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Structure optimization of Ta-O-N films prepared by reactive HiPIMS for more effective water splitting

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The TaON material is a promising candidate for application as a visible-light-driven photocatalyst splitting water into H_2 and O_2 and thus converting solar energy into chemical energy. The photo-generated electron-hole pairs act here as the active water splitting species. In order to work as a water splitting photocatalyst, the material must satisfy certain conditions: (i) band gap of proper width (preferably corresponding to visible light absorption) and (ii) suitable alignment of the band gap with respect to the water splitting redox potentials. The subsequent transport of the charge carriers through the material (particularly across the films thickness) plays an important role in the effectivity of the process.
In this work we first demonstrate that using reactive high-power impulse magnetron sputtering (HiPIMS) as the deposition technique followed by post-annealing of the deposited film at 900°C in a vacuum furnace, allows us to prepare a polycrystalline (non-textured) film exhibiting a pure TaON phase. Such film satisfies the above mentioned conditions for a water splitting photocatalyst (band gap of ~2.6 eV). In addition, the film exhibits a lower electrical resistivity as compared to the amorphous as-deposited film, allowing easier transport of the charge carriers in the film. As the monoclinic TaON phase exhibits anisotropic charge carrier conductivity, tailoring the texture of the film can further improve the charge carrier transport in a desired direction. In this work, we therefore also investigate the possibilities of the following approaches: deposition at elevated substrate temperatures (up to 850°C), deposition at high power densities in a pulse (up to 4 kW/cm^2) and/or deposition onto suitable substrates providing proper seeding layers (e.g., Pt, Ta, ZrO_2) to prepare textured TaON film allowing enhanced charge carrier mobility across the film thickness.

Keywords
Reactive HiPIMS
TaON
Water splitting