SYNTEHSIS AND PROPERTIES OF TITANIA FILMS CONTAINING ANATASE, RUTILE AND HIGH-PRESSURE TiO_2-II

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The metastable TiO_2-II phase of titania has attracted interest as a material that, compared to more stable anatase and rutile phases, could have advantages in photocatalytic applications because of its narrower band gap as suggested on the basis of some theoretical and experimental studies [1,2]. However, the existing data are too contradictory yet. Differently from the results of Wang et al. [2], our recent experiments demonstrated that, as predicted in theoretical studies, the formation of TiO_2-II in thin films together with rutile caused only minor band gap narrowing (by around 0.06 eV) compared to that of anatase [3]. As the band gap of the mixed anatase and TiO_2-II phases has been predicted to reach significantly smaller values [1], an additional study was performed to find possibilities to deposit this kind of films and characterize the optical properties of those. For this reason, TiO_2 was grown by atomic layer deposition from $TiCl_4$ and O_3 on α-Al_2O_3(0 0 0 1), α-Al_2O_3(0 1 -1 2) and SiO_2 substrates at growth temperatures (T_G) varied from 250 ºC to 450 ºC to obtain thin films with different phase compositions. X-ray diffraction and spectrophotometric measurements were carried out. The results obtained demonstrated that anatase phase grew on SiO_2 at T_G = 250–400 ºC. On α-Al_2O_3(0 1 -1 2), a mixture of anatase and rutile were formed at 250 ºC while at $T_G \geq$ 300 ºC, only rutile was obtained. In contrast, the films grown on α-Al_2O_3(0 0 0 1) at $T_G \geq$ 350 ºC contained high pressure TiO_2-II in addition to anatase and/or rutile. The relative amount of TiO_2-II in the films increased with the decrease in the film thickness and with the increase of T_G to 450 ºC. The studies performed for films grown at $T_G \geq$ 350 ºC on α-Al_2O_3(0 0 0 1) to different thicknesses revealed considerable band gap narrowing together with the formation of the TiO_2-II phase.

References

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