Machine Learning Prediction of HEA Properties

Nick Beaver, Nathaniel Melisso, Travis Murphy, Mohsen Kivy
Materials Engineering Department

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Research Goal

The goal of this research project is to study the ability of machine learning models for the prediction of phases in high-entropy alloys (HEA). A model that could reliably predict phases of HEAs could supplant conventional computational approaches to phase prediction.

What is a High-Entropy Alloy?

High-entropy alloys are a very new and promising development in the field of materials science. They are less than 20 years old, and come as an extension of the well-studied alloy systems that have been used in engineering for decades. A typical alloy system has one main element as its base, with small amounts of additional elements added in to tune its physical properties in desirable ways (Figure 1a). HEAs are different in that they are composed of multiple elements in similar amounts, which contributes to their more mixed (entropic) structure (Figure 1b).

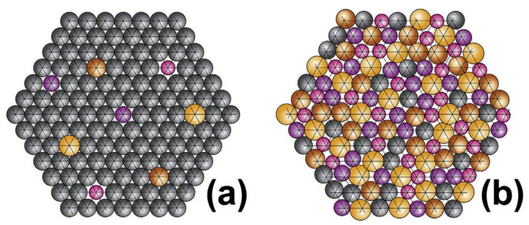


Figure 1a, 1b: (a) A typical engineering alloy, (b) a possible structure for an HEA [1]

There can be multiple possible atomic-scale structures (phases) in an HEA just like in other alloys, including single-phase structures, multi-phase structures (Figure 2), and intermetallic compounds. The unique phase effects seen in HEAs can give them very useful properties [1].

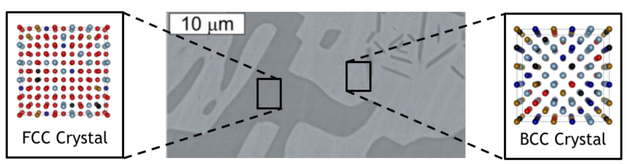


Figure 2: Illustrative example of a 2-phase HEA

Challenges with HEA Research

HEAs are challenging to study for a few key reasons. Common thermodynamic trends and models are misleading when applied to these alloys [1]. A result of this is the 'cocktail effect', where HEAs have a different microstructure (and therefore properties) than expected. This is partly because HEAs represent a much more complicated composition space than regular alloys due to them containing multiple components. Getting enough data to make meaningful models is one of the central challenges in the study of HEAs.

Computational Approach

An extremely common method to get data beyond previous experimental results is the use of CALPHAD (calculation of phase diagrams) software (Figure 3). This computational method uses thermodynamic equations in conjunction with experimental databases to predict the phases present in HEAs. Since the structure and mixture of phases in an alloy are fundamental to its physical properties, having the ability to simulate them based on our current understanding of thermodynamics is critical. However, this fails to describe the larger relationships between structure and composition necessary for making testable predictions on novel alloys.

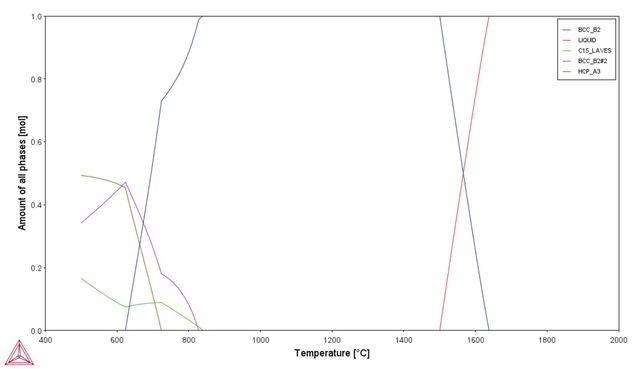
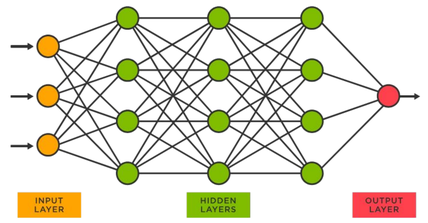


Figure 3: Single-composition phase diagram for TiVZrNbHf

The Machine Learning Approach

A promising method to explore HEAs is to use neural nets. Neural nets can approximate any function given enough data and training time, which in theory makes them ideal for finding the complex relationships between composition and structure present in HEAs. It was hypothesized that there was a relationship between the simple structure and the complex structure that a neural net could learn when given CALPHAD data. However, the relationship proved to be too complex to learn reliably given the amount of data we were able to obtain, so a new method was needed to model the data.




```
# make a sequential model with 3 dense layers
input_shape = y_val.shape[1]
model = keras.Sequential([
  layers.Dense(input_shape, activation='relu'),
  layers.Dense(4, activation='relu'),
  layers.Dense(4, activation='relu'),
  layers.Dense(4, activation='relu'),
  layers.Dense(1, activation='softmax'),  # Output layer
])
```

Figure 4: Example neural net and its code [2]

Future Research

Specialized machine learning models called autoencoders can be used to model systems with high-dimensional dynamics. They are used lower the dimensionality of these systems such that low-dimensional dynamics can capture the behavior of the more complex original behavior. This research will continue the coming academic year as a materials engineering senior project.

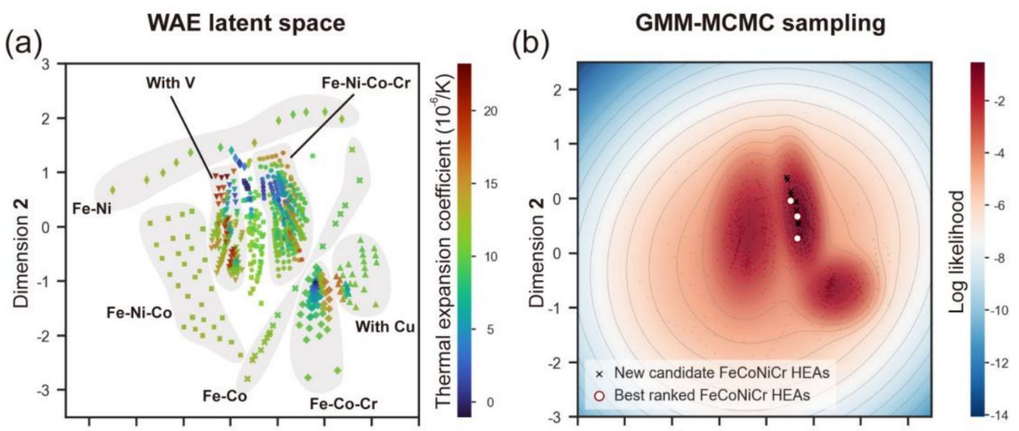


Figure 5a, 5b: (a) Latent encoding of Invar alloys, (b) labelled space with desired property [3]

The goal of future research is to use generative models to make predictions about alloy systems and assess those predictions experimentally. This will be done by encoding the vast compositional space of high-entropy alloys (HEAs) in a latent space, labeling the points in that space with a new independent property, and then finding low-dimensional dynamical models that allow for predictions about the property of interest.

Acknowledgements

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References

[1] Miracle, D.B., and O.N. Senkov. "A critical review of high entropy alloys and related concepts." Acta Materialia, vol. 122, 2017, pp. 448–511, https://doi.org/10.1016/j.actamat.2016.08.081.

[2] "What Is a Neural Network?" TIBCO Software, www.tibco.com/reference-center/what-is-a-neural-network. Accessed 28 Aug. 2023.

[3] Rao, Ziyuan, et al. "Machine learning–enabled high-entropy alloy discovery." Science, vol. 378, no. 6615, 2022, pp. 78–85, https://doi.org/10.1126/science.abo4940.