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Analysis of Helium Cluster Dynamics near Grain Boundaries of Plasma-Exposed Tungsten LIN HU, University of Massachusetts, Amherst, KARL HAMMOND, University of Missouri, Columbia, BRIAN WIRTH, University of Tennessee, Knoxville, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We report results of a systematic atomic-scale analysis of the kinetics of small mobile helium clusters near a model symmetric tilt grain boundary (GB) in tungsten (W). The small mobile helium clusters migrate toward the GB region by Fickian diffusion and drift due to an elastic interaction force that drives GB segregation. As the clusters migrate toward the GB, trap mutation (TM) reactions are activated at rates higher than those away from the GB and are the dominant kinetic processes for 4-member and larger mobile helium clusters. Each TM reaction produces a W interstitial atom on the GB, in the form of an extended interstitial configuration, and an immobile helium-vacancy complex with the W vacancy located at a short distance from the GB. These reactions are identified and characterized in detail based on analysis of a large number of molecular-dynamics trajectories. The mobility of the extended W interstitial on the GB depends on the location of the helium-vacancy complex. The identified cluster reactions are responsible for important structural, morphological, and compositional features in plasma-exposed tungsten.

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