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Hydrogen diffusion at surfaces, defects and interfaces

Monday, 23 November 2020 14:20 (20 minutes)

The presentation will summarize the work we recently achieved and is currently going on regarding the surface of tungsten. The title of the presentation reflects our full project to the CRP. However, this meeting presentation will only focus on the role of oxygen on tungsten and how it modifies the interaction of hydrogen.

We will start by presenting the work we carried out on the adsorption of hydrogen on both the W(110) and W(100) surfaces without oxygen. This way, we will present the methodology we follow; it is made of Density Functional Theory (DFT) calculations, thermodynamics and kinetics, with which we attempt to produce macroscopic data that can be compared with experimental results. In particular, we recently developed a model that determines the surface coverage in hydrogen of both the W(110) and W(100) surfaces depending on the pressure and the temperature. Thanks to the Low Energy Ions Scattering (LEIS) and Direct Recoil Spectroscopy (DRS) measurements from Rob Kolasinski at SANDIA National Lab, Livermore, we are now able to confront the predictions from the model to experimental measurements. The agreement will be presented and discussed.

Then we adsorbed oxygen on the bare W(110) surface. Despite many configurations were investigated, only the three-fold (TF) adsorption site was shown to be relevant for the rest of the study. The adsorption pattern we calculated at various coverages are in good agreement with experimental observations. The adsorption energy is nearly constant at -4.5eV per O atom up to saturation of the surface, which is obtained for 1 Mono-Layer (ML) of oxygen. Beyond saturation, oxygen still absorbs below the surface up to the formation of a WO2 layer that is very weekly bonded to the surface.

When hydrogen is added to the tungsten surface with oxygen, it is shown that oxygen blocks the TF sites and prevents the adsorption of hydrogen. Again, saturation is achieved for 1 ML of adsorbent, but regardless of the concentration of oxygen and hydrogen. It is also shown that the adsorption energy of hydrogen on the surface decreases with increasing coverage in oxygen.

In the end, a brief summary of the work we intend to do in the one or two coming years will be provided.

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