Materials discovery with artificial intelligence

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Using data to design materials

Materials design

- Experiment
- Physical intuition
- Materials selection
- Simulation
Schematic of a jet engine
Artificial intelligence

Composition

Yield stress
Hardness
Melting point
Oxidation resistance
Cost
Density
Fatigue life
Fracture toughness
Creep
Processibility
Microstructure
Testing the yield stress

Proposed theory
Testing the yield stress

Proposed theory

Yield stress / MPa

Temperature / °C

RR1000
Testing the yield stress

![Graph showing yield stress vs temperature](image)
Testing the oxidation resistance

- RR1000
- Proposed theory
- Proposed expt

![Graph showing mass gain over time for RR1000, Proposed theory, and Proposed expt. The x-axis represents time in hours, the y-axis represents mass gain per square meter, and the lines show how the mass gain changes over time.]
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

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## Fragmented databases

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Merging simulation and experiment

Composition

Artificial intelligence

Computed strength

Melting point

Hardness

Strength
Merging simulation and experiment
Merging simulation and experiment
Merging simulation and experiment

Combine
Designing a lithium cathode

Experiment  Computational
Database verification

Database contains $>10^7$ separate entries
Analyze databases with artificial intelligence to discover four new alloys

Merge fragmented computational and experimental databases

Materials database verification and completion