Strain engineering of epitaxial perovskite-based heterostructures for efficient photoelectrochemical water splitting

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Photocatalysis, harnessing sunlight, is crucial for addressing energy generation and environmental pollution. Perovskites are extensively studied as potential photocatalysts, particularly, for water splitting reaction. Strategies for enhancing the photoelectrochemical (PEC) activity of complex oxide materials involve adjusting their intrinsic structural, topographical, and stoichiometric properties. Here, we focus on the fabrication of perovskite thin films using Pulsed Laser Deposition (PLD) and evaluate their PEC performance in terms of film thickness, deposition pressure and heterostructure's arhitecture. We examine the influence of the structural parameters with film thickness and oxygen content in epitaxial LaFeO3 (LFO) thin films, noting the formation of self-assembled nanodomains for films thicker than 14 nm due to strain induced by differences in lattice constants between the material and the substrate. The multilayer configuration based on LFO/BFO/STON and BFO/LFO/STON exhibits a strong dependence on the interface/surface properties of the film. By utilizing Nb:SrTiO3 as a conductive substrate and 0.5 M NaOH aqueous solution for PEC measurements, we analyze the relationship between photocurrent density, onset potential, and the structural, topographical, and optical characteristics of complex oxide-based photoelectrodes using X-ray diffraction, high-resolution transmission electron microscopy, and ellipsometry. The catalytic activity under dark condition is evidenced Potentiodynamic PEC analysis reveals the highest photocurrent density values (up to 1.2 mA/cm2) and excellent stability over time for the thinnest LFO/Nb:SrTiO3 sample prepared at 0.6 mbar O2, showing both cathodic and anodic behavior. Further enhancement in photocurrent density is expected through the use of a multilayer photoelectrode incorporating LFO and BFO materials. Importantly, perovskite-based thin films exhibit efficient hydrogen evolution from water, confirmed by gas chromatography under constant illumination. The enhancement of photocurrent density can be achieved through the utilization of a multilayer photoelectrode incorporating LFO and BFO materials. The objective of this investigation was to merge the robust ferroelectricity of BFO with the excellent absorption properties and high chemical stability of LFO, thereby creating novel photocatalysts with improved activity in photocatalytic reactions.

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