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SEAKMC results of small He clusters near free surfaces in tungsten[1] ROGER STOLLER, Oak Ridge National Laboratory, ALEXANDER BARASHEV, University of Tennessee, Knoxville, HAIXUAN XU, Oak Ridge National Laboratory — The behavior of small helium and helium vacancy clusters is believed to crucial to understanding the plasma-surface interaction that gives rise to was has been called "fuzz" formation on tungsten metal surfaces exposed to low-energy helium plasmas at elevated temperatures. Detailed characterization of this behavior requires a computational approach capable of capturing the atomistic physical properties while reaching times well beyond those typically accessible by molecular dynamics. The recently developed self-evolving atomistic kinetic Monte Carlo (SEAKMC) method has been applied to investigate small He clusters in tungsten at a range of relevant temperatures, and as a function of distance from a free surface. A strong effect of the free surface on cluster behavior was found for clusters within about 4 lattices parameters of the surface. In some cases, cluster migration to the surface leads to the production of tungsten adatoms associated with Frenkel pair formation, resulting in atomic-scale surface roughening. The resulting He-vacancy cluster is immobile, and can be a stable trap for other He atoms. Capture of additional He atoms can lead to formation of additional Frenkel pair and adatoms. The possible role of these mechanisms in surface fuzz formation will be discussed.

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