MSE Seminar

In-Person and Virtual

Friday, Oct. 15, 2021

Goodwin Hall 155

10:40 AM – 11:10 AM

https://virginiatech.zoom.us/j/83958084105

Wenjiang Huang

Material Science and Engineering
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"Machine Learning and Atomistic Modeling of Defect Diffusion in Concentrated Ni-Fe Alloys"

Single-phase concentrated solid solution alloys including high entropy alloys are promising structural materials for various high-temperature applications including nuclear energy. Defect diffusion and evolution in these non-traditional alloys play central roles in governing their macroscopic properties. Here we use atomistic modeling and artificial neural network based machine learning method to study how the atomic configurations influence the vacancy diffusion in Ni-Fe concentrated alloys in the full composition range. Molecular dynamics are conducted to calculate the vacancy diffusivities in these alloys at different temperatures, alloy compositions, and atomic configurations. Based on many alloy properties obtained from atomistic modeling such as heat of mixing, vacancy formation energy distribution, migration barrier distribution, and short-range-order parameter, a machine learning based model concerning statistical uncertainties is developed to predict the vacancy diffusivities for different atomic configurations. The effects of these alloy properties on the vacancy diffusion are also analyzed from the machine learning mode.

Wenjiang Huang finished his master's degree at Arizona State of University. It is his 3rd year of Ph.D. work in Dr. Bai's group. His research focuses on studying and understanding the underlying mechanism of the defect diffusion of multi-component concentration alloys by mainly using the atomistic modeling techniques and machine learning methods.