

Characterization and photoelectrochemical behavior of mono- and co-doped sodium tantalate deposited by a combinatorial approach

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Sodium tantalate (NaTaO₃) has attracted significant attention due to its enhanced photostability and effectiveness in charge separation, which promote the efficiency of photoelectrochemical and photocatalytic systems. Doping NaTaO₃ with metal cations is considered an effective strategy to modify its electronic structure, improve optical absorption and photocatalytic activity [1]. Strontium and vanadium have been proven to be attractive doping elements for such purposes [2].

In this study, we have employed chemical beam vapor deposition (CBVD) to deposit Sr-doped, V-doped and Sr, V-codoped NaTaO₃ thin films *via* a combinatorial approach. CBVD technique relies on several punctual sources to emit, in high vacuum conditions, molecular beams of chemical precursors which thermally decompose on a heated substrate. A great variety of combinatorial configurations is achievable by changing the number and position of the active sources, enabling stoichiometry tuning [3]. X-ray diffraction analysis of the fabricated thin films confirmed the deposition of orthorhombic NaTaO₃ and a crystal lattice expansion upon the successful incorporation of the two dopants. Optical characterization revealed a marked band gap reduction in codoped samples. Finally, the photoelectrochemical properties were assessed by linear sweep voltammetry, photocurrent transients and electrochemical impedance spectroscopy. It was found that single doping with V and especially codoping with Sr and V improved the NaTaO₃ activity.

The combinatorial approach used in this work may promote new strategies in the development of increasingly efficient photocatalysts. CBVD technique can play a primary role in this scenario, allowing a fast screening of dopants and shedding light on the composition-dependent properties of photocatalysts.

[1] Physical Chemistry Chemical Physics, 2014,**16**, 16085-16094

[2] ACS Catalysis 2015, **5**, 3196–3206; Integrated Ferroelectrics, 127:1, 106-115,

[3] Nanomaterials 2022, **12**(6), 1012