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A Silicon Photocathode Protected with Epitaxially Grown SrTiO3 for Photoelectrochemical Water Splitting Application

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Silicon (Si) has been considered as one of the most promising materials for photoelectrochemical (PEC) devices due to its low cost, established manufacturing process, and high theoretical photovoltage and saturation current density. However, developing Si-based PEC devices has been challenging, primarily because of silicon highly susceptibility to (photo)corrosion under PEC conditions. To address this, a protective layer is necessary to both prevent corrosion and maintain efficient charge transfer within the photoelectrode. In this study, we prepared high-quality SrTiO3 (STO) thin films on p-Si substrates with reduced graphene oxide (rGO) as an interfacial layer. The STO thin film (~ 10 nm) was deposited using pulsed laser deposition (PLD) on both rGO-buffered and bare Si substrates to explore the effects of epitaxy i.e. crystallinity and interfacial properties on PEC performance. The results showed that the STO layer epitaxially grown on rGO-buffered Si exhibited lower onset potential compared to non-epitaxial counterparts. From linear sweep voltammetry (LSV) and chronoamperometry measurements, we concluded that the epitaxially protected photocathode had significantly improved performance compared to the non-epitaxial sample, thus highlighting the importance of a well-defined interfaces. The smooth surface of high-quality epitaxial STO layer with sub-nano roughness played a crucial role in protecting the underlaying p-Si substrate from corrosion, whereas the presence of pinholes in the non-epitaxial sample resulted in degradation rate similar to that of bare Si substrate without any protection. This study presents a novel approach for preparing a protective layer over the photoelectrode substrate ensuring both high efficiency and long-term stability in PEC devices.

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