Analyzing High Entropy Alloy Data Using Citrination

Undergraduate Researchers: Alec Saville & Nick Lipski
Graduate Researcher: Francisco Coury
Research Advisor: Amy Clarke
What is a High Entropy Alloy (HEA)?

- High Entropy Alloys
  - MPEAs, CCAs, etc.
- New class of materials
  - No principal element
- Examples
  - HfNbTaTi - BCC
  - $\text{Al}_{0.3}\text{CoCrFeNi} - \text{FCC}$
Current Research Focus

- Applications in extreme environments
- Tailorable microstructure and properties
  - Multiple possible compositions
- High-throughput property prediction
  - Accelerated alloy design

The Challenge

- Predicting mechanical properties
  - Yield Strength
- Complex phase formation
  - 6 dimensional phase diagrams required
- Thermodynamic simulations are best effort currently
- Possible alternative prediction method
  - Citrination

\[
\Omega = \frac{T_{mix} \Delta S_{mix}}{\Delta H_{mix}} \quad \delta = 100 \sqrt{\sum_{i=1}^{n} c_i (1 - r_i / r)^2}
\]
Working with Citrination

- Predicting empirical thermodynamic parameters (Takeuchi 2005)
  - Python script
  - Experimental data

- Creating training data set from published papers
  - Miracle et. al 2017
  - Citrination Data Generator
  - 50 HEAs included so far

- Models for phase equilibria
  - Predicts yield strength, but not elongation
<table>
<thead>
<tr>
<th>Error Metric</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Root mean squared error (MPa) (0.0 for a perfect model)</td>
<td>212.38942306025044</td>
</tr>
<tr>
<td>Non-dimensional model error (0.0 for a perfect model)</td>
<td>0.4557020204273737</td>
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<tr>
<td>Uncertainty calibration: fraction of actual values within the prediction error bars (0.68 is perfectly calibrated)</td>
<td>0.5732484076433121</td>
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<tr>
<td>Uncertainty calibration: root mean square of standardized errors (1.0 is perfectly calibrated)</td>
<td>1.3144560765766122</td>
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<tr>
<td>Error Metric</td>
<td>Value</td>
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<tr>
<td>Root mean squared error (0.0 for a perfect model)</td>
<td>0.9039119357169366</td>
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<td>Non-dimensional modal error (0.0 for a perfect model)</td>
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<td>Uncertainty calibration: fraction of actual values within the prediction error bars (0.68 is perfectly calibrated)</td>
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<td>Uncertainty calibration: root mean square of standardized errors (1.0 is perfectly calibrated)</td>
<td>2.2764148216709836</td>
</tr>
</tbody>
</table>
Future with Citrination

- Machine Learning Algorithm still work in progress
  - Many more papers to gain information from
    - 250 HEA’s in references
      - 70 extrapolated to date
- Identify new trends or candidates
  - Move away from empirical approach
Our Takeaway

- Machine learning has potential to greatly accelerate alloy design
  - Not just HEAs
- Utilize in future for investigative and predictive analyses
  - Graduate work and industry
- Continue to update and expand HEA database
Thanks Citrination for working with us!