Translational Inelasticity of Hydrogen Atoms Scattering off Hydrogen-Covered W(100) Surfaces

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Recent experiments show that translational energy loss is mainly mediated by electron-hole pair excitations [1], for hydrogen atoms impinging on clean metallic surfaces. Inspired by these studies, quasi-classical trajectory simulations are performed to investigate the energy transfer after scattering of hydrogen atoms off clean and hydrogen-covered tungsten (100) surfaces. The present theoretical approach examines the coverage effect of the preadsorbed hydrogen atoms, as was done for the case of the tungsten (110) surface [2]. Dispersion can be rationalized in terms of three different dynamical mechanisms, the contribution of which changes with coating. These allow, in particular, to understand why the shape of the energy loss spectra depends critically on whether the scattering is analyzed in the whole space or at a specular angle.

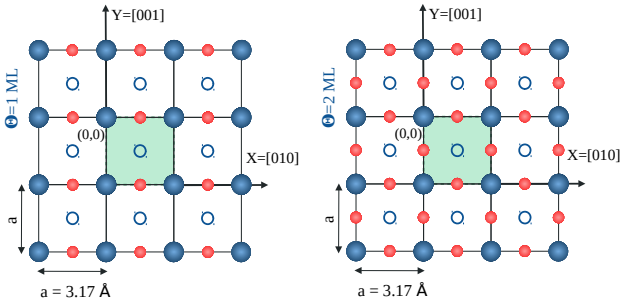

Figure 1: *Position of adsorbed H atoms (red points) on W(100) at Θ= 1 ML (left) and Θ= 2 ML (right). Blue circles show the position of the second layer tungsten atoms.*

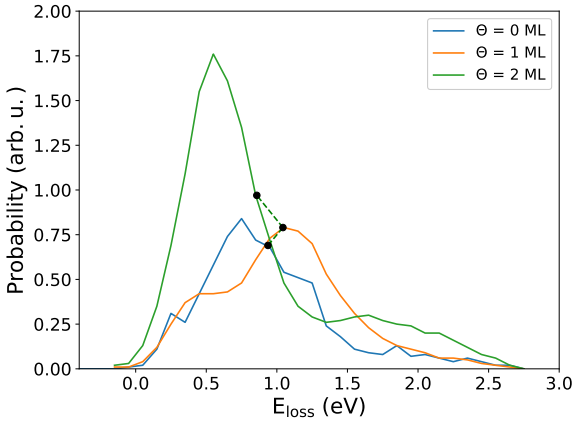

Figure 1: *Energy loss spectra for scattered atoms at specular angle, at Θ= 0 ML (blue), Θ= 1 ML (orange) and Θ= 2 ML (green). The distribution is normalized to the total number of trajectories. The black dots represent the average energy loss for each case.*

[1] O. Bunermann, H. Jiang, Y. Dorenkamp, A. Kandratsenka, S.M. Janke, D. J. Auerbach, and A. M. Wodtke, Science, vol. 350, no. 6266, pp. 1346–1349, 2015.

[2] R. Martin Barrios, O. Galsparsoro, A. Martinez-Mesa, L. Uranga-Piña, C. Créspos, and P. Larregaray. J. Phys. Chem. C, vol. 125, no. 26, pp. 14468–14473, 2021.