Materials discovery with artificial intelligence

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Approaches to materials design

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

Composition

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

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Testing the yield stress

Proposed theory
Testing the yield stress

![Graph showing yield stress vs temperature for RR1000 material. The graph includes a curve representing the proposed theory and data points for different temperatures.](image-url)
Testing the yield stress

![Graph showing yield stress over temperature with proposed theory and experiment data.]
Testing the oxidation resistance

- RR1000
- Proposed theory
- Proposed expt
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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Merging simulation and experiment
Merging simulation and experiment
Merging simulation and experiment

Combine

YS

X

YS

X

YS

X
Exploiting material correlations

Lithium cathode materials

Experiment \hspace{2cm} DFT
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