Influence of the presence of deuterium on damage in tungsten – an artificial dynamics MD-study

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Experimental results for the reported damage in tungsten under high energy tungsten-ion bombardment [1] as well as for exposure to low-energy hydrogen isotope exposure [2] indicate a pronounced influence of the presence of deuterium on the defect formation in the host material and experimentally different steady-state defect concentrations are derived from deuterium concentration profiles as measured by nuclear reaction analysis. The underlying atomic mechanism, however, is unclear at present.
Here we report on the results of artificial dynamics approaches on the influence of deuterium on the dynamic and eventually steady-state modification of tungsten samples based on molecular dynamics simulations. The evolution of the microstructural sample properties is modeled by an artificial dynamics approach using repeated atomic drag-and-drop cycles where atoms are randomly displaced in the system, followed by short relaxation periods. The dynamics of the model evolution with respect to a variety of system quantities like e.g. energy and vacancy concentration are studied for systems with and without hydrogen for different temperatures.
Especially the correlation analysis of lifetimes of vacancies with and without hydrogen present for systems in steady-state provides some additional insight into the experimentally observed effects and points towards a potential key process which needs to be scrutinized and confirmed by classical (but much more costly) MD.

[1] T. Schwarz-Selinger, J. Bauer, S. Elgeti, S. Markelj, Nuclear Materials and Energy 17 (2018) p. 228-234

[2] L. Gao et al, Nucl. Fusion 57 (2016) p. 016026 (11 pages)