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sputter-deposited nanocristalline Ta3N5/TaON for the photoelectrolysis of water under sunlight exposition

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Ta_3N_5 is a material under investigation for photo-electrolysis of water. Up to now, a lot of effort has been devoted to synthesize this material by chemical routes, substituting nitrogen to oxygen inside Ta_2O_5 commercial particles by annealing under ammonia. Yellow or green TaON crystals with an ideal bandgap around 2.3eV are produced in the same way by annealing under nitrogen gas. This leads generally to quite large particles and then to a small photo-catalytic activity.
Besides, little work has been done to investigate physical routes, for example vapor deposition processes for this kind of material despite certain advantages regarding the nanoscale roughness and the nano-morphology of deposited films. The reason for that might be the abundantly present δ–TaN phase that forms over wide ranges of nitrogen molar fractions and is a metallic phase without a bandgap. Impeding the formation of these crystallites is thus a first step to prepare the route for sputter-deposited TaON or Ta_3N_5 films.

For this study, films were prepared by various magnetron sputtering, from D.C to reactive high-power impulse magnetron sputtering in an $Ar/N_2/O_2$ gas mixture. The general process is to fully characterize the films: structurally () by grazing incidence X-ray diffraction, optically by photo spectrometry and chemically by elementary analysis and x-ray photoelectron spectroscopy. For sufficiently organized films, electrical properties are tested by conductive atomic force microscopy and photocurrent measurements and then photocatalytic activity are checked under solar equivalent radiation.
DC magnetron sputtering is used in this work, to our knowledge for the first time, to successfully deposit thin films of Ta_3N_5. The focus of this study is placed on the influence of the working gas composition Ar/N2/O2 on the film properties, notably the role of oxygen as a crucial ingredient.

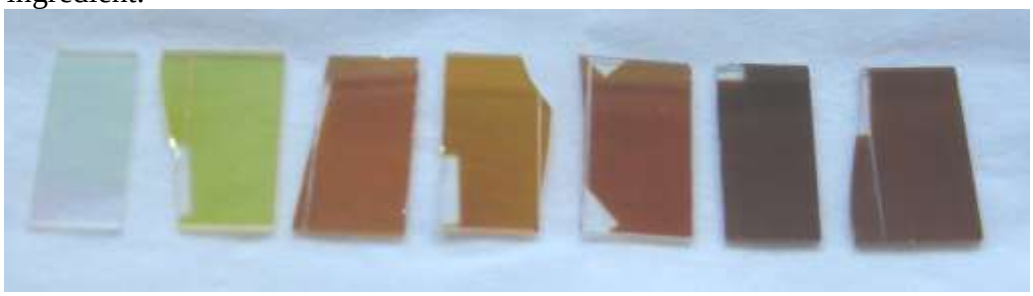

Fig. 1. Aspect evolution of the nanosize films while increasing nitrogen gas ratio in the plasma under a small amount of oxygen for DC magnetron sputtering..

We will show the evolution of the film properties with the synthesis process and in particular the addition of a small amount of oxygen in the reactor for various nitrogen flow-rate.