Title: Structural study of nanocrystalline titanium oxide films and their temperature stability

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Abstract:

TiO_2 thin films can exhibit photocatalytic activity and photoinduced superhydrophilicity depending on crystallinity, phase composition and microstructure. These parameters were studied by X-ray diffraction (XRD) and reflectivity (XRR) for magnetron deposited films – nanocrystalline and amorphous, namely their temperature and time evolution. For nanocrystalline films, it was found that higher partial oxygen pressure during the deposition is beneficial. Small anatase crystallites were stable up to about 450 °C. Depth-profiling XRD of some samples revealed that rutile phase was only present close to the substrate. For amorphous films it was found that the crystallization depends strongly on the film thickness and it is slower for very thin films. Evolution of the intensities of anatase diffraction peaks with annealing time could be described by a modified Avrami equation. XRD profile was relatively narrow from the very beginning of crystallization (at about 220 °C), which indicated relatively larger crystallites (> 100 nm), and hence, nanocrystalline films cannot be obtained simply by annealing of amorphous ones. Peak shifts with annealing time indicated generation of a tensile residual stress. These stresses in crystallized films were studied in detail at room temperature. The strain anisotropy in the films was observed and interpreted. Tensile residual stresses formed during the crystallization process increased rapidly with reducing film thickness and inhibited the further crystallization. Additional benefit of the work was the stimulation of further development of the software for total diffraction pattern, namely by inclusion of the effect of elastic anisotropic strain in the films.

Keywords: titanium dioxide, thin film, X-ray diffraction, reflectivity, texture, residual stress, hydrophilicity