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Helium interaction with tungsten surfaces and subsequent evolution from atomistic simulations

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The results of a computational study of helium-vacancy clusters in tungsten are reported. A recently developed atomistic kinetic Monte Carlo method employing empirical interatomic potentials was used to investigate the behavior of clusters composed of three interstitial-helium atoms near {111}, {110} and {100} free surfaces. Multiple configurations were examined and the local energy landscape was characterized to determine cluster mobility and the potential for interactions with the surface. The clusters were found to be highly mobile if far from the surface, but were attracted and bound to the surface when within a distance of a few lattice parameters. When near the surface, the clusters were transformed into an immobile configuration due to the creation of a Frenkel pair; the vacancy was incorporated into what became a He_3-vacancy complex. The corresponding interstitial migrated to and became an adatom on the free surface. This mechanism of cluster immobilization and adatom formation may provide a significant source of helium retention in and surface degradation in tungsten divertors. Clearly, the ejection of one adatom to the surface does not result in significant reconstruction of the surface. However, the cumulative effect of many such events should be studied to understand its potential as a unit process that may contribute to fuzz formation. These helium-vacancy clusters may also provide significant trapping sites for tritium and increase tritium retention. It should be noted that there are some differences between these results and molecular dynamics simulations reported recently by Hu et al. (Surf. Sci. 626, 2014, pp. 21-25); these indicate that atomic vibrations may play a stronger role in the energy landscape near free surfaces, leading to the Monte Carlo model somewhat underestimating the interaction between He clusters and free surfaces.