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New insights into the photochromism of yttrium oxyhydride thin films from in-situ muon spin rotation (MuSR) and positron annihilation spectroscopy (PAS) studies

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Thin films of rare-earth metal oxyhydrides, such as yttrium oxyhydrides ($\text{YH}_{3-2x}\text{O}_x$), show a pronounced photochromic effect where the transparency of the films decreases reversibly over a large range of sub-bandgap wavelengths upon exposure to UV light. This makes these materials suitable candidates for applications in smart windows. However, the exact mechanism behind the photochromic effect is unknown. We investigated the behavior of $\text{YH}_{3-2x}\text{O}_x$ thin films, with different O:H ratios, under dark and illuminated conditions using in-situ muon spin relaxation, employing low energy muons at the LEM spectrometer. Transverse Field (TF) measurements, complemented by ZF and LF experiments, revealed that the muonium (Mu^0) formation, inferred from the missing fraction in the TF depolarization curves, increases with increased O:H ratio corresponding to a larger semiconductor band gap. The temperature dependence of the muonium fraction was well described by a transition-state model, where Mu^0 formation and gradual Mu^+ recovery takes place, accompanied by the formation of a $\text{Mu}^+-\text{O}^{2-}$ complex and a polaron at the Y cation. The activation energy ($E_{A,dia}$) associated with Mu^+ recovery is dependent on lattice relaxation and is lower for thin films of higher H content ($E_{A,dia} = 29-45$ meV). In-situ illumination further reduces this energy barrier for all measured oxyhydrides, suggesting that the photochromic effect involves a reversible structural rearrangement during photodarkening. In the light of our muon spin rotation studies, we discuss several proposals for the identity of the light-absorbing species generated by the electron-hole pairs created upon UV illumination, such as the formation of metallic domains by H^- diffusion, hydroxide formation, color centers, and dihydrogen formation. We complement our discussion with recent findings from in-situ positron annihilation studies on similar films, that suggest that hydrogen vacancies are formed, as well as metallic domains that may play an important role in the mechanism of the photochromic effect.

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