Helium Bubble Growth in Tungsten Under Realistic Rates

Dr. Luis Sandoval
Los Alamos National Laboratory

Abstract

The growth process of He bubbles in W is investigated using molecular dynamics and parallel replica dynamics (ParRep) for growth rates spanning 6 orders of magnitude. ParRep enables the temporal parallelization of the state-to-state dynamics, hence allowing massively parallel resources to be leveraged in order to reach very long simulation time scales on systems of modest sizes. For example, some of our results were generated using 10 000 replicas distributed over 160 000 cores on the Titan supercomputer at Oak Ridge National Laboratory. Fast and slow growth regimes are defined relative to typical diffusion hopping times of W interstitials around the He bubble. Slow growth rates allow the diffusion of interstitials around the bubble, favoring the biased growth of the bubble towards the surface. In contrast, at fast growth rates interstitials do not have time to diffuse around the bubble, leading to a more isotropic growth and increasing the surface damage.