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Deuterium effect on defect evolution in tungsten, from bulk to surfaces

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Tungsten will be used as the plasma facing material in fusion reactors, and will be subjected to irradiation, which will affect its properties. Fusion fuels, such as hydrogen isotopes, will be implanted into the material, which will affect the material properties and be a problem as radioactive tritium is retained. Experimentally it has been seen that having deuterium present during irradiation will substantially affect the defect evolution of tungsten, compared to pure tungsten [1]. For instance, about double the amount more deuterium was trapped in the dual beam experiments compared to the case where tungsten first was irradiated and then as a second step subjected to deuterium. This indicates that the defect structure and defect production mechanisms are different. The tungsten surfaces have also been seen to be decorated by deuterium, which might affect the sputtering of the tungsten surfaces, when they are not pure tungsten anymore.

To remedy this, we carried out atomistic simulations with Molecular Dynamics to understand these phenomena better. In the bulk case we could reproduce the experimental trends by deuterium, as found the underlying mechanisms [2]. Among these were increased defect production and significantly less recombination if deuterium is present. We systematically studied the effect of different deuterium concentrations and vacancy cluster sizes. To shed some light on how deuterium affects the sputtering of tungsten surfaces, different deuterium decoration levels of the tungsten were studied. Sputtering simulations by various fusion relevant ions were studied under different conditions. We found that deuterium decoration will affect the tungsten sputtering, in addition to being sputtered itself. The next steps involve multiscale modelling to achieve longer timescales and Machine Learned interatomic potential development for these systems, for more accurate representation.

References:

[1] S. Markelj, T. Schwarz-Selinger, M. Pecovnik et al. Nucl. Fusion 59 (8) (2019) 086050
[2] V. Lindblad, D. R. Mason, F. Granberg, J. Nucl. Mater. 603 (2025) 155422

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