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Molecular Dynamics and Kinetic Monte Carlo Simulations on Defect Formation in Tungsten with and without Hydrogen

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Recent experiments have shown a number of unexpected phenomena in the interaction of tungsten and hydrogen.

One class of experiments (c.f. [1,2]) investigated the influence of hydrogen isotopes HI (i.e. hydrogen and deuterium) on the damage level in tungsten under high-energetic W-ion irradiation. Here tungsten samples were exposed to repeated sequential tungsten-ion irradiation with 20 MeV and low-energy deuterium plasma exposure. It was found that the maximum deuterium concentration for this cycles can exceed the value observed for damaging without the presence of deuterium by a factor of two or more. Here we present investigations using molecular dynamics simulations and subsequent kinetic Monte Carlo calculations which emphasize the importance of interstitial-hydrogen interactions in the explanation of the observed phenomena: The presence of hydrogen does hardly influence the primary damage production but reduces the damage annealing rate significantly by the temporary formation of I(W)-H-complexes.

Another class of experiments describe the formation of a stable hydrogen-enriched layer on the surface of tungsten samples exposed to low-energy hydrogen plasmas, where the upper limit of the ion-energy transfer to the sample atoms is below the nominal displacement threshold [3,4], thus initially no permanent sample modifications was envisaged. These supersaturated surface layers contain up to 10% of HI and have a thickness of the order of the ion range. Here molecular dynamics simulations suggest a surface-driven formation mechanism and – in contrast to the previous, high-energy damaging case - the importance of vacancy-hydrogen VH-complexes.

References:
[1] T. Schwarz-Selinger et al., Nucl. Mater. Energy 17, 228-234 (2018)
[2] S. Markelj et al., Nucl. Mater. Energ. 12, 169 (2017)
[3] L. Gao et al., Nucl. Fusion 57, 016026 (2017)
[4] L. Gao et al., Acta Mater. 201, 55 (2020)

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