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Retention of hydrogen and helium in monocrystal of tungsten[1]
JACK WELLS, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, PREDRAG KRSTIC, State University of New York, Stony Brook, NY 11794 — Beginning with either perfect or damaged mono-crystal of tungsten, we bombard the surface with a mix of isotopes of H and He at the impact energy range from 1-100 eV in order to predict the retention rate of the impinging atoms as well as their distribution inside the material, in particular inside the vacancies. Our calculation is based on molecular dynamics simulation using high-performance computing and bond-order potentials. The goal is to distinguish between the following alternative outcomes: (1) the retention rate is proportional to the number of vacancies – consistent with recent experiments on the retention of H in damaged W, (2) vacancies will be filled by aggregates of H or He, leading to unstable surfaces, e.g., bubbling and blistering of the surface, and (3) some fraction of hydrogen and helium will fill the interatomic space in the W crystal lattice, creating a "protective layer" or bubbles and blisters close to the surface, even in absence of significant tungsten lattice defects, and (4) the impact direction and the crystal surface cut influence significantly ratio of effects 1-3.

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