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magnetron-sputtered Ta3N5 thin films for water photoelectrolysis

M. Rudolph[1,2], B. Bouchet-Fabre[1] ,-M.-C. Hugon[2] , E. Foy[1], D. Stanescu[1],

J. Alvarez[3], H. Magnan[1], J.-P. Kleider[3], T. Minea[2]

1 NIMBE, CEA/CNRS, Université Paris-Saclay, 91191 Gif-sur-Yvette, France

2 LPGP, Univ. Paris-Sud/CNRS, Université Paris-Saclay, 91405 Orsay, France

3 GeePS, CentraleSupélec, Université Paris-Saclay, 91192 Gif-sur-Yvette, France

*Corresponding author. Tel: (+33) 630734793; Fax: (+33) 169081213; E-mail:bribouchet@gmail.com

Abstract

Ta_3N_5 has aroused interest in the scientific community as a small-band gap semiconductor able to split H_2O 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 $Ar/N_2/O_2$ 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 K_2SO_4 aqueous solution adjusted to ph=11 by KOH.

We show that variations scale with the O_2 flowrate: from amorphous at high O_2 flowrates, to Ta_3N_5 crystallization at reduced O_2 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 O_2 flowrate to reach minimum values around 10^{-9}S/m..

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

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