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Nanostructured Nb-Doped TiO_2 Photoanodes for Enhanced Charge Transport in Dye-Sensitized Solar Cells

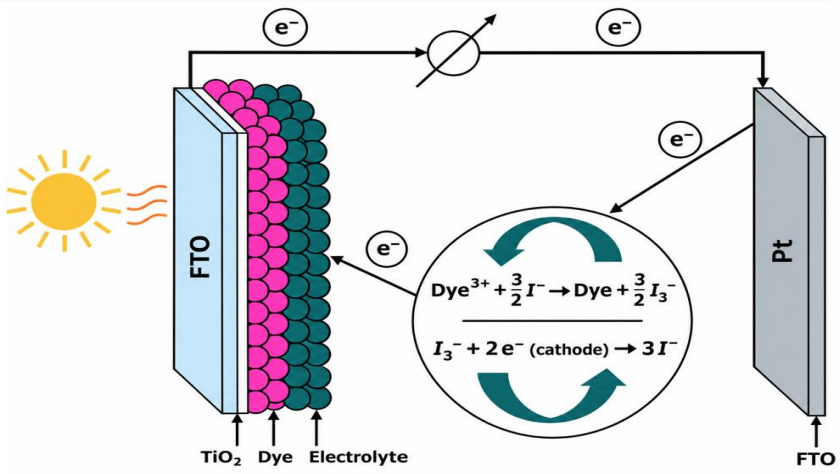
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INTRODUCTION

Dye-sensitized solar cells (DSSCs) combine low cost and simple fabrication [1–3], a dye-sensitized mesoporous TiO_2 photoanode injects and transports photoelectrons to the FTO collector. Efficiency is limited by slow electron transport and by recombination at the TiO_2/dye/electrolyte interface, both set by film morphology, crystallinity and defects. Replacing Ti^{4+} (0.605 Å) by Nb^{5+} (0.64 Å) in anatase supplies a donor electron, increasing conductivity and shifting the flat-band potential [4], but the benefit is not monotonic: reported optima fall at a few at% (e.g., 3 at% in [5]) and over-doping is expected to create defects and recombination centres.

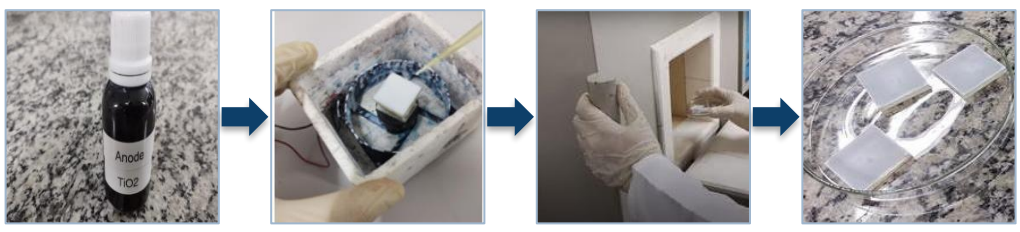
Objective: evaluate how the Nb content (1, 2 and 4 wt%) of spin-coated TiO_2 films on FTO, annealed at 450 °C, affects morphology (AFM), vibrational structure (Raman) and surface chemistry (FTIR), and define what remains to be demonstrated before performance gains can be claimed.



DSSC operation: the photoexcited dye injects e^- into the TiO_2 photoanode (FTO); I^-/I_3^- regenerates the dye and the Pt counter electrode closes the circuit.

RESULTS AND DISCUSSION

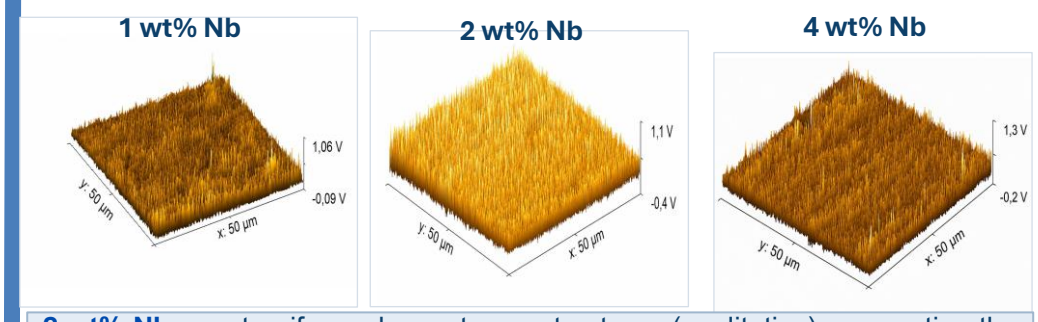
1. Experimental: Photoanode fabrication



Anode solution | Spin-coating deposition | Annealing in a muffle furnace (450 °C) | Finished Nb-doped TiO_2 anodes

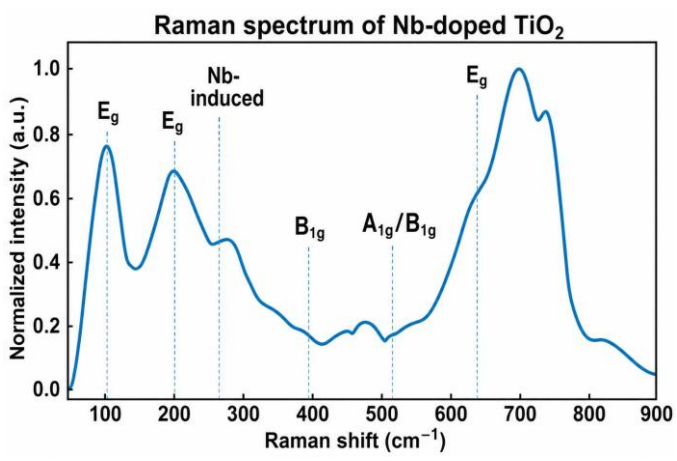
Nb-doped TiO_2 films (1, 2 and 4 wt% Nb) were deposited by spin coating on FTO substrates and thermally treated at 450 °C in a muffle furnace. Characterization: AFM (50 × 50 μm²), Raman and FTIR spectroscopy.

2. AFM surface morphology



2 wt% Nb: most uniform, densest nanostructures (qualitative), suggesting the largest accessible surface for dye loading. Caveat: z-scale is shown as probe signal (V); roughness (Ra/Rq), grain size and dye loading are not yet quantified.

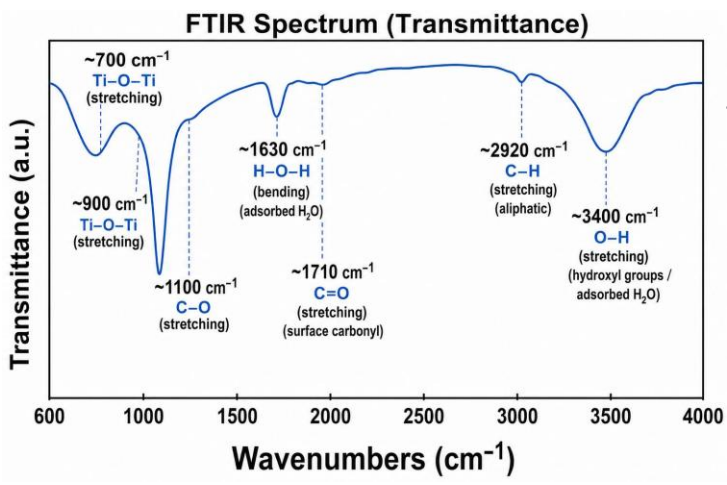
3. Raman spectroscopy



Bands (cm^{-1}, approx.)
103, 200: E_g
~265: Nb-induced
395: B_{1g}
515: A_{1g}/B_{1g}
638: E_g

Anatase reference [6]: E_g 144, E_g 197, B_{1g} 399, A_{1g}/B_{1g} 513, E_g 639 cm^{-1}. The lowest E_g appears at ~103 cm^{-1} and the dominant 700–740 cm^{-1} feature lies in the NbO_6 stretching region [7] (FTO contribution not excluded): phase purity cannot be inferred from Raman alone.

4. FTIR spectroscopy



Oxide network
Ti–O–Ti (~700, ~900)

Hydroxyl / water
O–H (~3400), H–O–H (~1630)

Organic residues
C–O (~1100), C=O (~1710), C–H (~2920)

FTIR confirms a hydroxylated Ti–O–Ti surface, but organic bands persist after annealing at 450 °C and no band was unambiguously assigned to Nb–O: FTIR alone does not demonstrate Nb incorporation.

CHARACTERIZATION SUMMARY AND CRITICAL ASSESSMENT

Technique	Observation	Critical assessment / next step
AFM	2 wt% Nb: most uniform and densest nanostructures (qualitative, 50 × 50 μm^2)	Area gain inferred visually; z-scale in V. Quantify Ra/Rq (nm), grain size and dye loading (desorption).
Raman	Anatase-like E_g, B_{1g}, A_{1g} bands; Nb shoulder (~265 cm^{-1})	XRD/XPS and spectra per Nb level.
FTIR	Ti–O–Ti network; O–H/H_2O; C–O, C=O and C–H signals	Organics persist at 450 °C; no Nb–O band, so doping is not proven. Add XPS (Nb 3d) and TGA.
Photovoltaic test	Not yet measured (η, J_{sc}, V_{oc}, FF, EIS, IPCE)	Morphology–efficiency link remains a hypothesis: test 1, 2 and 4 wt% Nb vs. undoped TiO_2 in complete DSSCs.

CONCLUSIONS

- Among the tested compositions, the 2 wt% Nb film showed the most uniform and densely packed surface features in the qualitative AFM images. Raman and FTIR indicate a Ti–O–Ti oxide network and a feature near 265 cm^{-1} associated with Nb, but do not alone confirm Nb incorporation or phase purity.
- FESEM/EDS and complementary characterizations are in their final stage and will provide further information on film morphology and composition.
- Complete DSSCs will then be evaluated by J–V, EIS and IPCE. Any improvement in charge transport or conversion efficiency remains to be experimentally demonstrated.

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