Unusual adsorption of hydrogen on supported ultrathin aluminium oxide films

Matic Poberžnik, Anton Kokalj
Jožef Stefan Institute, Ljubljana, Slovenia

It is well known that (ultra)thin oxide films can exhibit different properties with respect to their bulk counterparts and in this contribution, we report on an unusual binding site for hydrogen on the surfaces of ultrathin aluminium oxide films supported on aluminium. In particular, we find that hydrogen preferentially adsorbs on surface Al atoms instead of oxygen atoms (as one would expect based on chemical intuition). By performing systematic Density Functional Theory (DFT) calculations on a model oxide film of varying thickness (α-Al_2O_3 supported on Al(111), shown in Figure 1a) we establish that this binding mode is favoured for ultrathin films, where hydrogen adsorbs in hydride form, with the excess charge originating from Al atoms at the metal-oxide interface (Figure 1b). Finally, we propose that hydrogen bonding to surface Al ions is connected to the experimentally observed hydrogen evolution in pits formed during the pitting corrosion of aluminium.

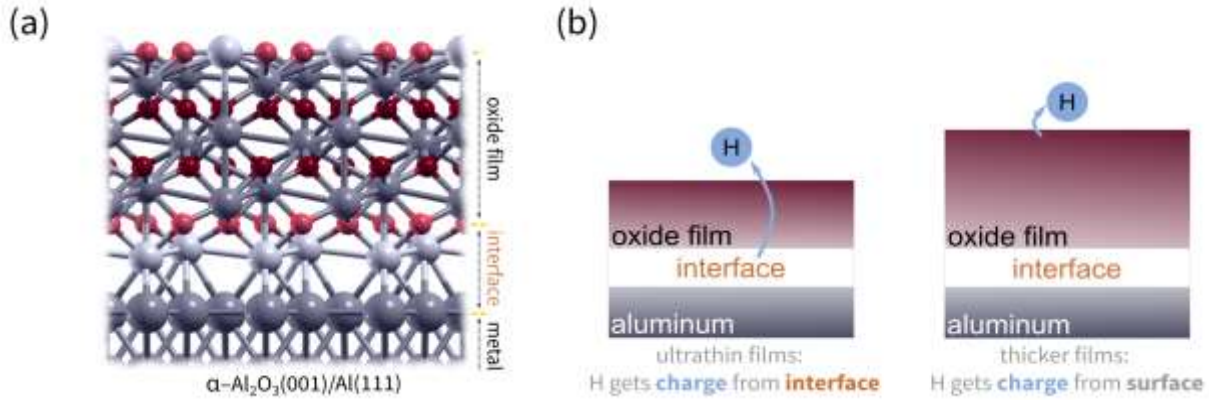

Figure 1. (a) A side-view of the model of the surface employed in DFT calculations. (b) On ultrathin films the charge on hydrogen originates at the oxide-metal interface