XPS and VUV studies of N-doped TiO₂ Sol-Gel Films

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Information about the structural environment of nitrogen anions in TiO₂ host matrices is necessary in order to tailor a glass composition with optimized spectral properties for photocatalytic applications.

The present study is aimed at determining the influence of the N ions on the structural glass environment around Ti cations in amorphous TiO_2 matrices (oxynitride films). For this purpose, thin film samples of $TiO_{2-x}N_x$ compositions, with N concentrations up to x = 0.75 (25 at.%), were prepared by sol-gel processing followed by spin-coating onto Si(100) wafers, glass slides and CaF_2 substrates. The samples were then studied by X-ray photoemission spectroscopy (XPS) and Vacuum ultraviolet (VUV) light scattering, after being annealed up to $500^{\circ}C$. These measurements allowed the determination of the concentrations of the different Ti-O-Ti, N-Ti-O and Ti-N-Ti bonding sequences. XPS data were correlated to thermal behavior and optical properties. Photoabsorption spectra of oxynitride thin films are reported in the energy range 3.9-10.8 eV (320-115 nm). Electronic state assignments have been suggested for each of the observed absorption bands.

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