Heteroepitaxial growth of $ZnTiN_2$ photoabsorbers on GaN for photoelectrochemical CO_2 reduction applications

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Photoelectrochemical (PEC) devices can generate sustainable liquid fuels from carbon dioxide and water using sunlight as a renewable energy source. Such devices must withstand degradation in the harsh electrochemical environments necessary for PEC CO_2 reduction while maintaining high photocatalytic performance. As such, a co-design approach was used to identify a novel photoabsorber system based on zinc titanium nitride, $ZnTiN_2$, which was theorized to have a crystal structure compatible with established semiconductor device processing as well as a mechanism for self-passivation under electrochemical conditions through the formation of stable surface oxides.

Our recent work demonstrating the synthesis of wurtzite-structured $ZnTiN_2$ has shown preliminary results that indicate the optoelectronic properties and chemical stability mechanisms of this novel nitride semiconductor are highly suitable for photoelectrochemical CO_2 reduction applications [1]. However, to fully realize this photoabsorber material in functional photoelectrochemical devices, efforts must now focus on optimizing material quality and successfully integrating it with other devices layers.

In this work, we report improvements made to the crystallinity and optoelectronic properties of $ZnTiN_2$ thin films through heteroepitaxial growth and optimization of growth parameters in radiofrequency co-sputtering deposition. X-ray diffraction and electron microscopy are used to monitor the crystallinity, epitaxial alignment to the substrate and film microstructure. Hall effect, spectroscopic ellipsometry, and transient absorption measurements are used to evaluate the electrical, optical, and optoelectronic properties of the films. The combination of these characterization techniques, along with high-throughput combinatorial synthesis, are used throughout the process to assess and guide the optimization of the $ZnTiN_2$ thin films.

References

[1] A. L. Greenaway *et al.* Zinc Titanium Nitride Semiconductor toward Durable Photoelectrochemical Applications. J. Am. Chem. Soc. 2022;144(30);13673–13687.