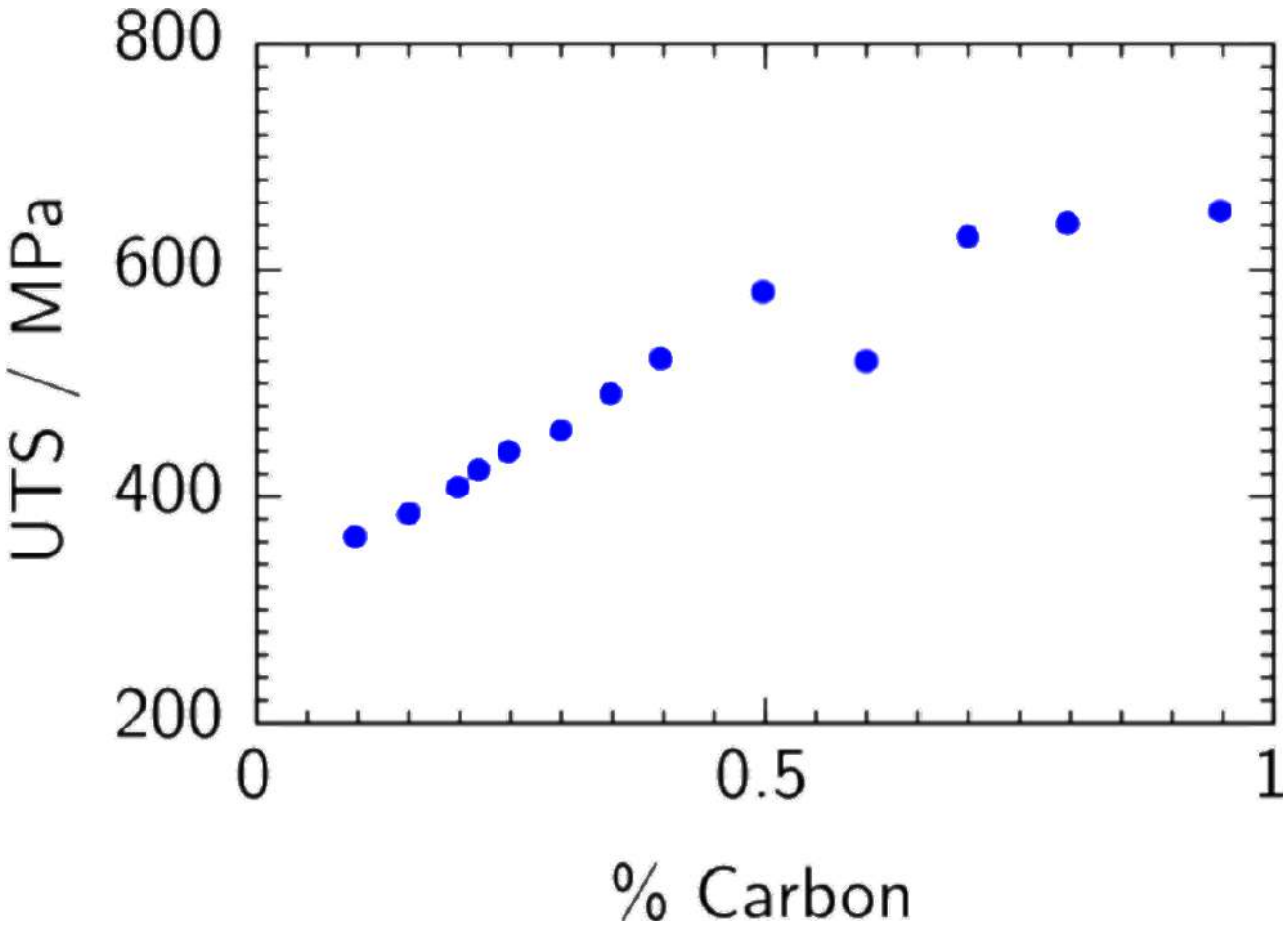
Lithium cathode materials

Database verification



Database contains >10^7 separate entries

Example: steels



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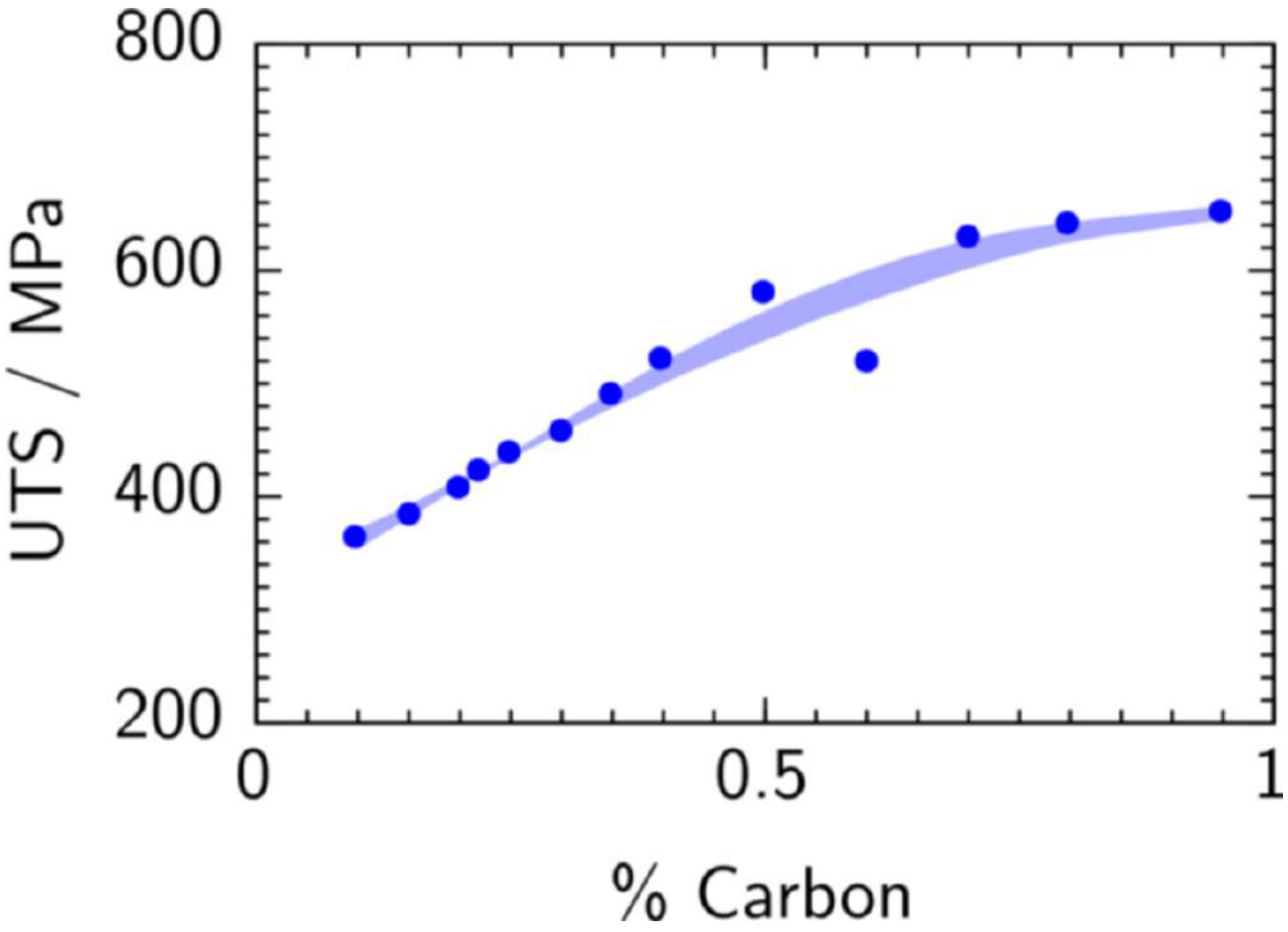

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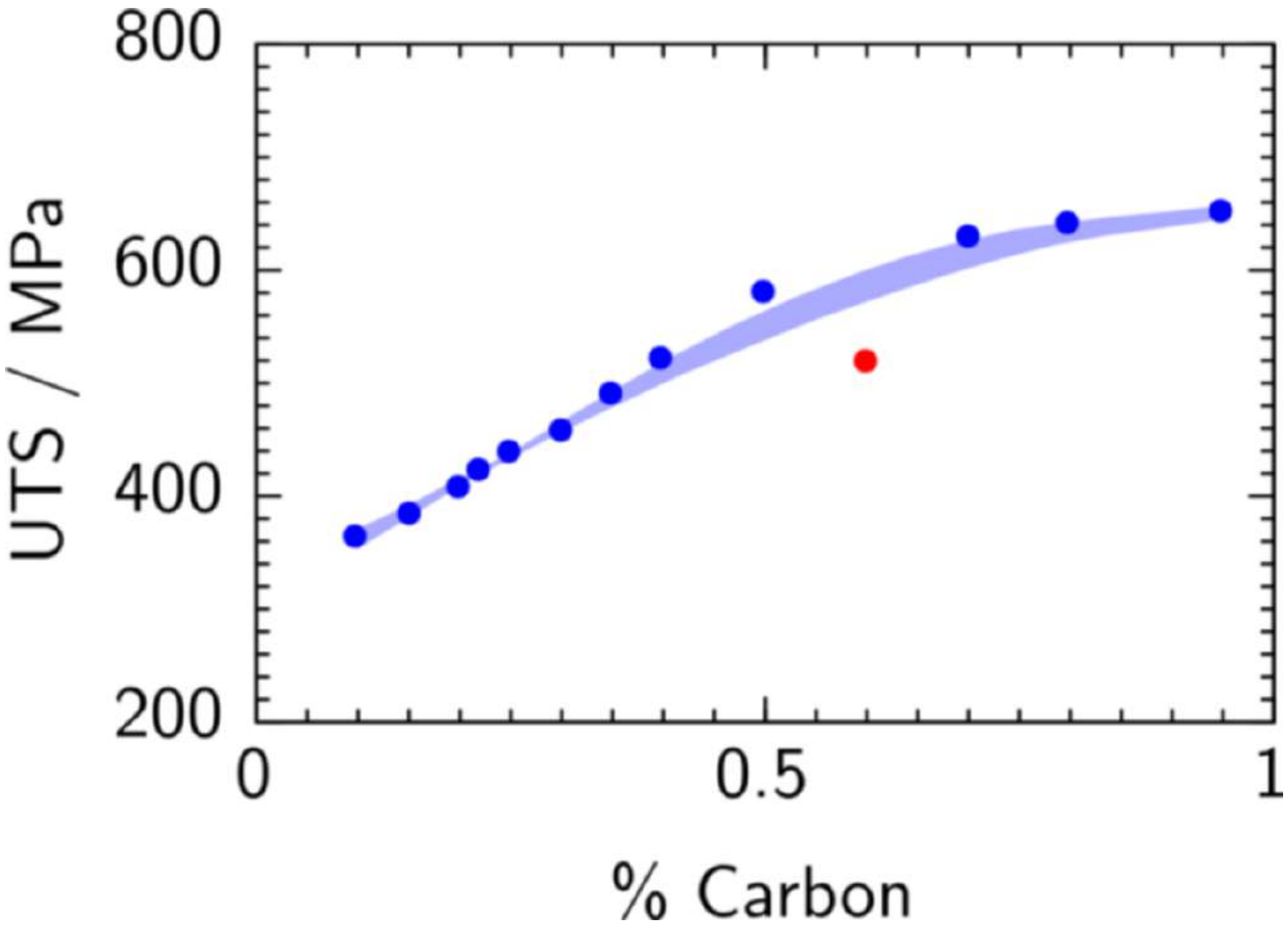

Summary

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