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Multi-scale modelling of H interactions on W surfaces and W/Cu interlayers

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In this contribution, we will provide an overview of the approach we have been developing over the last few years to model the interaction of hydrogen isotopes (HIs) with fusion-relevant materials. This approach now allows us to model the material from the plasma-exposed surface to the coolant boundary. Following a multiscale (MS) approach, our modeling relies upon electronic structure calculations based on density functional theory (DFT), classical molecular dynamics (MD), kinetic, and/or thermodynamic theory. DFT enables an accurate description of the material's structure at a scale of hundreds of atoms. MD allows us to simulate larger systems of hundreds of thousands of atoms, while kinetic and thermodynamic theories use atomic data as input and deliver macro-scale physical quantities as output. We applied this MS approach to tungsten and copper, considering perfect material structure, point defects, and extended 2D defects such as interfaces [1]. In tungsten, this led us to determine the macroscopic physical conditions that make the surface processes the rate-limiting step for HIs transport. Based on these findings, a kinetic model has been developed and further incorporated into the macroscopic code MHIMS [2]. These results will be briefly reviewed to illustrate the MS approach we developed. Then we will focus the presentation on our latest developments that extend to the coolant side of the divertor plasma-facing components. Two models of W/Cu interface are built to obtain the HIs solution and diffusion properties there. DFT models allow us to determine the stable interstitial sites where HIs could be placed. While thermodynamic and kinetic models were developed to study their solubility within and out of thermal equilibrium conditions. Finally, with MD, we investigated the impact of the mismatch on the copper structure near the W/Cu interface: it leads to the formation and propagation of defects like vacancies and dislocation lines.

[1] Y. Silva-Solis et al, NME 37 (2023) 101516.
[2] E. A. Hodille et al, NF 57 (2017) 056002.
[3] J. Denis et al, NME 19 (2019) 550-557.

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