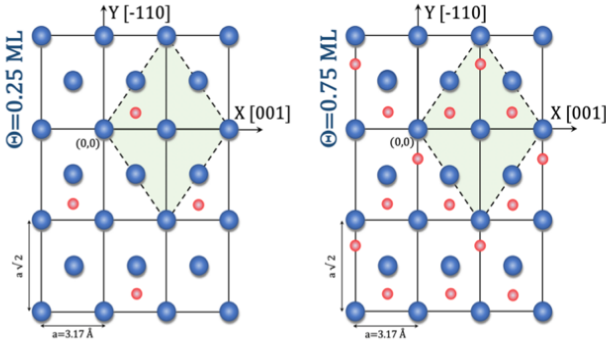
Hydrogen Atom Scattering off Tungsten Surfaces: recent developments.

Pascal Larregaray[1]

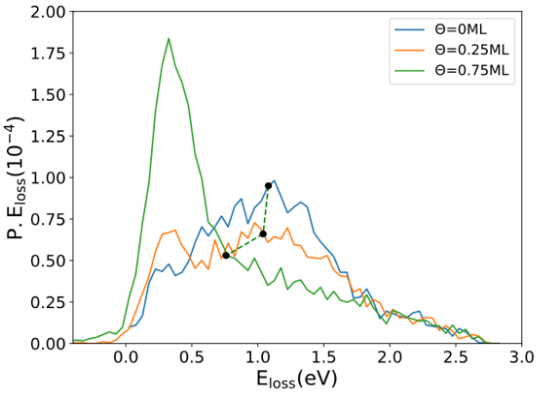
[1] Univ. Bordeaux, CNRS, Bordeaux INP, ISM, UMR 5255, F-33400 Talence, France

Pascal.larregaray@u-bordeaux.fr

Quasi-classical trajectory simulations are performed to investigate the energy transfer upon scattering of hydrogen atoms off clean and hydrogen-covered (110) tungsten surfaces. For hydrogen atoms impinging clean metal surfaces at energies of the order of few electronvolts, translation energy loss has been recently demonstrated to be mainly mediated via electron-hole pair excitations. The present theoretical approach scrutinizes this effect, in particular, the influence of coverage by hydrogen pre-adsorbed atoms. Scattering can be rationalized in terms of three distinct dynamical mechanisms, the contribution of which changes with coverage. These allow in particular to understand why the shape of the energy loss spectra critically depends on whether scattering is analyzed in the whole space or at specular angle.



Position of the adsorbed H atoms (red points) on W(110) at Θ=0.25 ML (left) and Θ=0.75 ML (right).



Energy loss spectra for atoms scattered at specular angle, for Θ=0 (blue), 0.25(orange) and 0.75(green) ML. The distributions are normalized to the total number of trajectories. Black circles represent the average energy loss.