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# Multilayer titanium-based thin films for photocatalytic dye degradation

A titanium-based multilayer thin-film system fabricated via magnetron sputtering represents a highly promising architecture for visible-light-driven photocatalytic applications. In this heterostructured design, each constituent layer is deliberately engineered to perform a distinct yet synergistic role in enhancing light absorption, charge transport, and surface redox reactions. The multilayer consists of a TiN base layer, an intermediate Ag layer, and a top TiON layer, collectively forming a functional TiN/Ag/TiON [1,2] architecture optimized for efficient photocatalytic activity under solar irradiation.

The TiN base layer, with a thickness of approximately 100 nm, serves as a highly conductive electron migration and collection layer. Owing to its metallic or semi-metallic nature, TiN facilitates rapid electron transport and acts as an electron sink, effectively suppressing charge carrier recombination within the photocatalytic system. Additionally, TiN provides mechanical stability and promotes improved interfacial adhesion for the subsequent layers, thereby enhancing the overall structural integrity of the multilayer film.

A thin silver (Ag) interlayer, typically in the range of 5–10 nm, is introduced between the TiN and TiON layers to further improve charge separation and optical performance. Silver plays a crucial role as a plasmonic and charge-mediating layer, where localized surface plasmon resonance (LSPR) effects can enhance visible-light absorption and local electromagnetic fields at the interface. Moreover, Ag acts as an efficient electron bridge, promoting directional charge transfer from the photoactive TiON layer toward the TiN base, while also serving as a recombination barrier that prolongs charge carrier lifetimes.

The top TiON layer, with a thickness of approximately 50 nm, functions as the primary photoactive component of the multilayer system. Titanium oxynitride exhibits a tunable and narrowed bandgap in the range of ˜2.0–3.5 eV, depending on oxygen and nitrogen content, making it highly responsive to visible light. Upon illumination, the TiON layer efficiently absorbs photons and generates electron–hole pairs. Its mixed anionic composition provides abundant surface defect states and active sites that are favorable for photocatalytic redox reactions, particularly at the solid–liquid interface.

A type-II band alignment at the TiN/Ag/TiON interfaces plays a critical role in facilitating effective charge separation. This alignment enables photogenerated electrons to migrate from the TiON conduction band toward the Ag interlayer and subsequently into the TiN layer, while holes remain in the TiON valence band. Such spatial separation of charge carriers is driven by favorable band offsets, interfacial electric fields, and the formation of Schottky or quasi-Schottky junctions at the metal–semiconductor interfaces. These effects collectively minimize electron–hole recombination losses and enhance the availability of long-lived charge carriers for surface reactions.

The optimized thicknesses of the individual layers are crucial for maximizing photocatalytic efficiency. The relatively thick TiN layer ensures efficient electron transport and surface reaction kinetics, while the thin Ag layer balances plasmonic enhancement and charge transfer without excessive optical shielding. The TiON top layer thickness is carefully chosen to provide sufficient light absorption while maintaining efficient charge extraction at the interfaces. Together, these parameters enable enhanced generation of reactive oxygen species (ROS), such as superoxide radicals ($O_2$•$^-$) and hydroxyl radicals (•OH), which are essential for organic pollutant degradation, antimicrobial activity, and water-splitting reactions.

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References:

[1] Lawley, C., Nachtegaal, M., Stahn, J., Roddatis, V., Döbeli, M., Schmidt, T. J., ... & Lippert, T. (2020). Examining the surface evolution of LaTiOxNy an oxynitride solar water splitting photocatalyst. Nature communications, 11(1), 1728.

[2] Kim, D. (2010). The structural and optoelectrical properties of TiON/Au/TiON multilayer films. Materials letters, 64(6), 668-670.

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