Materials discovery with artificial intelligence

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Approaches to materials design

Simulation

Physical intuition

Experiment

Materials selection
Designing a new alloy: what is required?

Required properties for new alloy:

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

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

Composition

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

Composition

Yield stress
Hardness
Melting point
Oxidation resistance
Cost
Density
Fatigue life
Fracture toughness
Creep
Processibility
Sample data
Modeling the data
Exceeding the target
Maximizing likelihood of exceeding the target
Microstructure
Microstructure
Testing the yield stress

Proposed theory
Testing the yield stress

Proposed theory

RR1000

![Graph showing the relationship between yield stress and temperature for RR1000 material. The graph plots yield stress in MPa against temperature in °C. There are data points indicated by blue triangles, and a solid line representing the proposed theory.]
Testing the yield stress
Testing the oxidation resistance

![Graph showing the mass gain over time for RR1000, Proposed theory, and Proposed expt. The graph plots mass gain per square centimeter against time in hours.]
Alloys discovered

Ni disc alloy
EP14157622
US 2013/0052077 A2
Alloys discovered

**Discovery algorithm**
EP14153898
US 2014/177578

**Ni disc alloy**
EP14157622
US 2013/0052077 A2
Alloys discovered

**Combustor alloy**
EP14153898
US 2013/0052077 A2

**Discovery algorithm**
EP14153898
US 2014/177578

**Ni disc alloy**
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Alloys discovered

Combustor alloy
EP1408536
US 2014/177578

Discovery algorithm
EP14153898
US 2014/177578

Mo-Hf forging alloy
EP14161255
US 2014/223465

Mo-Nb forging alloy
EP14161529
US 2014/224885

Ni disc alloy
EP14157622
US 2013/0052077 A2
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

**Mo-Hf forging alloy**
EP14161255
US 2014/223465

**Ni disc alloy**
EP14157622
US 2013/0052077 A2

**Mo-Nb forging alloy**
EP14161529
US 2014/224885
Merging simulation and experiment
Merging simulation and experiment

\[ y \]

\[ x \]

\[ y \]

\[ x \]
Merging simulation and experiment
Artificial intelligence

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Exploiting material correlations

Alloy for direct laser deposition

3D printability  Weldability
Combustor liner
Artificial intelligence

Composition

Simulations

Artificial intelligence

Physical intuition

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Simulations

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Exploiting material correlations

Alloy for direct laser deposition

3D printability → Weldability

Lithium cathode materials

Experiment → DFT
Nickel-Cobalt-Manganese (NCM) battery materials
NCM-424 battery structure

$\text{LiNi}_{0.4}\text{Co}_{0.2}\text{Mn}_{0.4}\text{O}_2$
Traditional approach

0.4Ni → 7.2 atoms
0.2Co → 3.6 atoms
0.4Mn → 7.2 atoms

153153000 possible permutations = 42000 years

Access any composition
Information on order
Li migration
Approach: characterize with a local order matrix

$N_{\text{yellow-yellow}} = 1$

$N_{\text{yellow-red}} = 2$
Approach: characterize with a local order matrix

\[ N_{\text{yellow-yellow}} = 1 \]

\[ N_{\text{yellow-red}} = 2 \]

\[ N_{\text{red migrate}} = 1 \]
Recursive learning
Recursive learning
How many calculations are required
### Local order matrix

<table>
<thead>
<tr>
<th>Matrix element</th>
<th>Optimal</th>
<th>From NMR</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_{\text{Co-Co}}$</td>
<td>0.34</td>
<td>0.2</td>
</tr>
<tr>
<td>$N_{\text{Ni-Ni}}$</td>
<td>0.16</td>
<td>0.3</td>
</tr>
<tr>
<td>$N_{\text{Mn-Mn}}$</td>
<td>0.09</td>
<td>0.0</td>
</tr>
<tr>
<td>$N_{\text{Li-Li}}$</td>
<td>0.08</td>
<td>0.0</td>
</tr>
<tr>
<td>$N_{\text{Co-Ni}}$</td>
<td>2.5</td>
<td>2.1</td>
</tr>
<tr>
<td>$N_{\text{Co-Mn}}$</td>
<td>0.2</td>
<td>0.1</td>
</tr>
<tr>
<td>$N_{\text{Ni-Mn}}$</td>
<td>3.4</td>
<td>3.1</td>
</tr>
<tr>
<td>$N_{\text{Ni-Li}}$</td>
<td>0.32</td>
<td>0.2</td>
</tr>
<tr>
<td>$N_{\text{Co-Li}}$</td>
<td>0.21</td>
<td>0.1</td>
</tr>
<tr>
<td>$N_{\text{Mn-Li}}$</td>
<td>1.37</td>
<td>1.2</td>
</tr>
<tr>
<td>$N_{\text{Ni}}$</td>
<td>1.82</td>
<td>1.1</td>
</tr>
<tr>
<td>$N_{\text{Co}}$</td>
<td>0.02</td>
<td>0.3</td>
</tr>
<tr>
<td>$N_{\text{Mn}}$</td>
<td>0.01</td>
<td>0.1</td>
</tr>
</tbody>
</table>
Database contains $>10^7$ separate entries
Example: steels
Example: steels
Example: steels
Database verification
Database verification

- Error checking: Internal
- Database completion: Internal
- Materials prediction: External
- Model creation: External
Database verification

Error checking
Internal

Database completion
Internal

Materials prediction
External

Model creation
External
Summary

Used artificial intelligence in materials discovery

Discovered four new alloys, experimentally verified, now real-world testing

Merge simulations and experiments into holistic design tool

Materials database verification and analysis