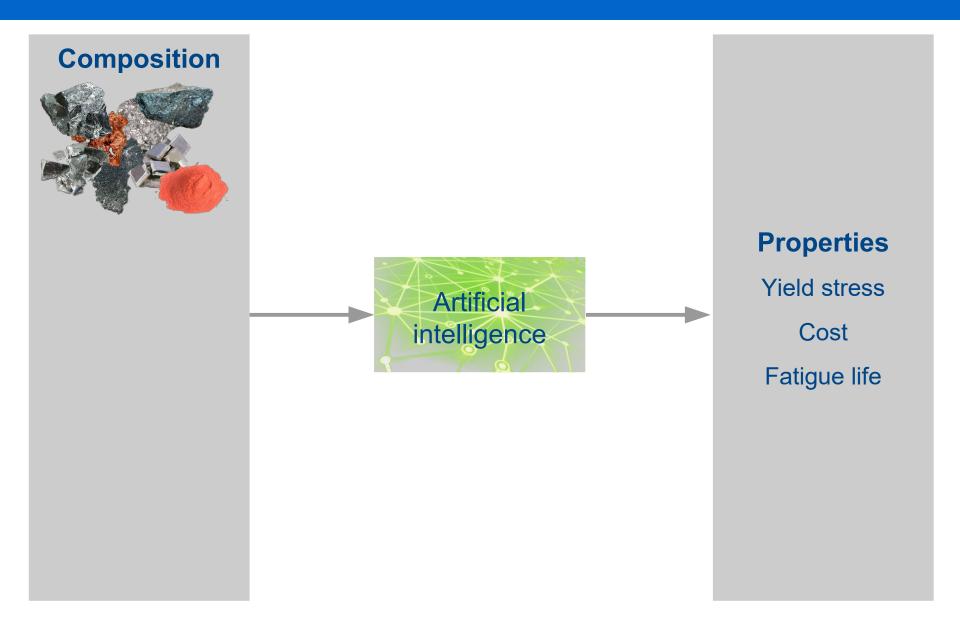


Materials discovery with artificial intelligence

Gareth Conduit

TCM Group, Department of Physics

Neural networks for materials design



Neural networks for materials design

Composition



Properties

Yield stress

Cost

Fatigue life

Simulations

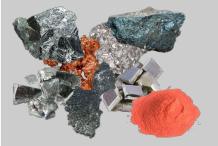
Density Functional

Molecular dynamics

Finite element



Composition



Properties

Yield stress

Cost

Fatigue life

Simulations

Density Functional

Molecular dynamics

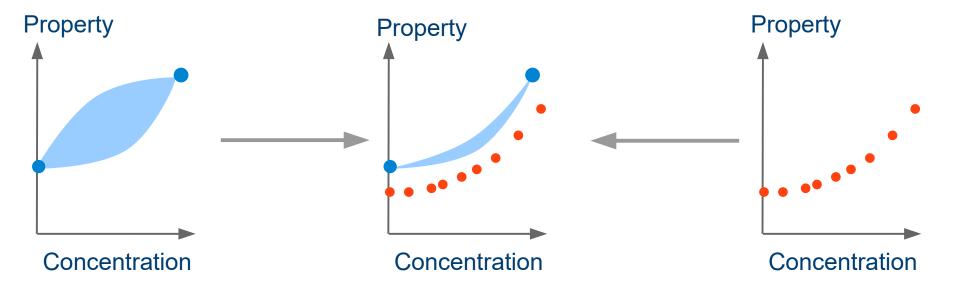
Finite element

Neural networks for materials design

Experiment

Combined

Simulation



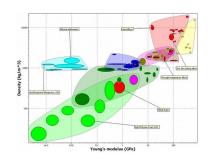
Materials design

Experimental





Experimental





Structural and experimental





Materials design

DFT and experimental





DFT and experimental



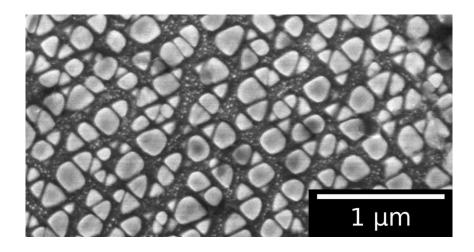


Quantum mechanics and experimental

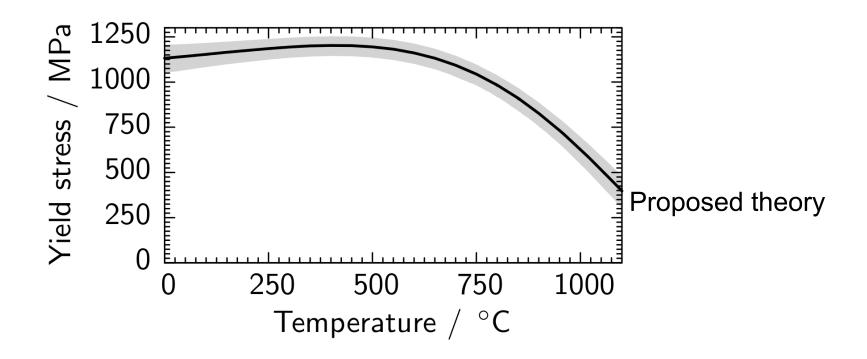




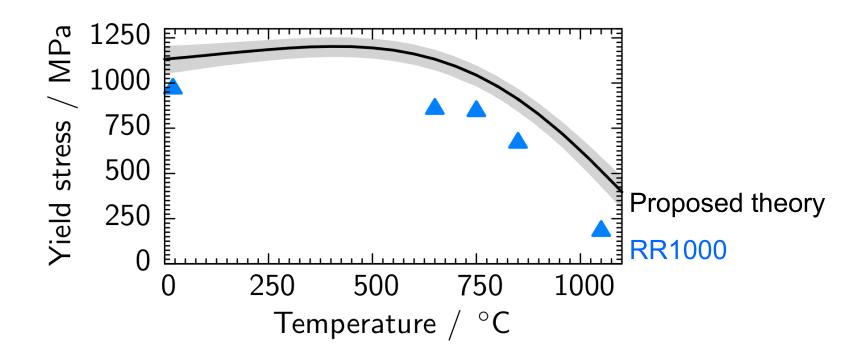
Microstructure



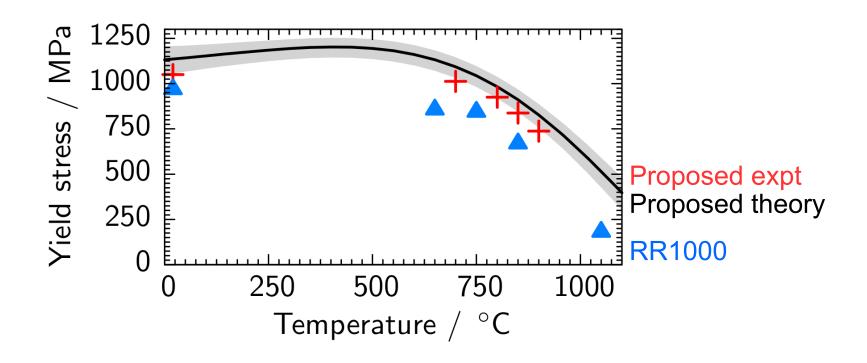
Testing the yield stress



Testing the yield stress

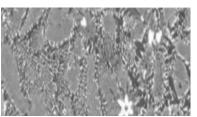


Testing the yield stress



Alloys discovered

Cr-Cr₂Ta alloys Intermetallics, 48, 62

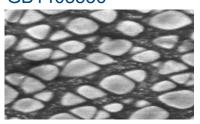


Ni disc alloy

EP14157622

US 2013/0052077 A2

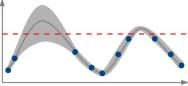
Combustor alloy GB1408536



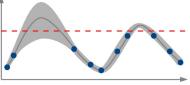
RR1000 grain growth Acta Materialia, 61, 3378



Discovery algorithm EP14153898

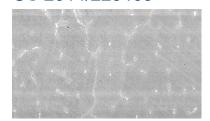


US 2014/177578



Mo-Hf forging alloy

EP14161255 US 2014/223465



Mo-Nb forging alloy EP14161529 US 2014/224885



Summary

Used artificial intelligence to discover materials

Handle fragmented data

Merge experiments and simulations into holistic design tool

Proposed four new alloys, experimentally verified

Worked with six different companies, formed startup intellegens