Mesoporous TiO_2 thin films by soft-templating : How to reach crystallization without mesostructure collapse?

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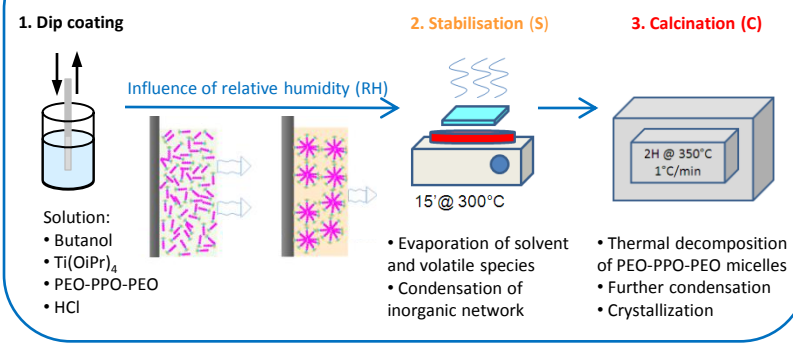
Introduction

Dye Sensitized Solar Cells (DSSC) are attracting a lot of interest as cheap alternatives to the current Si-based technology for photovoltaic conversion. Light is absorbed by dye molecules impregnated on a porous TiO_2 electrode, therefore high surface area is necessary to enhance dye loading.

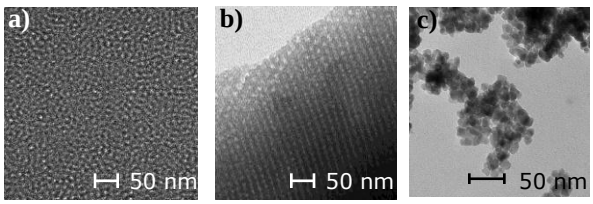
Mesoporous TiO_2 films obtained by surfactant-assisted sol-gel techniques such as Evaporation-Induced Self Assembly (EISA) offer good pore accessibility. However, as-obtained films are amorphous and must be crystallized into the anatase phase to achieve good performances. At the same time, it is necessary to control the crystallite growth to prevent a collapse of the mesostructure. This requires a careful tuning of the heat treatment.

Film preparation



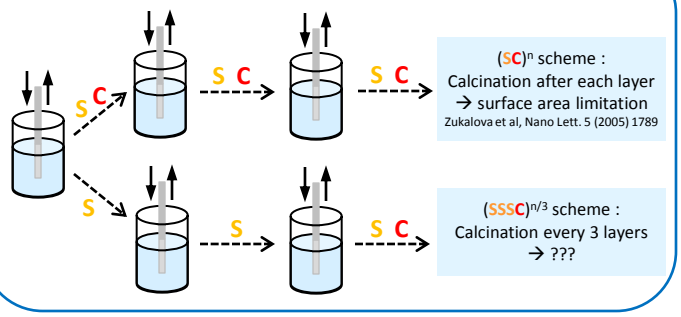
Mesostructures

Higher relative humidity leads to long-range ordered mesoporosity. Too high temperatures or too long treatments result in collapse of mesostructure.



Worm-like (RH 10 %) | Grid-like (RH 30-60 %) | Collapsed (due to over-heating)

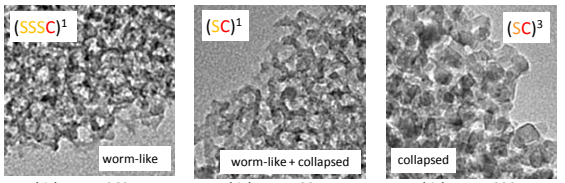
Multilayer deposition



Comparison of $(SC)^n$ and $(SSSC)^{n/3}$ schemes

Single layer films on oxidized silicon substrates were characterized by poroellipsometry, transmission electron microscopy and grazing incidence X-ray diffraction.

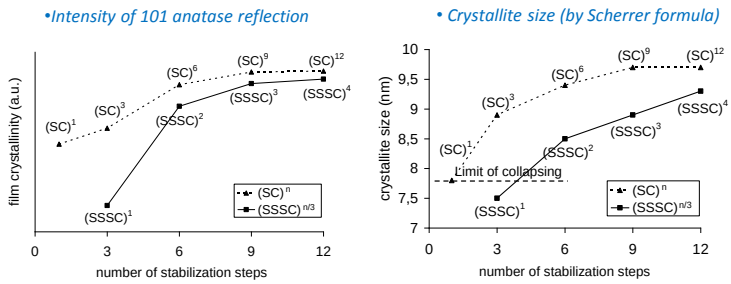
Thickness and mesostructure



Thickness = 362 nm, Surface area =255 m²/cm³ | Thickness = 335 nm, Surface area = 235 m²/cm³ | Thickness = 330 nm, Surface area =190 m²/cm³

It turns out that the worm-like network collapses in all single layer films submitted to more than one calcination treatment.

Crystallization and crystallite size

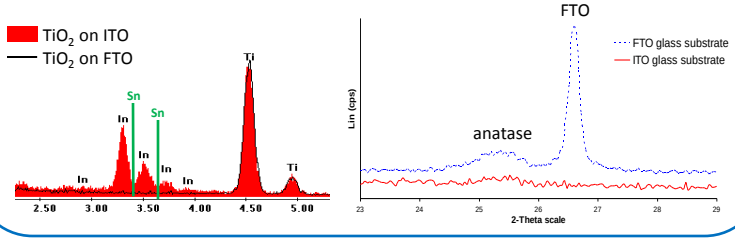


CONCLUSION of comparison $(SSSC)^1$ /$(SC)^1$

→ Less film contraction and larger surface area in $(SSSC)^1$ due to improved condensation of inorganic network at 300°C
→ Lower crystallite size in $(SSSC)^1$ prevents mesostructure collapse
→ Additional stabilisation steps delay crystallization in $(SSSC)^1$

Delayed crystallization due to indium diffusion

Films on indium tin oxide (ITO)-coated glass or fluorine-doped tin oxide (FTO)-coated glass were heated at 350°C for 2 h and characterized by EDX analysis and grazing incidence X-ray diffraction.



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Acknowledgments

- Walloon Region, MINERGIBAT program (PHOTOCEL – 0616464/0616465)
- Belgian Science Policy, Interuniversity Attraction Poles program (INANOMAT - P6/17).