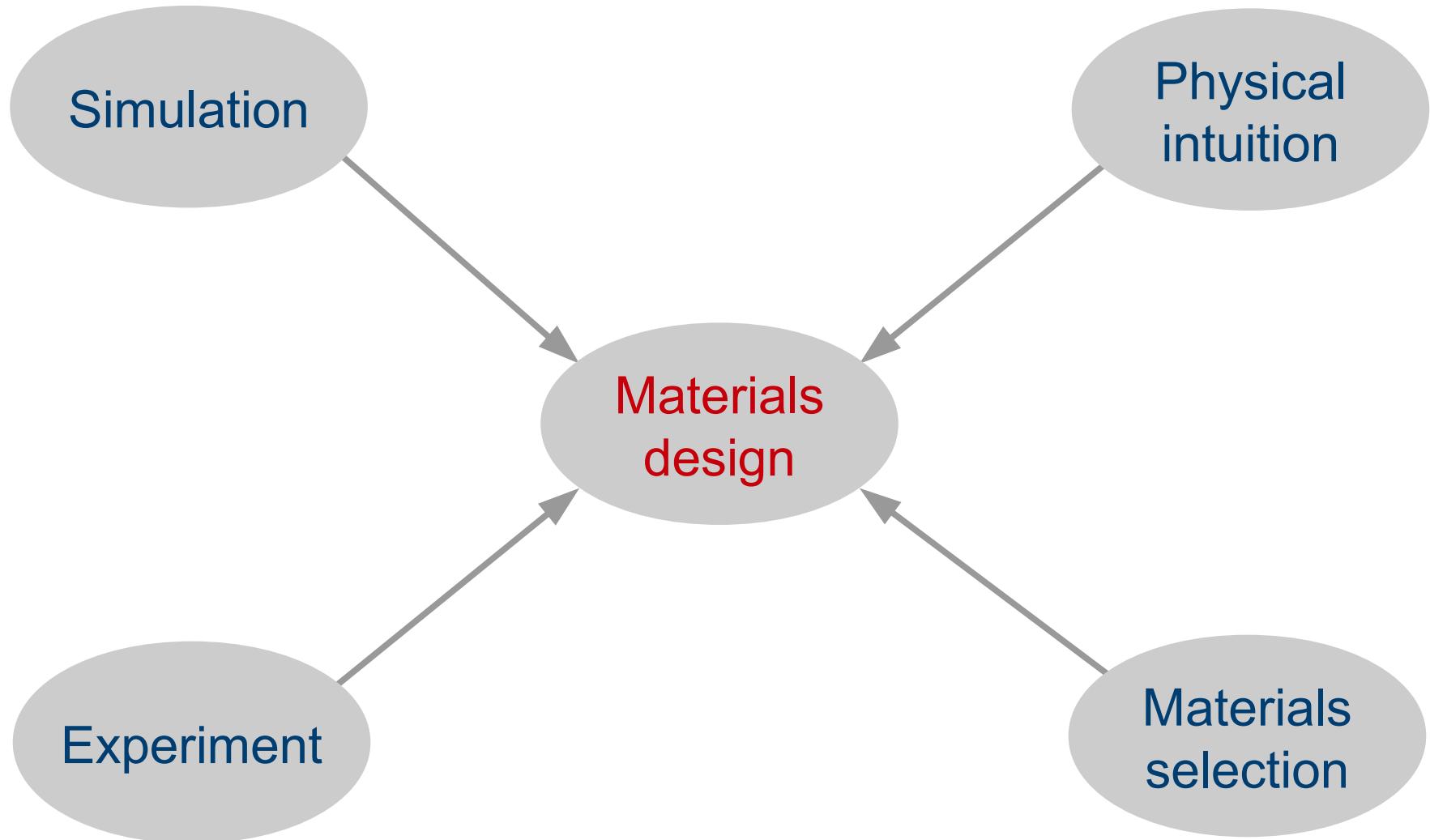


Materials discovery with artificial intelligence

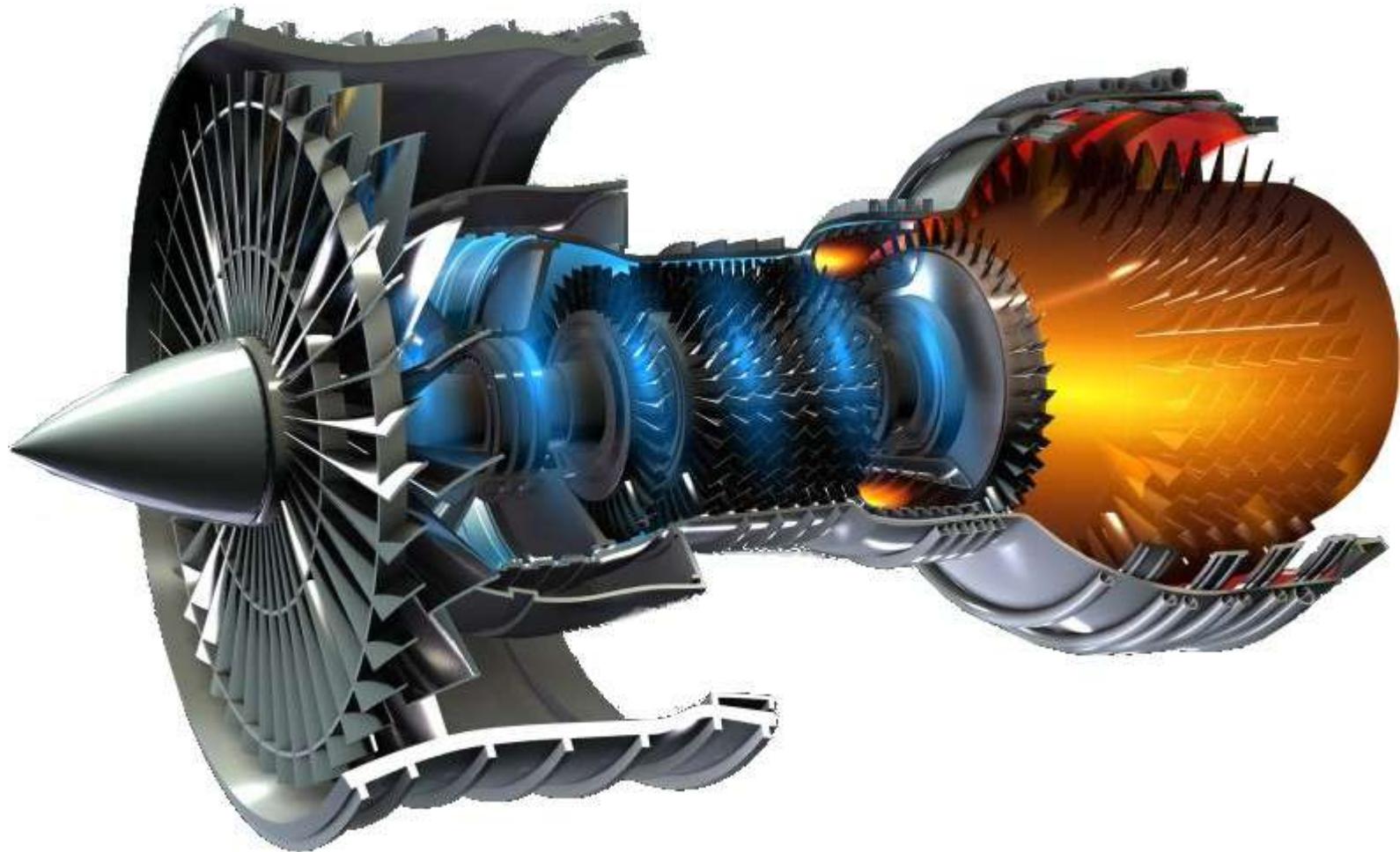
Gareth Conduit

TCM Group, Department of Physics

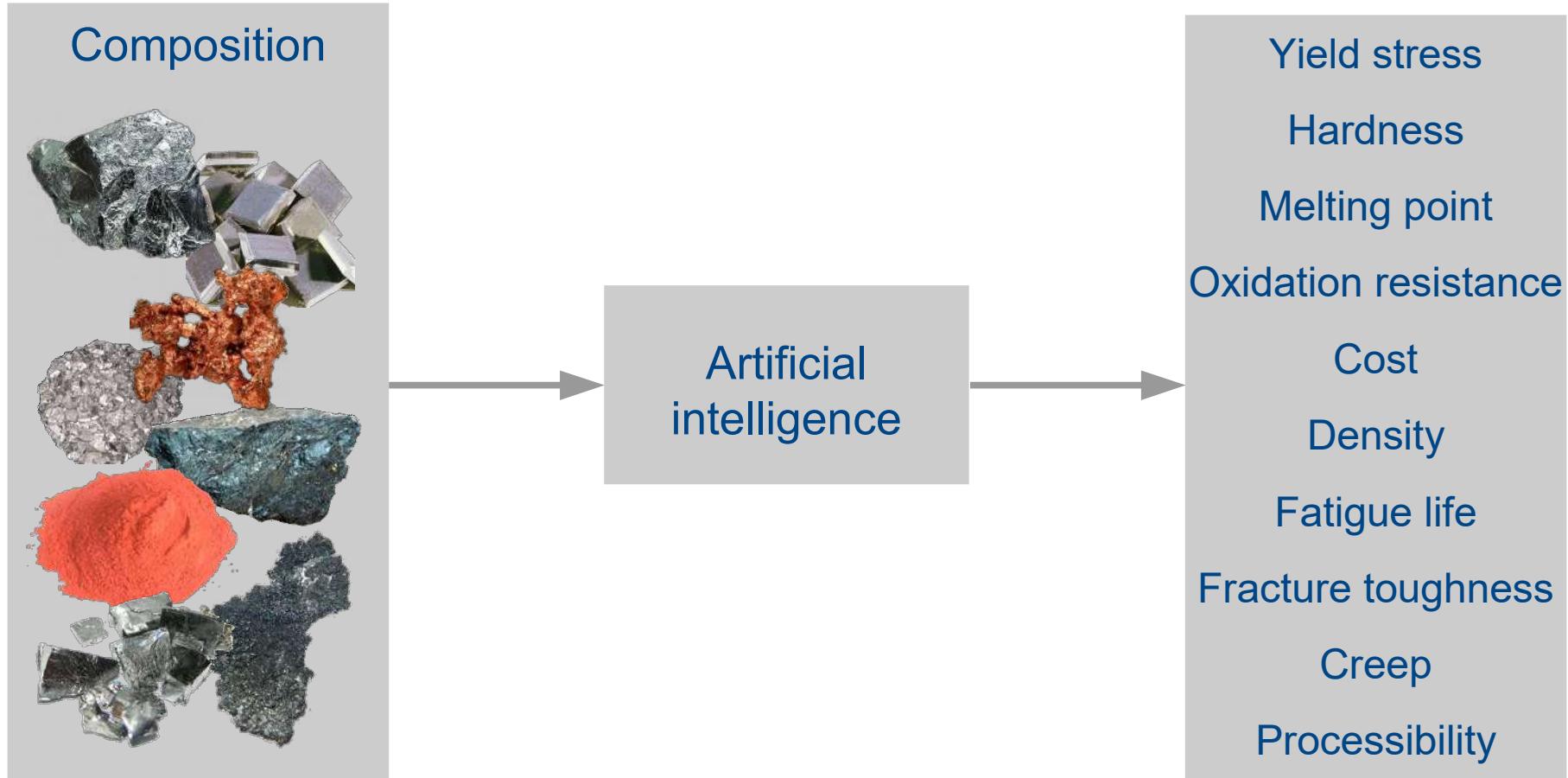
Approaches to materials design



Schematic of a jet engine



Artificial intelligence



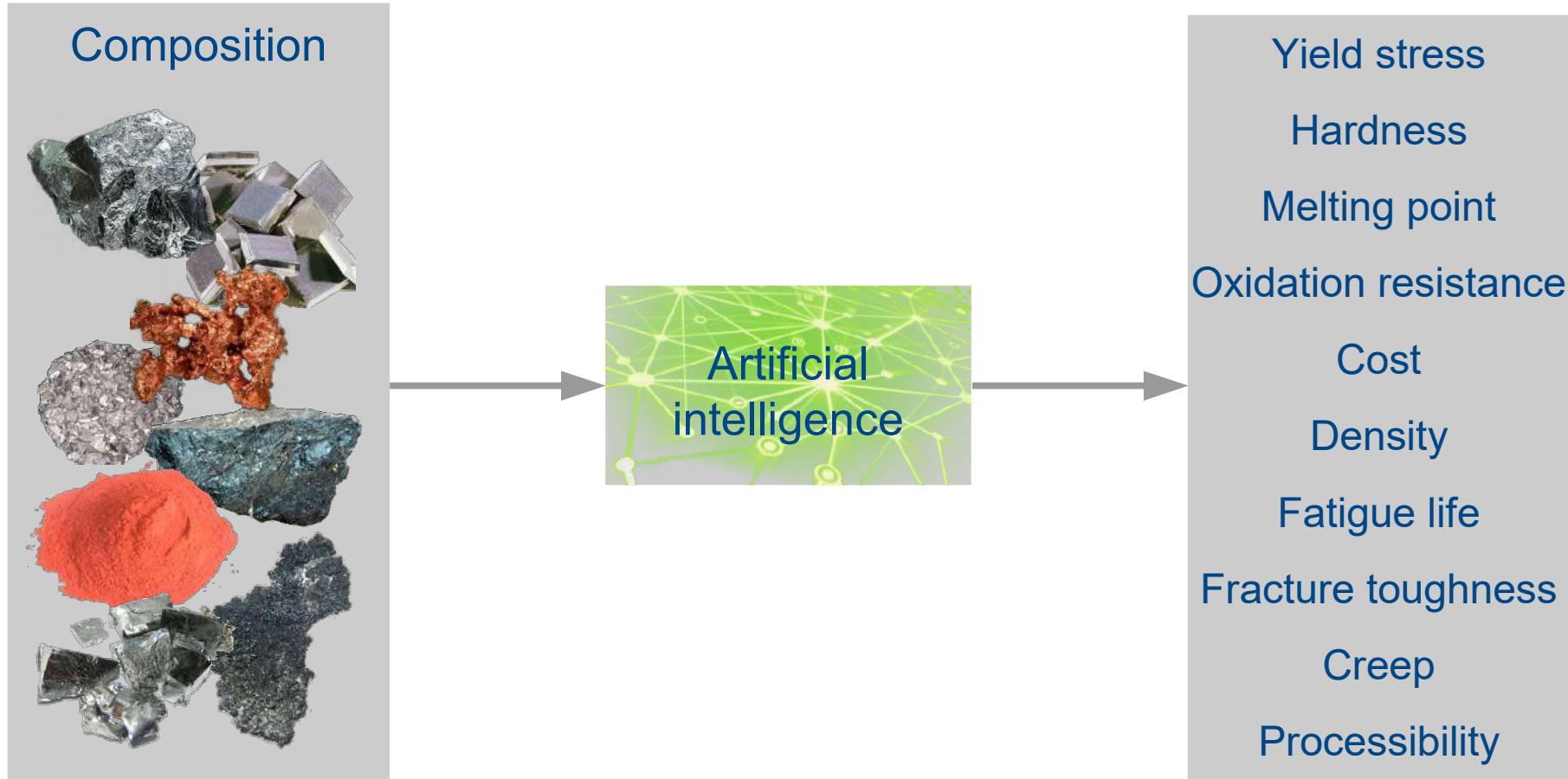
Artificial intelligence



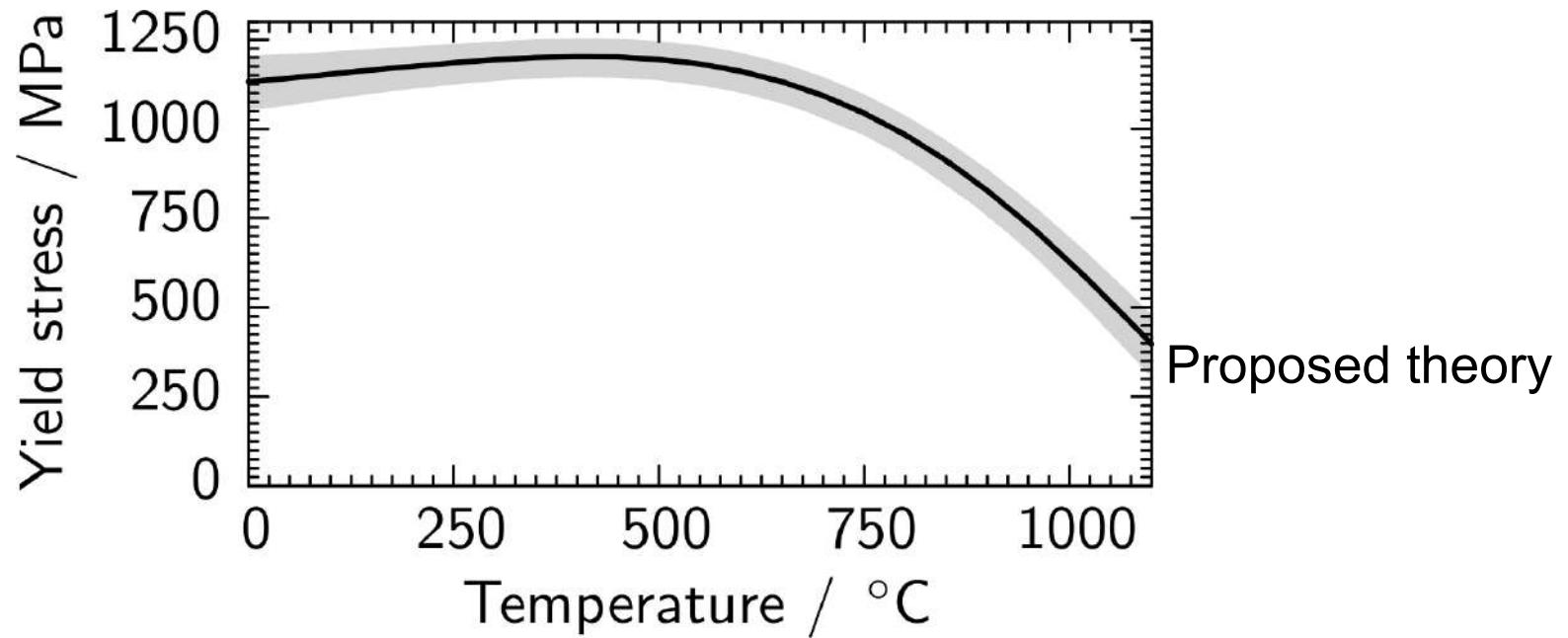
Artificial
intelligence

2	9	3	9	2	8	7	6	4	7	9	0	9	0	4
0	2	1	3	6	4	0	1	0	3	6	0	2	0	2
6	3	6	5	8	4	9	7	0	5	0	8	1	8	3
7	0	3	8	1	8	4	0	6	4	6	5	0	1	7
5	0	1	0	6	3	9	7	4	4	6	5	0	2	9
7	1	5	2	6	9	0	9	4	6	7	4	4	9	5
0	1	1	4	0	4	4	9	7	4	9	4	8	0	2
4	8	8	6	8	5	7	3	1	1	0	9	9	3	1
2	0	3	3	3	2	7	2	1	9	9	4	9	9	5
9	7	6	5	7	9	9	4	2	4	3	4	1	8	3
3	9	4	0	4	6	7	0	3	9	6	0	3	9	1
5	9	7	6	9	2	8	6	8	1	1	2	3	9	2
3	7	6	4	1	3	4	2	0	4	8	7	3	4	1
3	6	6	5	2	4	4	7	2	7	7	3	7	8	1
1	4	4	2	1	9	8	1	3	2	6	6	1	0	9
8	0	5	5	5	6	0	6	9	5	2	6	6	4	3
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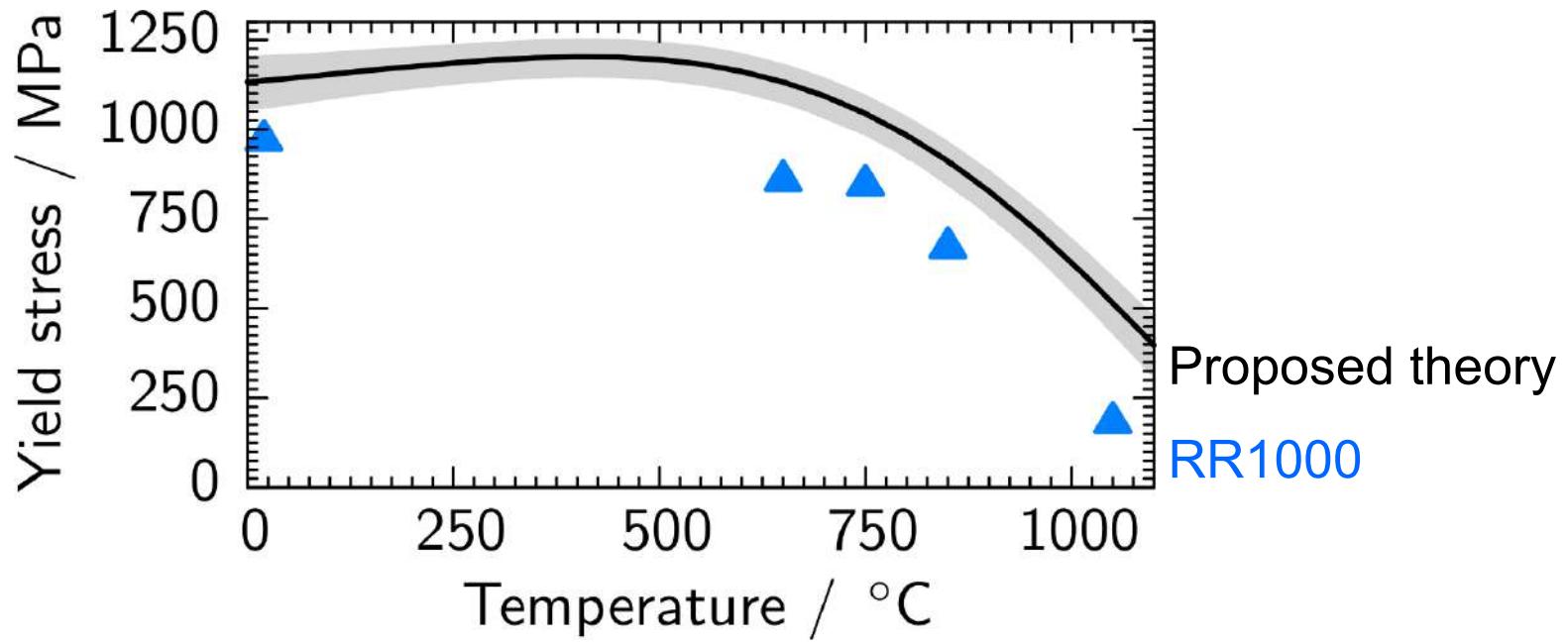
Artificial intelligence



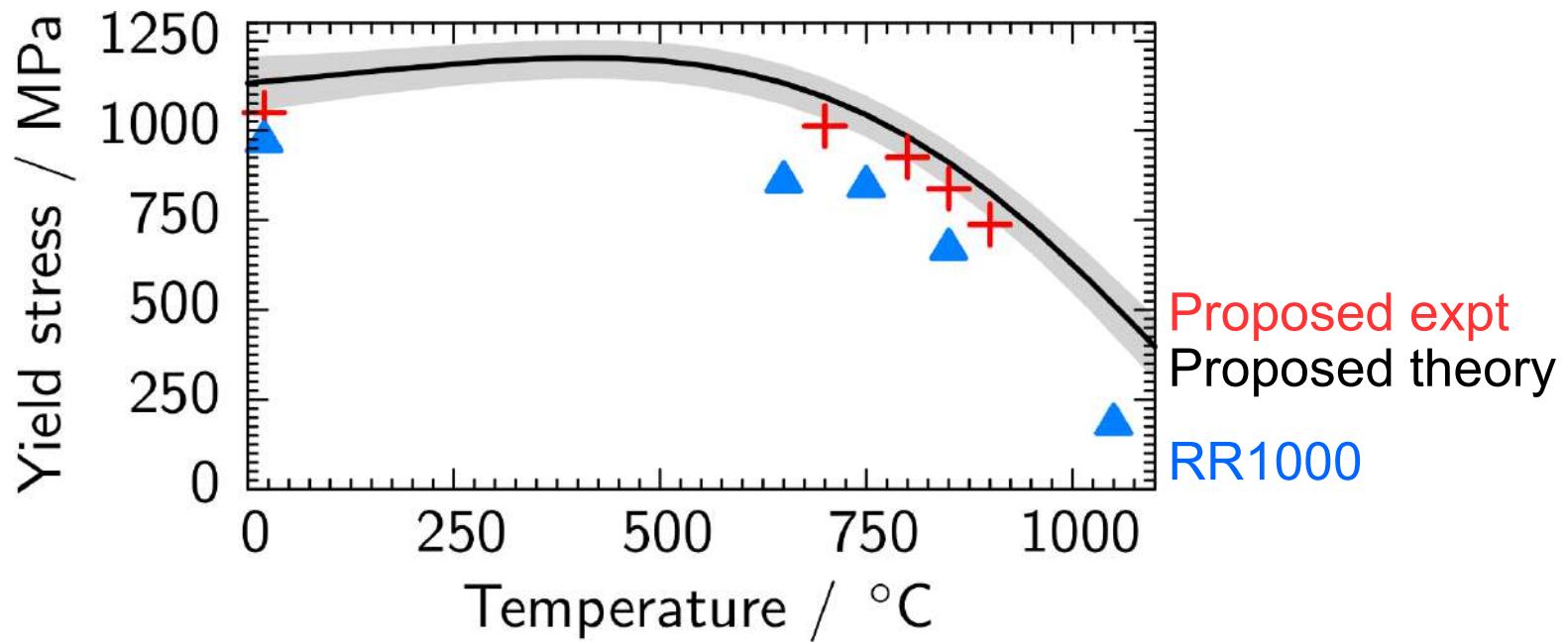
Testing the yield stress



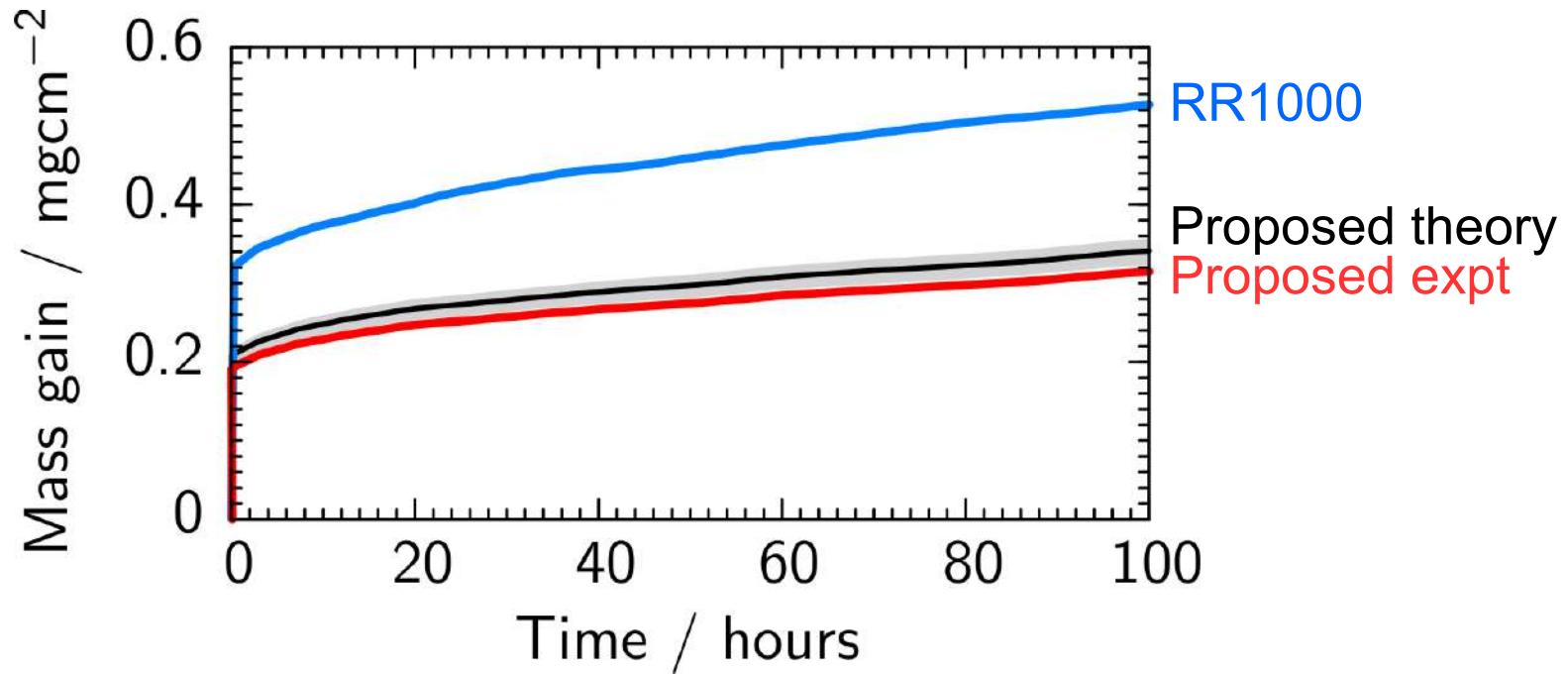
Testing the yield stress



Testing the yield stress



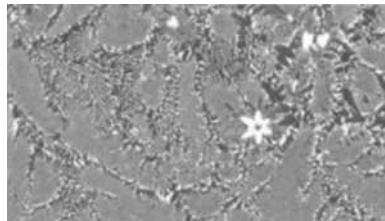
Testing the oxidation resistance



Alloys discovered

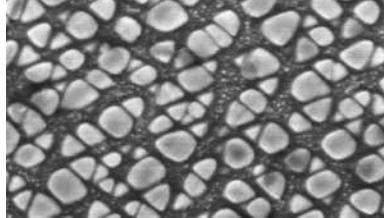
Cr-Cr₂Ta alloys

Intermetallics, 48, 62



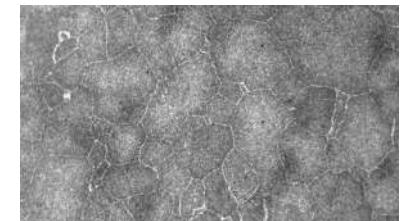
Combustor alloy

GB1408536



RR1000 grain growth

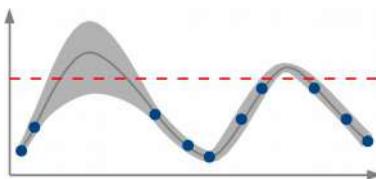
Acta Materialia, 61, 3378



Discovery algorithm

EP14153898

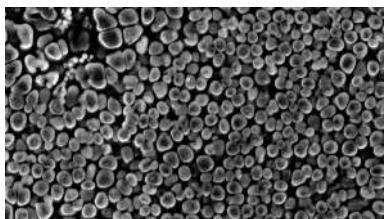
US 2014/177578



Ni disc alloy

EP14157622

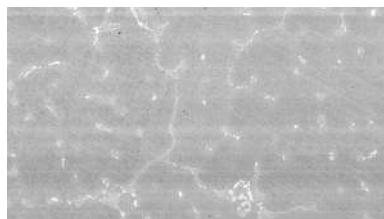
US 2013/0052077 A2



Mo-Hf forging alloy

EP14161255

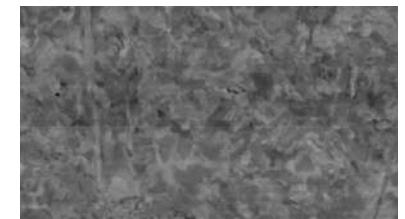
US 2014/223465



Mo-Nb forging alloy

EP14161529

US 2014/224885

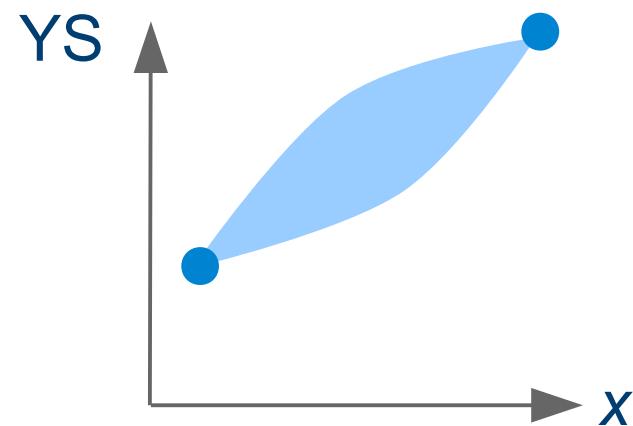


Materials databases

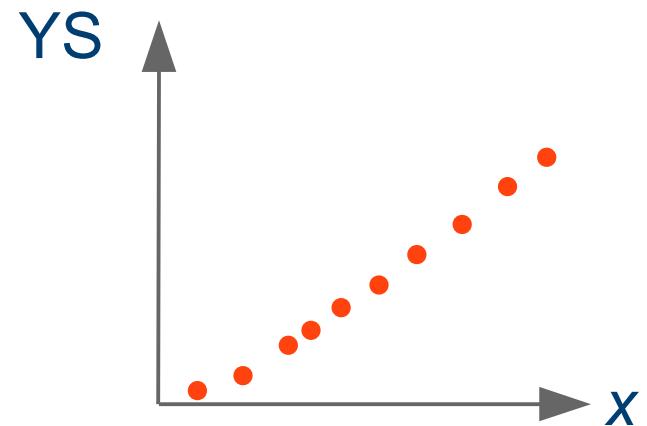
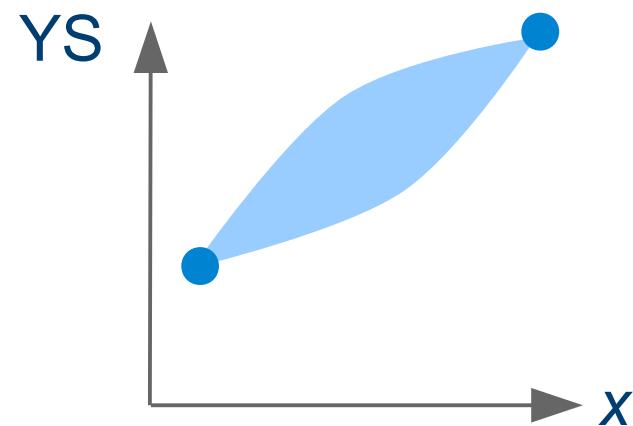
Fragmented databases

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

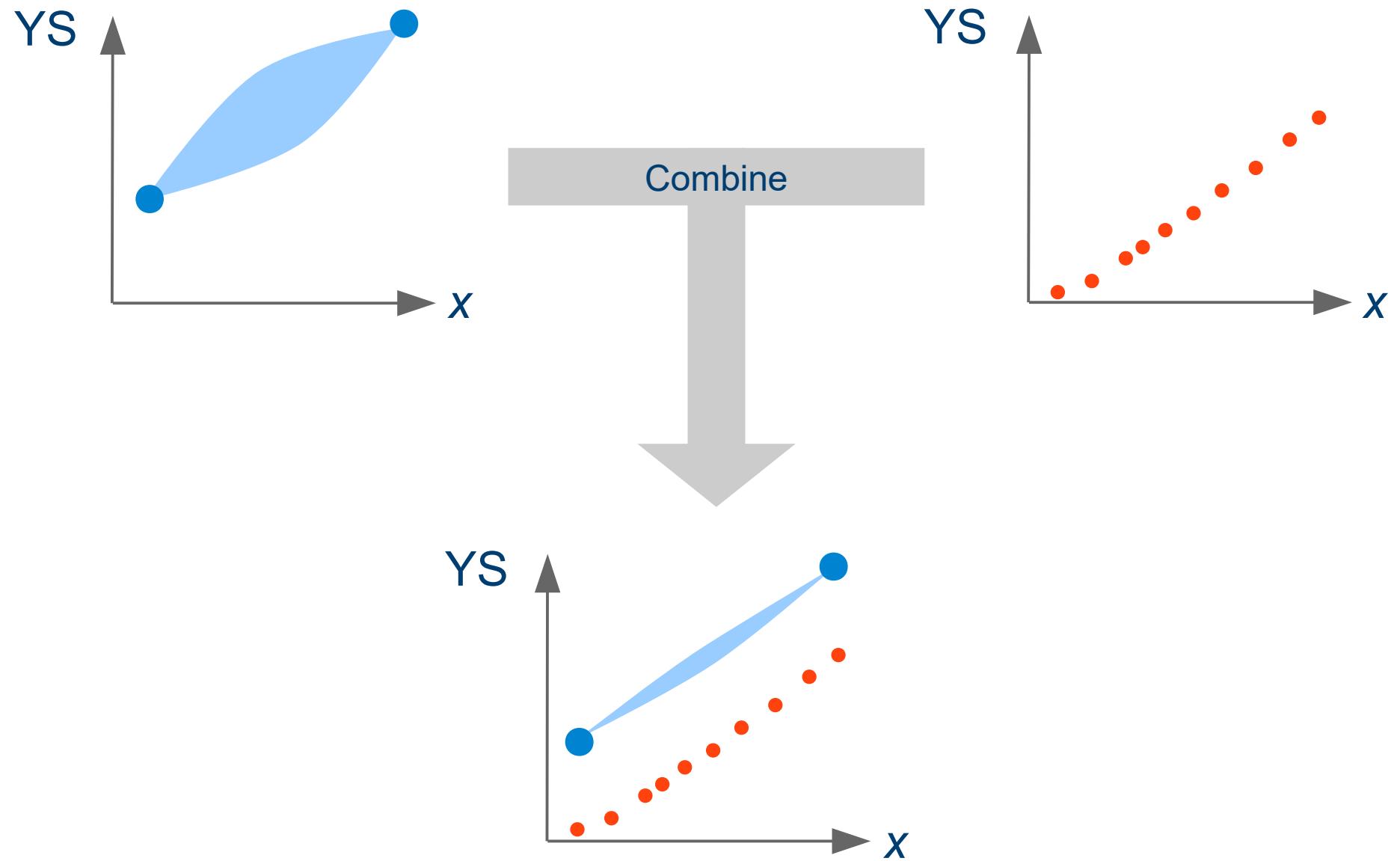
Merging simulation and experiment



Merging simulation and experiment



Merging simulation and experiment



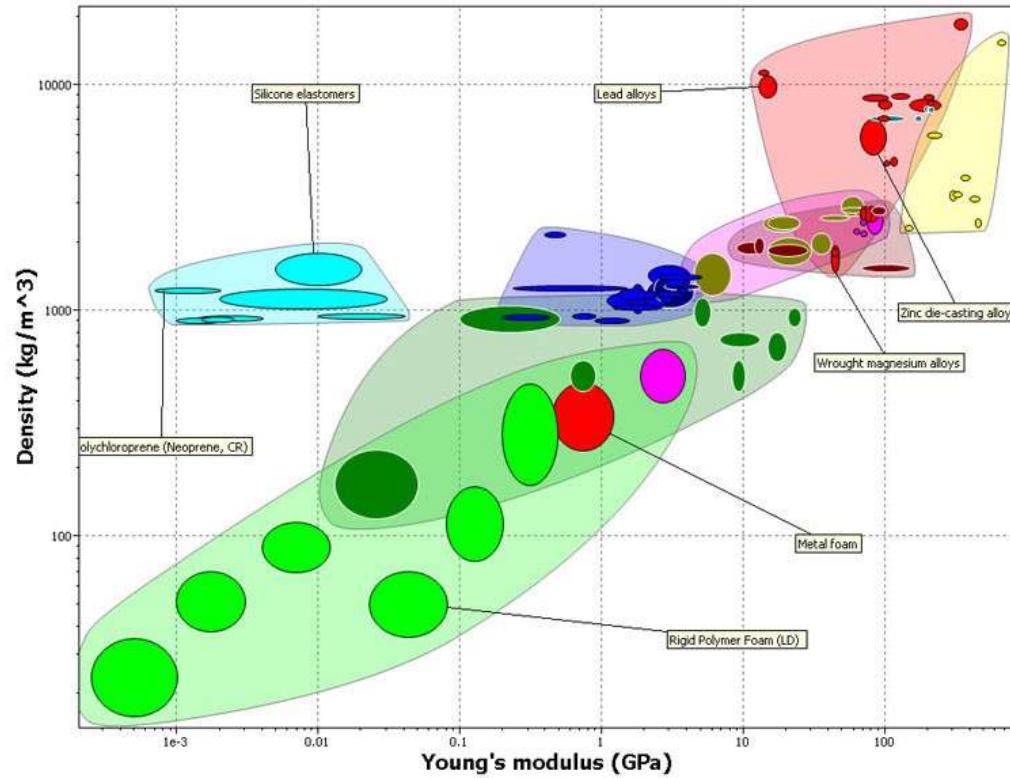
Exploiting material correlations



Lithium cathode materials

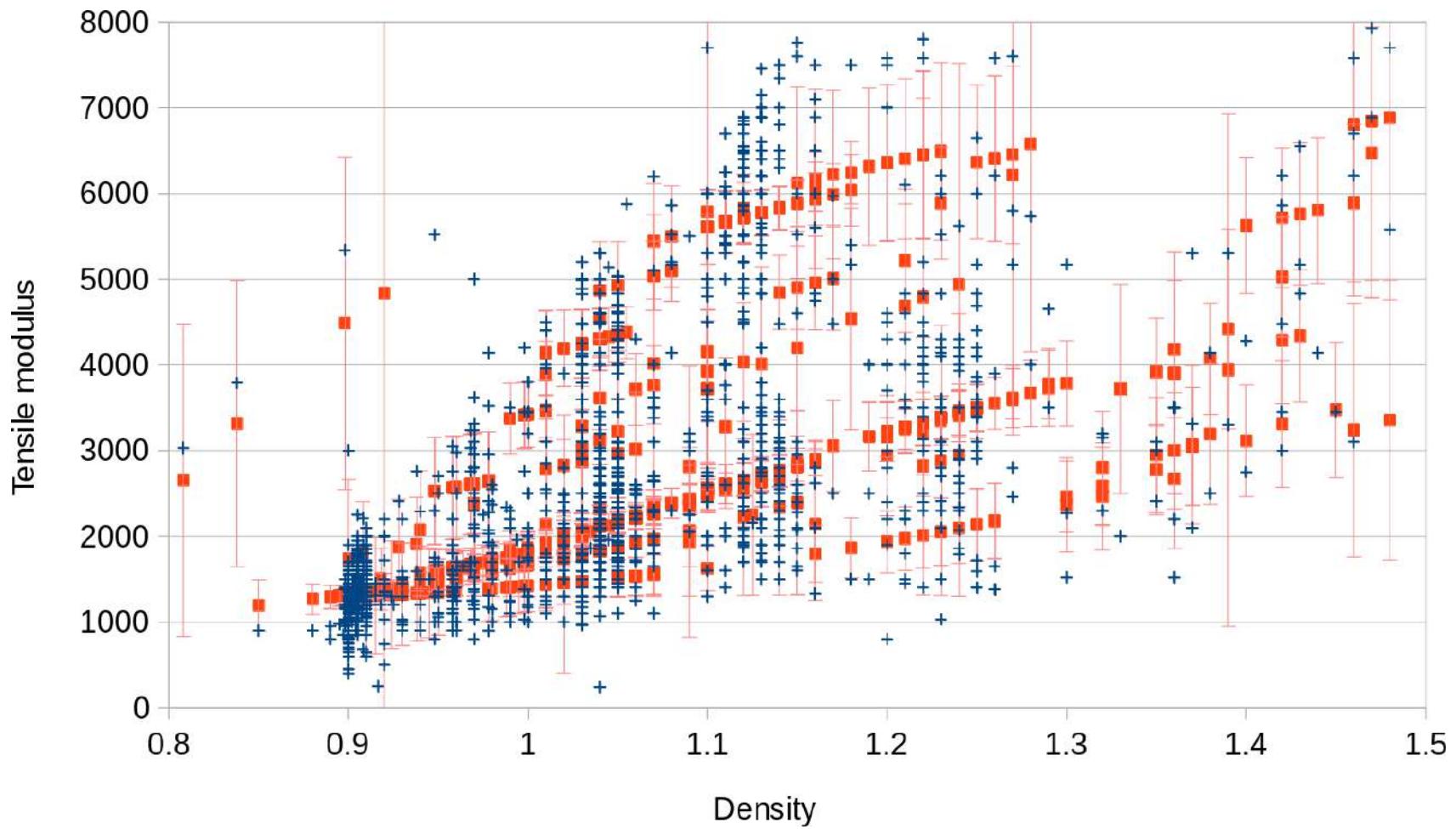


Database verification



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