

Abstract Submitted  
for the DPP15 Meeting of  
The American Physical Society

**A Molecular Dynamics Study of Sub-Surface Mixed Hydrogen-Helium Bubbles in Tungsten** ZACHARY BERGSTROM, MARY ALICE CUSENTINO, BRIAN WIRTH, Univ of Tennessee, Knoxville, PSIDAC PSI COLLABORATION — Fusion reactor materials experience high ion fluxes and operating temperatures which pose significant problems to plasma facing components. Among these issues is the formation of sub-surface helium and hydrogen bubbles in the divertor, of which tungsten is the prime candidate. Bubbles below the surface can grow by loop punching producing significant surface roughening and deformation. Molecular dynamics (MD) simulations are used to provide insight on the migration of hydrogen and helium within and around a sub-surface cavity in tungsten as a function of bubble size and partial pressures of helium and hydrogen to be compared to theoretical assessments of tritium partitioning to bubbles based on Sievert's Law. In this study, a cavity is created from a lattice of tungsten by removing atoms from inside a centered spherical region 2.5 nm below a free surface and approximately 2 nm in diameter. Hydrogen and helium are inserted into the cavity at random positions and allowed to find their local minimum. MD simulations are then performed for times on the order of nanoseconds for various concentrations of H and He, temperature, and surface orientations. The MD simulations provide quantitative information on the H and He distributions and partitioning amongst the bubbles and surfaces required to further understand the H and He synergies to estimate tungsten divertor lifetimes in ITER due to tritium retention, as well as provide insight into possible approaches to mitigate gas-driven damage to the tungsten divertor.

Zachary Bergstrom  
Univ of Tennessee, Knoxville

Date submitted: 24 Jul 2015

Electronic form version 1.4