High-Throughput Optimization of Mo-Doped $BiVO_4$ Thin Films Using SPECM for Enhanced Photoelectrochemical Performance

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Significance and Relevance

This study presents the successful optimization of molybdenum-doped BiVO4 thin films, achieving a significant enhancement in photocurrent density for water splitting applications. Using a combinatorial sputtering method, we identified optimal doping levels and conditions that reduce electron-hole recombination, extend light absorption, and improve structural stability. These results provide a scalable approach to developing efficient and durable photoanodes for solar-driven hydrogen production.

Preferred choice for the topic: Photocatalysis and photoelectrocatalytic approaches, solar energy utilization

2nd choice for the topic: H2 storage and transportation, green H2 production, hydrogen vectors

Preferred presentation: Poster

Introduction and Motivations

$BiVO_4$ is a promising material for photoelectrochemical (PEC) water splitting due to its suitable bandgap and stability. However, its performance is limited by high electron-hole recombination and low charge mobility.[1] Molybdenum (Mo) doping addresses these issues by modifying the band structure, improving light absorption, and enhancing charge transport.[2] This study explores the synthesis, optimization, and PEC performance of Mo-doped $BiVO_4$ thin films using combinatorial sputtering.

Materials and Methods

Mo-doped $BiVO_4$ thin films were fabricated using RF magnetron sputtering with a combinatorial approach to create a gradient of Mo doping concentrations across the samples. The films were deposited on FTO-coated glass substrates under controlled conditions. Two sputtering targets were used: a pure $BiVO_4$ target and a 10 at.% Mo-doped $BiVO_4$ target. During the deposition, the RF power for the pure $BiVO_4$ target was fixed at 200 W, while the RF power for the 10 at.% Mo-doped $BiVO_4$ target was varied between 0 W and 200 W to produce a series of samples with varying Mo doping concentrations. This combinatorial sputtering method generated thin film libraries with doping gradients. To evaluate the photoelectrochemical (PEC) properties, Scanning Photoelectrochemical Microscopy (SPECM) was employed, enabling high-throughput analysis of local photocurrent responses across the doping gradient. Structural and optical characterizations were performed using SEM, XRD, and UV-Vis spectroscopy to correlate the film properties with their PEC performance.

Results and Discussion

The SPECM analysis of the combinatorial thin film libraries enabled the rapid identification of the optimal Mo doping concentration. At an RF power of 100 W for the Mo-doped target, the photocurrent density reached a maximum of 0.8–1.0 mA/cm^2 at 1.23 V vs. RHE. This corresponded to an optimal doping level of 2–3 at.%. The localized PEC measurements revealed significant suppression of electron-hole recombination and enhanced charge carrier mobility in the optimally doped regions. XRD patterns showed the formation of well-defined crystalline structures with reduced defect densities, while UV-Vis spectroscopy indicated an extended light absorption range due to bandgap narrowing. SEM mapping confirmed uniform distribution of Mo within the optimized thin films. Figure 1 highlights the relationship between RF power and photocurrent density, demonstrating the efficiency of the SPECM-driven optimization process.

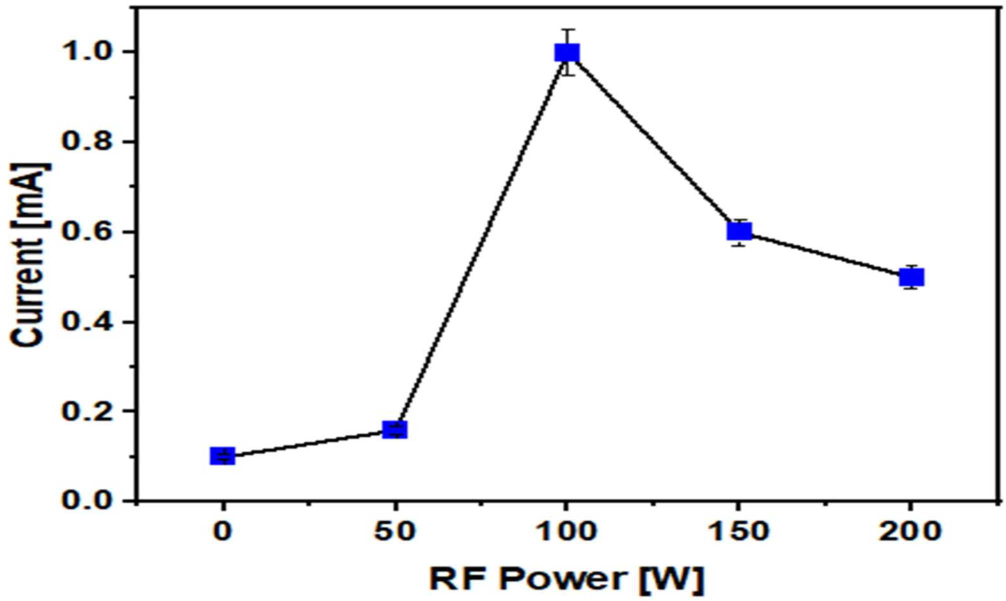

Figure 1. Relationship between RF power for Mo-doped $BiVO_4$ target and photocurrent density measured by SPECM at 1.23 V vs. RHE

References

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