Machine Learning Prediction of Interfacial Segregation in Complex Concentrated Alloys

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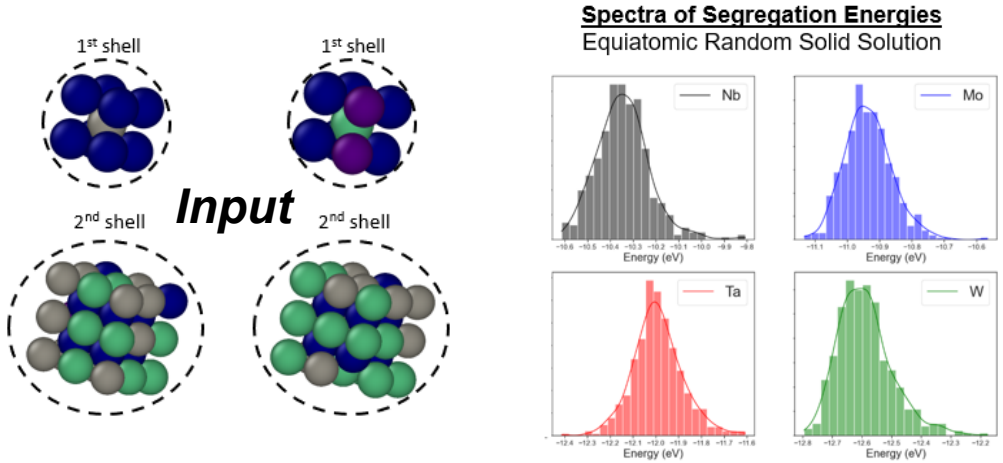
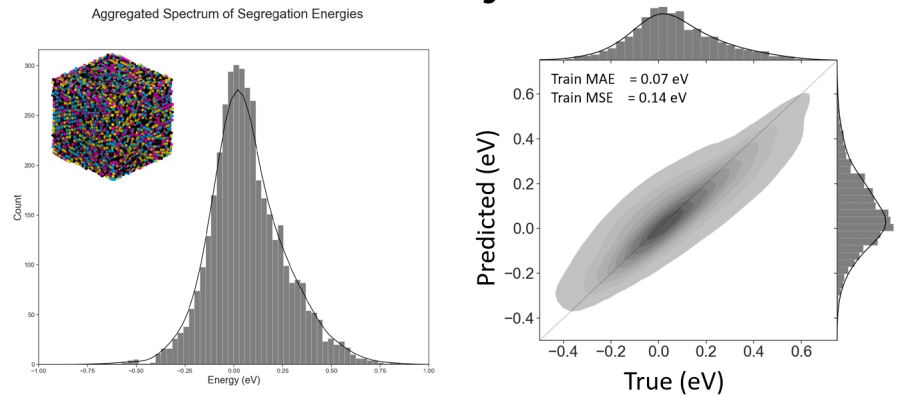
In this work, the grain boundary co-segregation behavior in a NbMoTaW refractory complex concentrated alloy was investigated with atomistic simulations and machine learning tools.

- A random solid solution was simulated with atomistic simulations and local atomic environments were converted into vector descriptions, which were fed into an artificial neural network to predict the segregation behavior.
- Preliminary results from a deep neural network model offer good prediction power.
- This method will allow researchers to predict the partitioning of elements at different internal features in complex concentrated alloys without the need to run expensive atomistic simulations.

Deep Neural Network Model



Preliminary Results



Aksoy D, Apelian D, Ong SP, Luo J, **Rupert TJ**, "Predicting Interfacial Co-segregation in a Refractory Multi-Principal Element Alloy with Machine Learning" (in preparation)