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Modeling of W-based High Entropy Alloys Proposed as PFM for Fusion Reactors MUHAMMAD ABDELGHANY, University of Illinois at Urbana-Champaign, JEAN PAUL ALLAIN, Pennsylvania State University — High-Entropy Alloys (HEAs) have great potential to be employed in the extreme environments of nuclear systems. However, we have very little knowledge about the occurrence, structure, and properties of their crystalline phases. One way of filling this gap is by predicting their behavior computationally. In this study, we are employing some methods to computationally develop an interatomic potential for a W-based HEA proposed by our collaborators at LANL as a PFM for fusion reactors. The proposed alloy is composed of W-Ta-Cr-V which is already tested experimentally and showed promising behaviors under irradiation. The first method is based on using a genetic-algorithm that combines the single-element potentials to generate binary potentials which are optimized such that the MD calculations of selected surface properties converge to the DFT calculations of these properties. The second method employs machine learning to connect the first principle calculations with MD calculations to produce a potential that works well for both the bulk and surface. BCA calculations were also performed for this alloy to capture the mixing effect in response to ion bombardment. For that, DYNAMIX code was used to calculate the partial scattering yield, surface, and depth profiles under ion irradiation.

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