Mesoporous TiO_2 Thin Films for Photovoltaic Applications

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Introduction

Thin films of nanocrystalline, mesostructured titanium dioxide are very promising materials to build low cost and efficient photovoltaic devices. TiO_2 present a high chemical stability and electronic properties such as photoinduced electronic transfer properties associated with the anatase phase. [1,2,3]

For many applications, highly porous nanostructured thin films with accessible pores are preferable to dense ones. Indeed, high accessible porosity leads to high surface area increasing the electron transfer area.[1,3,4]

Synthesis process

The synthesis is based on the "Evaporation Induced-Self Assembly" method using titanium isopropoxide as inorganic source, Pluronic F127 copolymer as structuring and porogeneous agent and ethanol as solvent. The films were obtained by dip-coating various substrates in the solution. When the solvent evaporates from the film, the surfactant concentration increases and reaches the critical micellar concentration. Micelles form and organize into an ordered mesostructure. Finally the films are thermally treated to condense the inorganic network and eliminate the surfactant.

Results and discussion

Relative humidity

As displayed in **Fig.1**, TEM analysis shows that a higher relative humidity (RH) leads to a better organization of the mesostructure. For 10% RH during both the dip-coating and after deposition we have obtained a « wormlike » mesostructure, whereas a « gridlike » structure is obtained for 30% RH during the dip-coating and 60% after deposition.

Thermal treatment

The thermal treatment is a critical parameter. It has to cristallize the film in form of active anatase while avoiding the mesostructure collapse. Too high temperatures or too long treatments lead to the mesoporous network destruction (**Fig.2**).

Withdrawal rate

As mentioned in litterature[5,6], a higher withdrawal rate leads to a thicker film. Moreover, RBS measurements show that thicker films are less dense and therefore more porous (**Fig.3**).

Diffusion of conducting glass substrates

As displayed in **Fig.4**, XRD analysis shows a better anatase crystallization for films dip-coated onto a FTO glass substrate than for an ITO one. By elemental analysis on scratched films (**Fig.5**), we can conclude that the ITO conducting layer diffuses into the film whereas FTO does not. The cations diffusion seems to hinder the film crystallization. This observation is mostly described in specific litterature for the Na^+ and Si^{4+} ions.[4,7]

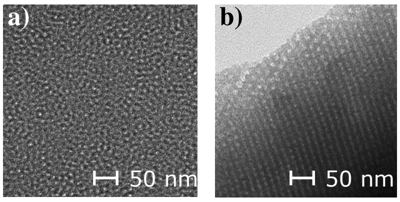

Fig.1: TEM micrographs of films obtained in a) 10% RH ("wormlike"), in b) 30%-60% RH ("gridlike")

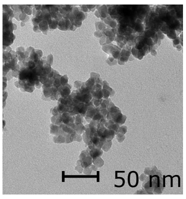

Fig.2: TEM picture of a film collapsed.

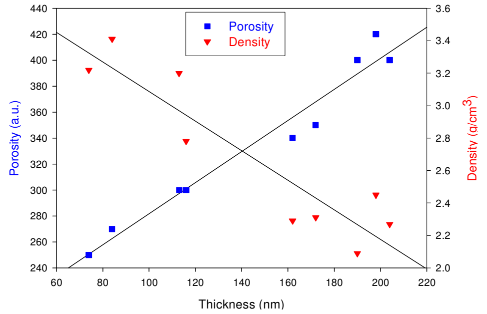

Fig.3: Thickness dependency of the porosity (left) and density (right) determined by RBS

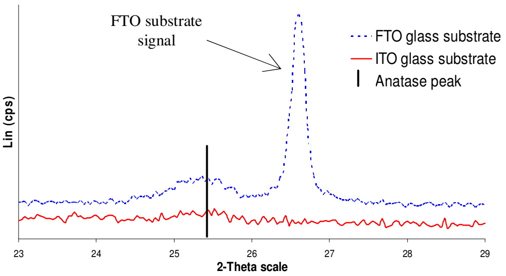

Fig.4: XRD patterns of films dip-coated onto ITO or FTO substrates.

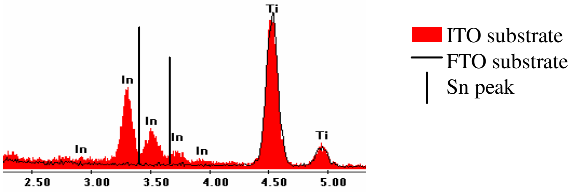

Fig.5: Elemental analysis of films dip-coated onto ITO or FTO substrates.

Conclusions

As showed by TEM and RBS, experimental parameters such as dip-coating and ageing relative humidity and withdrawal speed influence the mesostructure.

Moreover the post-deposition thermal treatment had to be accurately adjusted in order to maximise the crystallisation of the inorganic network while avoiding the collapse of the porous mesostructure.

The conducting oxide layer also influences the the crystallization of the anatase network.

References

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