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magnetron-sputtered Ta₃N₅ thin films for water photoelectrolysis

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Abstract

Ta₃N₅ has aroused interest in the scientific community as a small-band gap semiconductor able to split H₂O molecules under sunlight illumination (3). Although its band gap of 2.1eV is highly suited (1), its synthesis is difficult. In this work, DC magnetron sputtering is used to successfully deposited thin films of Ta₃N₅ : the influence of the working gas composition Ar/N₂/O₂ on the film properties is studied, notably the role of oxygen as a crucial ingredient for the structure. Previous attempts using magnetrons employed RF sputtering and investigated primarily temperature effects (2,4) .

The films were characterized structurally, optically (transmission/reflection spectrophotometry), electrically, chemically and subjected to photocatalytic measurements in 0.1M K₂SO₄ aqueous solution adjusted to pH=11 by KOH.

We show that variations scale with the O₂ flowrate: from amorphous at high O₂ flowrates, to Ta₃N₅ crystallization at reduced O₂ flowrate. Photo-spectrometry analyzed with a Tauc-Lorentz oscillator model shows that the band gap scales with the oxygen flowrate, from a metallic behavior to a maximum gap of 2.5 eV. Photocurrent measurements corrected by the conductivity in darkness show an insulating character for all films. Nevertheless the photo-conductivity drops by 9 orders of magnitude with increasing O₂ flowrate to reach minimum values around 10⁻⁹S/m..

Keywords: magnetron sputtering; structural properties; optical gap; oxy-nitride; photoelectrolysis

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