

The role of vacancies and hydrogen in the photochromism of YO_xH_y thin films examined by in-situ Positron Annihilation Spectroscopy and μ SR

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Yttrium oxyhydride (YO_xH_y) is a promising mixed-anion material in view of its special photochromic properties, offering prospects for application in smart windows [1]. Doppler Broadening Positron Annihilation Spectroscopy (DB-PAS) depth profiling was applied to probe the electronic structure and the evolution of vacancies in YO_xH_y thin films and related materials. A strong systematic variation in the S- and W-parameters of Y, $YH_{1.9+\delta}$, YO_xH_y and Y_2O_3 thin films is observed, caused by distinct differences in their electronic structure that spans the range from metals to a large band gap insulator [2]. Positron Annihilation Lifetime Spectroscopy (PALS) reveals the presence of vacancies and positronium formation in the YO_xH_y films. In-situ optical illumination of the semiconducting YO_xH_y films above the band gap leads to an increase in S-parameter, plausibly induced by the generation of vacancies or growth into small vacancy clusters [2]. Intriguingly, the S-parameter does not relax during optical bleaching under dark conditions, indicating persistent local rearrangements of vacancies and hydrogen ions.

Furthermore, low-energy Muon Spin Rotation (μ SR) experiments on $YH_{1.9+\delta}$ and YO_xH_y thin films indicates the formation of μ^+H pairs at tetrahedral sites. In-situ illumination of YO_xH_y films leads to a clear reduction in muonium formation, that could be affected by photo-excitation of charge carriers during photochromic darkening, relaxing slowly upon bleaching.

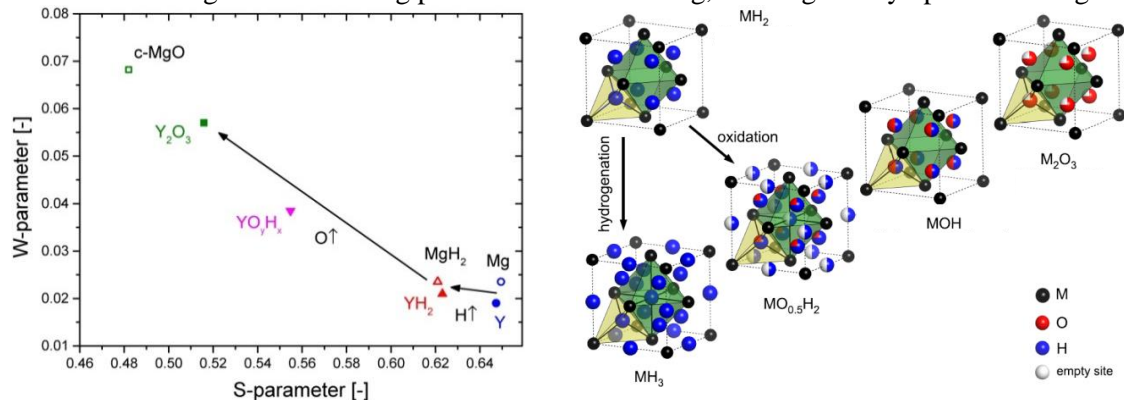


Figure 1 (a) S-W diagram (best-fit values) for Y, $YH_{1.9+\delta}$, YO_xH_y and Y_2O_3 thin films [2], (b) Schematic crystal structures of rare-earth oxyhydrides with different H^-/M and O^{2-}/M ratios [3].

References

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