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Atomistic Simulation of Radiation Resistivity of Tungsten-based High Entropy Alloys Proposed as Plasma-facing Materials MUHAMMAD ABDELGHANY, ASHLEY ZHAO, JEAN PAUL ALLAIN, University of Illinois at Urbana-Champaign — High Entropy Alloys (HEAs) are proposed as potential plasma-facing materials for fusion reactors for their high structure stability and radiation resistivity. An atomistic simulation study of surface changes due to plasma irradiation of W-based HEA, W-Ta-Cr-V, has been performed. The main challenge is to develop a proper surface potential of this alloy, that can capture the properties of the system especially at the surface in such far from equilibrium condition. A genetic-algorithm is used to find an optimized Embedded Atom Method (EAM) potential. This algorithm combines the single-element potentials to generate binary potentials, which are combined to form multi-component alloy potentials. The main idea is to optimize the binary potential of each pair such that the Molecular Dynamics (MD) calculations of selected surface properties obtained using these potentials approach the Density Function Theory (DFT) calculations of the corresponding properties of these pairs. This optimized potential is used to do an MD simulation of the surface changes. DYNAMIX, a binary collision approximation code, is used to understand ion-surface interactions. Surface characterization is being done using IGNIS, in-situ facility, to experimentally validate this computational study.

Muhammad Abdelghany
University of Illinois at Urbana-Champaign

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