Materials discovery with artificial intelligence

Gareth Conduit
Neural network algorithm to

**Merge** simulations, physical laws, and experimental data

**Reduce** the need for expensive experimental development

**Accelerate** materials and drugs discovery

**Generic** with **proven** applications in materials discovery and drug design
Neural network: a black box

Crystal structure
Neural network: train on complete data

Materials design

Materials design
Neural network: train on complete data

Crystal structure → [Image] → Crystal structure
Neural networks: architecture

\[
tanh(A_{11}x_1 + B_1) \rightarrow h_1
\]
\[
tanh(A_{12}x_1 + B_2) \rightarrow h_1
\]
\[
tanh(A_{21}x_2 + B_1) \rightarrow h_2
\]
\[
tanh(A_{22}x_2 + B_2) \rightarrow h_2
\]
\[
h_1 \rightarrow y
\]
\[
h_2 \rightarrow y
\]
\[
C_1 h_1 + D
\]
\[
C_2 h_2 + D
\]
Neural network trains on fragmented data
Neural network predicts on fragmented data
Black box for materials design

Composition

Properties
- UTS
- Hardness
- Cost
Training the neural network
Neural network for materials design

Composition

Properties
- UTS
- Hardness
- Cost
Neural network that can exploit all correlations

Composition

Properties
UTS
Hardness
Cost

Simulations
Density Functional
Molecular dynamics
Finite element

Composition

Properties
UTS
Hardness
Cost

Simulations
Density Functional
Molecular dynamics
Finite element
Neural network trained on experimental data

Experiment vs. Composition diagram
Further information is provided by a simulation.
Neural network combines the two sources of data
Schematic of an engine
<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost</td>
<td>$&lt; 33.7/kg⁻¹</td>
</tr>
<tr>
<td>Density</td>
<td>$&lt; 8281/kgm⁻³</td>
</tr>
<tr>
<td>γ’ content</td>
<td>vol% $&lt; 50.4</td>
</tr>
<tr>
<td>Phase stability</td>
<td>vol% $&gt; 99.0</td>
</tr>
<tr>
<td>Fatigue life</td>
<td>cycles $&gt; 10^{3.9}</td>
</tr>
<tr>
<td>Yield stress</td>
<td>MPa $&gt; 752.2</td>
</tr>
<tr>
<td>Ultimate tensile strength</td>
<td>MPa $&gt; 960.0</td>
</tr>
<tr>
<td>300hr stress rupture</td>
<td>MPa $&gt; 674.5</td>
</tr>
<tr>
<td>Cr activity</td>
<td>$&gt; 0.14</td>
</tr>
<tr>
<td>γ’ solvus</td>
<td>°C $&gt; 983</td>
</tr>
<tr>
<td>Tensile elongation</td>
<td>% $&gt; 11.6</td>
</tr>
</tbody>
</table>
Proposed alloy

Cr: 15.8  Co: 20.0  Mo: 0.5  W: 0.5  Ta: 4.9  Nb: 1.1  Al: 2.4
Ti: 3.0  Fe: 3.9  Mn: 0.2  Si: 0.2  C: 0.02  B: 0.06  Zr: 0.18
Ni: 47.2

900°C  30 hours
Microstructure
Predict the yield stress

![Graph showing the relationship between yield stress and temperature. The graph indicates a decrease in yield stress as temperature increases, with a proposed theory line highlighting the trend.](Image)
Test the yield stress

Yield stress / MPa

Temperature / °C
Test the yield stress

![Graph showing yield stress vs. temperature with proposed theory and experiment results.](image-url)
Test the oxidation resistance

- RR1000
- Proposed theory
- Proposed experiment

![Graph showing mass gain over time for different conditions.](image)
More materials designed

3D printed alloy designed from 7 data entries

Identified and corrected errors in materials database

Battery design with DFT and experimental data
Even more materials designed

Designing lubricants with DFT and experimental data

Thermometer with quantum and experimental data

Drug design
CARBON AND LOW-ALLOY STEELS

This network can be used for carbon steels and low-alloy steels containing only the alloying elements listed below, within the specified ranges. The predicted values represent typical properties for the wrought and annealed condition. Composition should be entered in weight %.

<table>
<thead>
<tr>
<th>Name</th>
<th>Input</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>C (carbon)</td>
<td></td>
<td>(0.0 - 0.965)</td>
</tr>
<tr>
<td>Cr (chromium)</td>
<td></td>
<td>(0.0 - 1.2)</td>
</tr>
<tr>
<td>Mn (manganese)</td>
<td></td>
<td>(0.0 - 1.75)</td>
</tr>
<tr>
<td>Mo (molybdenum)</td>
<td></td>
<td>(0.0 - 0.25)</td>
</tr>
<tr>
<td>Ni (nickel)</td>
<td></td>
<td>(0.0 - 3.5)</td>
</tr>
<tr>
<td>Si (silicon)</td>
<td></td>
<td>(0.0 - 0.25)</td>
</tr>
<tr>
<td>Young's modulus</td>
<td></td>
<td>(205.1 - 213.0)</td>
</tr>
<tr>
<td>Yield strength (elastic limit)</td>
<td></td>
<td>(134.7 - 469.6)</td>
</tr>
<tr>
<td>Tensile strength</td>
<td></td>
<td>(260.5 - 815.6)</td>
</tr>
<tr>
<td>Elongation</td>
<td></td>
<td>(12.6 - 43.9)</td>
</tr>
<tr>
<td>Fracture toughness</td>
<td></td>
<td>(52.4 - 166.5)</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td></td>
<td>(39.7 - 75.3)</td>
</tr>
<tr>
<td>Specific heat capacity</td>
<td></td>
<td>(434.3 - 499.6)</td>
</tr>
<tr>
<td>Thermal expansion coefficient</td>
<td></td>
<td>(11.0 - 13.2)</td>
</tr>
</tbody>
</table>
Apply deep learning to high-value fragmented data

Merge experiments and simulations into holistic design tool

Experimentally proven materials and drugs design with 7 companies, founded startup intellegens.ai

Steels demonstrator: http://app.intellegens.ai/app/network/#/327