Threshold Displacement Energy Study in Tungsten: Combining Machine Learning and Classical MD Simulations

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In this study, we employ a combination of machine learning techniques and classical molecular dynamics (MD) simulations to compute the threshold displacement energy (TDE) in both pure tungsten (W) and deuterated configurations. We use interatomic potentials based on Gaussian Approximation Potential (GAP) framework, a 3-body Tersoff potential with the Ziegler-Biersack-Littmark universal screening function, and Embedded Atom Method (EAM) potential tailored for modeling W-H interactions with hybrid simulations for EAM/GAP. The primary knock-on atom (PKA) is considered in an energy range of 20 to 120 eV, and random velocity directions. Our investigation delves into the probability of stable defect formation, drawing correlations between PKA energy levels, and velocity orientations by a machine learning based software workflow FaVAD (Fingerprinting and Visualization of Atomic Defects) to characterize their configurations and strain profiles. All investigated MD-potentials report a minimum TDE along the <001> orientation for pure W with values of 53 eV with the Tersoff, 50 eV employing GAP, and 45 eV for EAM (Fig 1, left panel). Meanwhile, for samples with a D atom present in the same unit cell as the kicked W-atom, the angle-averaged TDE is reduced to 45 eV for <001>, 65 eV at <101>, and 70 eV along <111>. With increasing D-content the TDE is decreasing for the Tersoff potential to 45 eV along <001>, 60 eV along <101>, and 65 eV along <111> where FAVAD was applied to identify D decorated defects with PCA method (Fig 1, right panel).

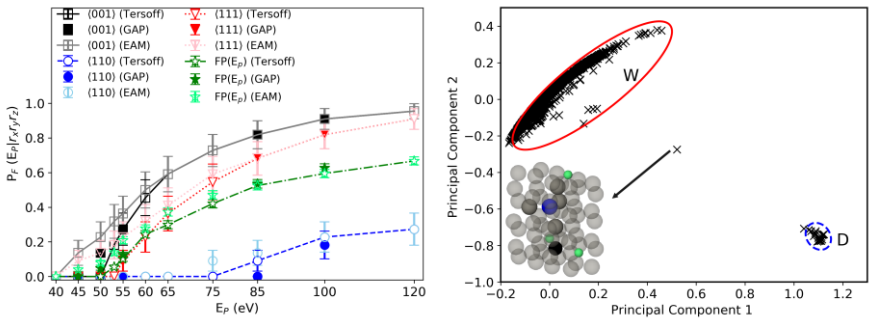

Figure 1: *TDE values for pure W matrices (left panel) and FAVAD applied to find D decorated W point defects in W samples with high concentrations of D atoms.*