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H trapping and migration in W: A DFT investigation that includes temperature dependency

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In this talk, the plasma wall interaction is focused on the hydrogen-tungsten system that we investigate by mean of Density Functional Theory (DFT). Because DFT is limited to small models of about one hundred atoms at zero temperature, this work is complemented by a statistical approach with the aim to yield temperature dependent data that can be directly compared with macro-scale thermodynamic and kinetic experimental data.

It follows that DFT data are included in a statistical model based on transition state theory and thermodynamic. Such model allows revising the solubility and diffusivity of hydrogen in tungsten. The discrepancy between the experimental diffusion coefficient from Frauenfelder *et al*[1] and other DFT results[2] is understood and two diffusion regimes are proposed depending on the temperature.

The trapping of multiple hydrogen atoms in tungsten vacancies is also investigated. The hydrogen population in vacancies and the vacancy concentration in tungsten are shown to depend on the temperature. Using a crude kinetic model, TDS spectra are simulated, which despite the simplicity of the model exhibit a reasonably good agreement with experimental results recorded on single crystalline samples[3,4].

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