

Porous Nanostructured Titania

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Abstract:

The excellent electrical and mechanical properties of porous nanostructured titania (NST) make it an ideal material for many different applications including dye sensitized solar cells (DSSC). While DSSCs are cheaper to manufacture than silicon-based cells, they are also less efficient. The efficiency of the DSSCs depends on how well the sensitizing dye coats the cell and how well the electron recombination source infiltrates into the porous NST [1]. Consequently, the structure of the NST has a great effect on the efficiency of the cell.

Different processing parameters were studied to determine their effects on pore size and surface area. Overall, it was found that increasing the deposition rate and the thickness of the original titanium film increased the pore size of the NST. Also, it was found that increasing the concentration of the hydrogen peroxide used to oxidize the titanium, increased the pore size of the NST. In general, it was also found that as pore size increased, surface area decreased.

Introduction:

Traditional NST production techniques, such as sol-gel processing, screen-printing, and reactive sputtering, all result in the formation of cracks throughout the NST. These processes also do not allow for *in situ* control over the pore size of the NST. However, we have developed a simple technique that is compatible with current micro-electronic manufacturing practices and produces crack-free NST with a sponge-like structure. It is proposed that control over the porous nature of this NST will allow for better dye sensitization and yield more efficient solar cells.

Procedure:

The process we have developed for producing crack-free, porous NST is relatively simple. First a layer of titanium is evaporated onto a layer of silicon dioxide that is grown either thermally or by plasma enhanced chemical vapor deposition (PECVD) (see Figure 1) [2]. Following the titanium evaporation layer, a sacrificial mask layer of SiO₂ is deposited by PECVD. Then 20 μm

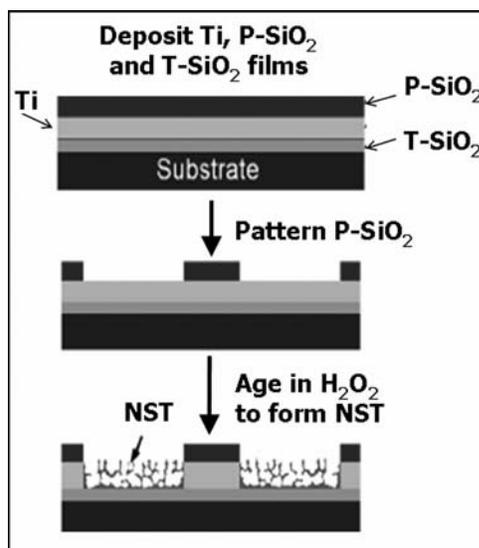


Figure 1: Schematic of NST production process.

pads are etched into an SiO₂ mask. The size of these pads effectively stops cracks from forming in the NST.

The exposed titanium is then oxidized using a hydrogen peroxide solution in order to produce titania. The titania is then annealed at 300°C for 10 hours which produces crystalline porous NST. The average pore sizes of the NST samples can then be found using gas absorption techniques. The effect of the parameters on surface area is also determined from the data.

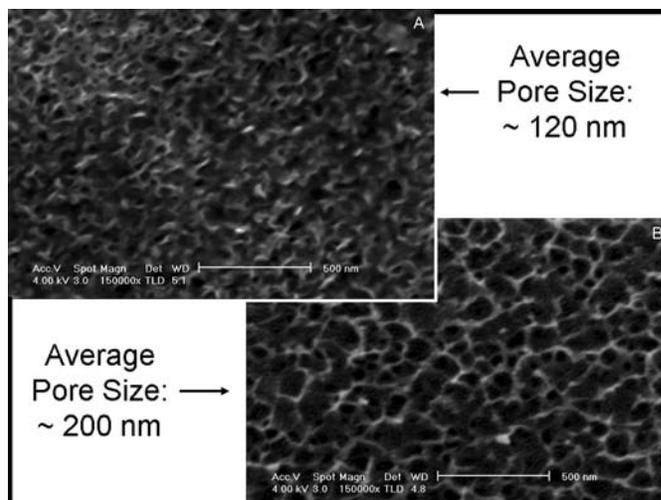


Figure 2: 500 nm thick Ti deposited at A) 2.5 Å/s. B) 4.5 Å/s.

Results and Conclusions:

Overall, the effects of three different process parameters were tested. The first parameter tested was the deposition rate of the titanium layer, which was varied between 0.5 and 4.5 Å/s. It was found that increasing the deposition rate increased the pore size. This can be seen in Figure 2 where the NST deposited at 4.5 Å/s has an average pore size of 200 nm while the NST deposited at 2.5 Å/s has an average pore size of 120 nm. It is proposed that this result is mainly due to fact that titanium films deposited at higher rates have larger average grain sizes.

The second parameter tested was the concentration of the hydrogen peroxide solution used to oxidize the titanium. The concentrations were varied from 5% to 20% and it was found that increasing the hydrogen peroxide concentration increased the average pore size. This can be seen in Figure 3 where the deposition rate is held constant and the concentration is allowed to vary.

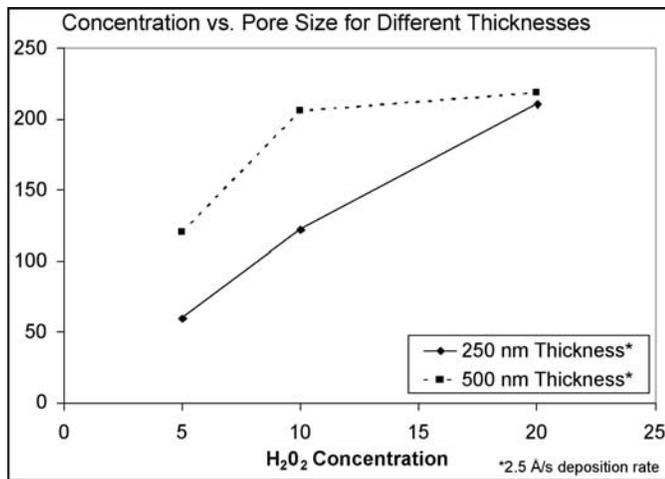


Figure 3: Variations in pore size by H_2O_2 concentration and Ti thickness.

Overall, this result is related to fact that higher hydrogen peroxide concentrations significantly reduce the oxidation time of the titanium because the diffusion of oxygen through the top gel layer formed during the nucleation stage is much faster. Faster diffusion could be one mechanism that produces the larger pores.

Finally, the effect of the thickness of the titanium layer was tested. Overall, it was found that as the thickness increased, the pore size increased as well. This can be seen in Figure 3, where 500 nm thick films generally have larger pores than 250 nm thick films. However, it appears that this result diminishes as the H_2O_2 concentration rises and becomes the dominant factor in pore size determination.

The effects of these three parameters on the surface area of the NST were also tested. Overall, it was found that as the deposition rate increased, the surface area decreased. Also, as the hydrogen peroxide concentration increased, the surface area of the NST decreased. Overall, these results show a clear negative correlation between pore size and surface area. This negative correlation can also be seen when the thickness of the Ti layer is increased. That is, doubling the thickness does not double the surface area because pore size increases reduce the surface area.

Future Work:

In order to implement these new results into actual DSSCs, much more testing must be done. Since the one major component on the effectiveness of such solar cells is dependent on how well the electron recombination source infiltrates into the NST, increasing the pore size is proposed to produce better cells. However, the effectiveness of the cells is also dependent on how much surface area is covered by the electron recombination source. This means that increasing the pore size too much could actually reduce the effectiveness of the cells because the surface area is decreased. Therefore, in the future, tests must be done in order to determine the best combination of pore size and surface area.

References:

- [1] Gratzel, Michael. "Photoelectrochemical Cells." *Nature*. 414, 338-344 (2001).
- [2] Zuruza, A. S., Ward, M. S., MacDonald, N. C., "Fabrication and characterization of patterned micrometer scale interpenetrating Au-TiO₂ network nanocomposites", *Nanotechnology*, 16, 1-6 (2005).

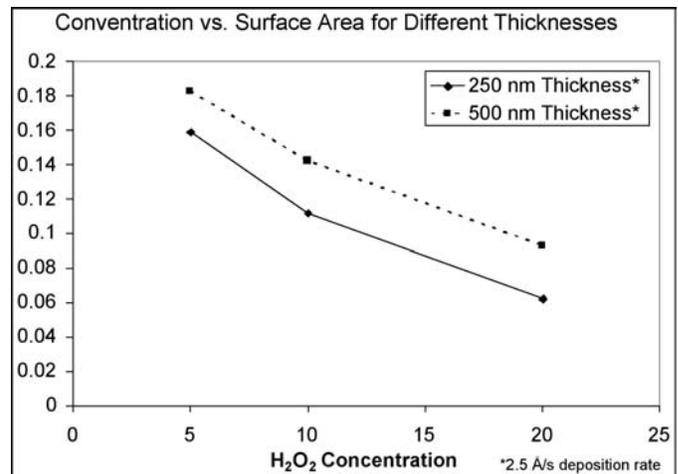


Figure 4: Variations in surface area by H_2O_2 concentration and Ti thickness.