Surface Analysis of the Evolution of Oxynitride Thin Films During Photoelectrochemical Water Splitting

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# Keywords

Oxynitride - Thin Films - Water Splitting - Surface - Low Energy Ion Scattering - Secondary Ion Mass Spectroscopy

# Introduction

Solar Water Splitting has been extensively studied during the last years as an effective approach to generate hydrogen as a renewable energy resource replacing fossil fuels. In this process, a semiconductor material, known as photocatalyst, is used to convert solar energy into chemical energy by splitting water into oxygen and hydrogen. Upon light illumination, an electron is excited to the conduction band (CB) of the semiconductor where it is injected to the electrolyte resulting in water reduction. The produced hole in the valence band (VB) contributes in the water oxidation reaction evolving oxygen.

For an efficient water splitting the semiconductor must be stable, have a band gap in the visible light range and band edges that are well-aligned with the redox potentials of water. To date, none of the investigated materials has shown to be an efficient photocatalyst for water splitting. For instance, oxides with high stability and well positioned band edges show limited performance due to their large band gaps which utilizes a small percent of the solar spectrum. WO3 and Fe2O3 are exceptional oxides with band gap in the visible light range, however their conduction bands are lower than the water reduction potential. Thus, they can’t be used for overall water splitting to produce stoichiometric amounts of oxygen and hydrogen simultaneously and they must be coupled to other semiconductors that are active for water reduction.(2,3 of thin film paper).

The partial substitution of O in oxides by N results in a reduction in the band gap due to the hybridization of the O 2p and N 2p orbitals shifting upward the valence band maximum. (ref.) Additionally, the conduction band minimum can be altered with the N substitution because of the change in anion electronegativity and/or lattice distortion.(markus paper) The resulting oxynitride material has, hence, a bandgap in the visible light range. For this purpose, different oxynitride materials have been investigated for water splitting such as the TaON and the perovskite oxynitrides (LaTiO2N, BaTaO2N, SrTaO2N, LaTaON2 and CaNbO2N).

For photoelectrochemical (PEC) water splitting, the photocatalyst material is deposited on a conducting substrate and used as a photoanode in a three-electrode system. In most of the previous reports, particulate photoanodes are typically used which are prepared by electrophoretic deposition of the oxynitride particles.(ref.) Another approach for fabricating the oxynitride photoanodes is through thin film deposition.(ref.) Recently, we have shown that thin films with their well-defined surfaces and good crystalline quality are ideal for surface studies to investigate fundamental properties of the oxynitride materials.

In this work, the surface and composition of CaNbOxNy and LaTiOxNy thin films is studied by low energy ion scattering (LEIS) and secondary ion mass spectrometry (SIMS). Additionally, the evolution of the surface during the PEC water splitting measurement for the two oxynitride thin films is investigated. The results show that …

# Materials and Methods

## Thin Film Preparation

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# Results

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# Discussion

This should explore the significance of the results of the work, not repeat them. Avoid extensive citations and discussion of published literature. A combined Results and Discussion section is often appropriate. The Results and Discussion should deals with the interpretation of the results in the light of previously published findings.

# Acknowledgements

Collate acknowledgements in a separate section at the end of the article before the references. List here those individuals who provided help during the research (e.g., providing language help, writing assistance or proof reading the article, etc.).