Materials discovery with artificial intelligence

Gareth Conduit

TCM Group, Department of Physics
Approaches to materials design

- Experiment
- Physical intuition
- Materials selection
- Simulation
Schematic of a jet engine
Combustor liner
Designing a new alloy: what is required?

- Processibility
- Yield strength
- Cost
- Density
- Fatigue life
- Creep
- Oxidation resistance
- Corrosion resistance
- Fracture toughness

Required properties for new alloy
Multidimensional design space

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<th>Cr</th>
<th>Co</th>
<th>Mo</th>
<th>W</th>
<th>Ta</th>
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and 4 different manufacturing processes
Artificial intelligence

Composition

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

Composition

Yield stress
Hardness
Melting point
Oxidation resistance
Cost
Density
Fatigue life
Fracture toughness
Creep
Processibility
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*Processing conditions:*

- Temperature ($T$): 900°C
- Time ($t$): 30 hours
Microstructure
Microstructure
Testing the yield stress

Proposed theory
Testing the yield stress

Proposed theory
RR1000
Testing the yield stress

Proposed theory

Proposed expt

RR1000

Yield stress / MPa

Temperature / °C
Testing the oxidation resistance

![Graph showing mass gain over time for RR1000, Proposed theory, and Proposed expt.](chart.png)
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
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Merging simulation and experiment
Merging simulation and experiment
Merging simulation and experiment

Combine

YS

YS

YS

YS

YS
Artificial intelligence

Composition

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

Composition

Simulations

Artificial intelligence

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

Alloy for direct laser deposition

3D printability ⇐ Weldability
Exploiting material correlations

Alloy for direct laser deposition

3D printability \[\rightarrow\] Weldability

Lithium cathode materials

Experiment \[\rightarrow\] 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
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