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Energetics of large helium-vacancy clusters in tungsten NIKLAS JUSLIN, RYAN SWEET, BRIAN WIRTH, University of Tennessee, PSI-SCIDAC TEAM — The divertor in a fusion reactor is subject to intense, low energy (1-100 eV) hydrogen isotope and helium bombardment from the plasma. Tungsten is the leading candidate material for the divertor plates. Helium in a material can cause changes in thermal and mechanical properties, such as swelling, change in ductile to brittle transition temperature, bubbles and nanofuzz formation. Molecular dynamics (MD) simulations is a valuable tool for studying energetics, structures and many radiation damage phenomena that happen on short time and length scales. Using MD simulations we have studied a wide range of size and composition of He bubbles in tungsten. By annealing a bubble and calculating the formation energy, a clear trend is found, which can be fit to a semi-empirical expression and thus providing the energetics of a bubble of any size. As helium is added to a bubble and the bubble pressure grows, W interstitials are punched out to relieve pressure, depending on bubble size and temperature. As nanofuzz formation has only been observed for helium plasma exposure we also compare the bubble formation mechanisms with neon based on ab initio data and a new W-Ne potential.

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