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Large-scale MD simulations investigating H plasma interactions with Tungsten surfaces MARY ALICE CUSENTINO, BRIAN WIRTH, University of Tennessee Knoxville — Tungsten is a prime candidate material for the divertor in future fusion reactors such as ITER. However, the tungsten divertor will need to be able to withstand high fluxes, on the order of 10^{24} $m^{-2}s^{-1}$, of low energy hydrogen. It is crucial to understand both the tungsten surface response as well as the hydrogen retention and recycling for the divertor region. Molecular dynamics (MD) is a useful tool to study these effects. One issue with MD is that implantation fluxes tend to be very high, on the order of 10^{27} $m^{-2}s^{-1}$, due to time and computational limitations. By performing large scale MD on supercomputers, it is possible to reach more realistic fluxes of 10^{25} $m^{-2}s^{-1}$. Results will be presented from MD simulations from a 50 nm x 50 nm x 25 nm tungsten box at 1200 K and 2000 K. Hydrogen is implanted every 10 ps based on the 60 eV depth distribution calculated by SRIM, which amounts to a flux of 4 x 10^{25} $m^{-2}s^{-1}$. A modified version of the Juslin bond order W-H potential is used to describe the W-H interactions. Preliminary results show an initially high retention of hydrogen that accumulates in a sub-surface region. These simulations provide insight into the early stages of surface deformation as well as hydrogen retention for the tungsten divertor.

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