Investigation of open volume in photochromic YH_xO_y thin films by positron annihilation lifetime spectroscopy

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YH_xO_y thin films have attracted considerable interest due to the photochromic effect induced by UV illumination that was discovered in 2011 [1], leading to a large potential for their application in smart windows and sensors. However, only limited information on the microstructure of sputtered YH_xO_y thin films and its relationship to the photochromic effect is yet available. In this study, positron annihilation lifetime spectroscopy is used as a sensitive technique to study the size and concentration of open volume defects in YH_xO_y, YH_2, Y and Y_2O_3 thin films, deposited on fused silica substrates by magnetron sputtering. POSWIN is utilized to decompose the positron lifetime spectra. Three lifetime components are obtained for the metallic Y and YH_2 thin films, while four lifetime components are necessary to accurately describe the lifetime spectra of the semiconducting YH_xO_y and insulating Y_2O_3 thin films. A two-defect trapping model [2] is applied to extract the bulk lifetime and defect concentrations for all thin films. It is found that cation monovacancies are dominant in Y and YH_2 thin films, at a concentration of the order of 10^{-5} per Y atom. In the YH_xO_y and Y_2O_3 thin films, larger vacancy clusters are present and the formation of positronium (Ps) in nanopores is observed. The porosity of YH_xO_y films increases with applied deposition pressure, that in turn leads to a higher oxidation degree of these films. Assuming the nanopores in the YH_xO_y films are spherical in shape, the Tao-Eldrup model [3, 4] applied to the Ps lifetime component τ_4 yields radii between 0.25 and 0.29 nm. This corresponds to vacancy clusters of around 7-10 missing atoms, i.e., of the size of around half a unit cell. Interestingly, vacancy clusters of similar size are indicated by the third lifetime component that we attribute to positron annihilation in such nanopores.

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