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Multiscale modelling of H and He in W

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In this talk, we will overview our work on using binary collision approximation (BCA), density-functional theory (DFT), classical molecular dynamics (MD), kinetic Monte Carlo (KMC), and rate equation (RE) modelling of how H and He escaping from a fusion plasma interacts with W. We will first present a brief overview of the simulation tools used, and in particular discuss our interatomic potential development approach.

We will then present results on several timely aspects of H and He interactions with W. We will show how DFT, MD and KMC simulations were used to explain why H and He bubble formation depths are very different in W [1,2,3]. We will further describe a systematic collection of BCA, MD, DFT data for describing the migration, trapping and detrapping energies of H in W, and how this data was used in a RE model to reproduce experimental data of D depth profiles before and after annealing. Analysis of the results show that a single monovacancy in W can hold about 5 H atoms [4,5]. We will finally present how a combination of MD and an entirely new KMC model has been used to study formation of W fuzz formation during high-fluence He irradiation, and in particular explain the origin of the experimentally observed sqrt(time) dependence for W fuzz formation [6,7].

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