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Electronic structure of TiO_2 thin films for photoelectrochemical and gas sensing applications studied by XPS and XAS

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Titanium dioxide is one of the best known transition metal oxides of an exceptional importance due to a wide range of applications that include photoelectrochemistry [1] and gas sensing [2]. Determination of the electronic structure of TiO_2 is one of the main aims of the current research as it has the biggest impact on its performance in the practical devices. Thin films of TiO_2 were prepared by reactive sputtering in ultra-high-vacuum system under controlled conditions. Constant substrate temperature of 350°C, constant power density of 10W/cm² and varied oxygen-to-argon flow ratio were applied to deposit a series of films of thickness within the range of 250-300 nm. The XPS analyses were carried out in a PHI VersaProbeII Scanning XPS system using monochromatic Al Kα (1486.6 eV) X-rays focused to a 100 µm spot and scanned over the area of 400 µm x 400 µm. The photoelectron take-off angle was 45° and the pass energy in the analyzer was set to 117.50 eV for survey scans and 46.95 eV to obtain high energy resolution spectra for the C 1s, O 1s and Ti 2p regions. All XPS spectra were charge referenced to the unfunctionalized, saturated carbon (C-C) C 1s peak at 285.0 eV. XAS studies were performed at Ti L_{23} and O K edges of TiO_2 thin films deposited on Si substrates at SOLARIS National Synchrotron Radiation Centre in Kraków, Poland. Surface-sensitive total electron yield (TEY) mode in 440-520 eV range for Ti L_{23} edge and 515-570 eV for O K edge was applied. The results of XPS performed on Ti 2p lines indicate that Ti^{4+} is mostly present at the surface of TiO_2 thin films. Oxygen XPS 1s spectrum confirms that the film is almost free from contamination as the higher energy peak is very small. XAS in TEY mode probes the properties of the near surface region of the thickness comparable to that of the XPS. Therefore, the information concerning surface electronic structure, crystal splitting and band occupancy has been provided by XAS. Correlation between these results and the performance of TiO_2 thin films in photoelectrochemical and gas sensing devices will be discussed.

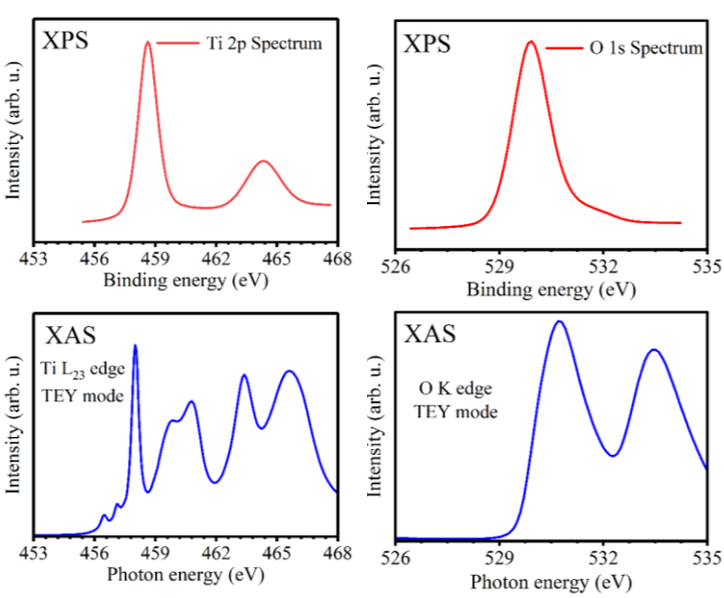

Figure 1. XPS and XAS spectra of TiO_{2-x} thin films deposited at 15% O_2 in the sputtering of Ti target

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References

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