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Development of Drift-Diffusion Models of Mobile Helium Cluster Dynamics Near Surfaces of Plasma-Exposed Tungsten DIMITRIOS MAROUDAS, LIN HU, Department of Chemical Engineering, University of Massachusetts, Amherst — We report on the development of continuum drift-diffusion models for the dynamics of mobile helium (He) clusters in near-surface regions of materials exposed to He plasmas in fusion reactors. In addition to Fickian diffusion, the models account for drift fluxes driven by surface/interface segregation forces; such thermodynamic driving forces become significant near surfaces/interfaces and areal defects such as grain boundaries (GBs). The continuum models for the evolution of the mobile cluster concentrations are linked hierarchically with molecular-dynamics simulations of mobile cluster migration and are parameterized based on atomistic computations over the range of mobile cluster size for various surface/GB orientations; these computations yield the energy profiles of structurally relaxed He-cluster configurations in the direction normal to the surface/GB and optimal cluster migration/reaction pathways. The atomistic predictions of diffusivities and segregation potentials provide the required constitutive information for the closure of the drift-diffusion transport equations. The transport modeling also is extended to cases of combined drift effects near multiple sinks, such as in regions where GBs intersect with the surface.

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