

INFLUENCE OF THE SURFACE STATE ON H₂-SORPTION PROCESS OF LIGHT HYDRIDES: THE CASE OF MAGNESIUM.

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Magnesium hydride (MgH₂) is a sustainable hydride able to accumulate high amounts of hydrogen (7.6 % wt H₂) [1]. However, thermodynamic restrictions and poor H-kinetics preclude its use in applications. MgH₂ nanostructures are being widely investigated to overcome these drawbacks, promoting the hydrogenation process by reducing the activation energies related to bulk processes such as H-diffusion, hydride nucleation, etc. However, the critical role of the surface on the hydrogenation process has been much less investigated. Theoretical calculations have shown the poor ability of clean magnesium surface to dissociate the H₂-molecule [2], but barely experimental works have been performed [3]. Moreover, the high reactivity of the magnesium promotes the formation of several phases such as oxides, hydroxides and carbonates, which could drastically affect H₂-dissociation and H-diffusion into few atomic layers. The composition and role of those phases at the surface on the hydrogenation properties are not clarified yet, giving controversial results [4]. This work will try to shed light on this issue.

To this aim, film geometry is chosen as an ideal playground due to its well-controlled synthesis and appropriate characterization techniques [5]. The H₂-sorption mechanisms were investigated by “in situ” optical measurements under different temperatures and H₂-pressures. All films were characterized by profilometry, XRD and STEM using EELS, EDS and HAADF techniques. Results show a drastic influence of oxide/hydroxide layer on the H₂-sorption processes, even with acting the palladium catalytic layer. Activation energies and control mechanisms would be revealed, giving clues about the key influence of the surface state on magnesium hydrogenation/dehydrogenation processes.

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