Dynamic Photocatalytic Strain Development in a Single Gold Nanoparticle Embedded in Au/TiO_2 Heterostructures

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Photocatalysis is a promising technique for harvesting solar energy efficiently and has the potential to address the global energy crisis [1]. However, the structure–activity relationships of photocatalysts during wavelength-dependent photocatalytic reactions remain largely unexplored because they are difficult to evaluate under the actual operating conditions. In this study, we investigated, for the first time, the photocatalytic strain evolution of a single Au nanoparticle (AuNP) supported on a TiO_2 film by conducting three-dimensional Bragg coherent X-ray diffraction imaging under an external light source (Figures 1 and 2) [2-4]. The findings reveal that wavelength-dependent generation of reactive oxygen species (ROS) significantly affects the structural deformation of the single AuNP on the TiO_2 support, leading to its strain evolution. Density functional theory calculations rationalize the strain induced by the adsorption of the generation ROS on the AuNP surface. These observations provide valuable insights into the impact of photocatalytic activity on the structural deformation of AuNPs, contributing to a general understanding of the catalytic adsorption process at the atomic level.

References

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Figures

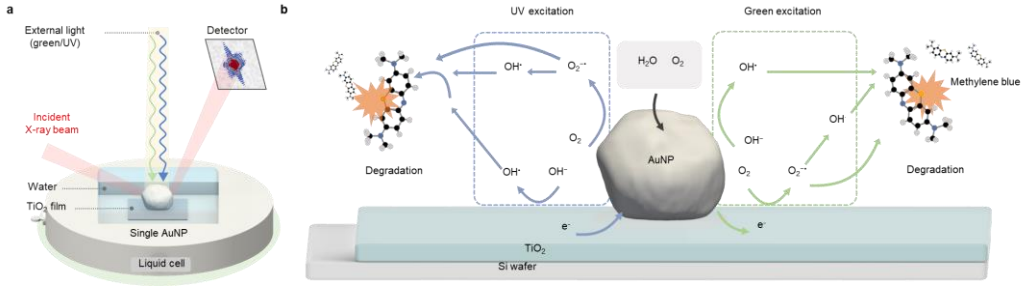

Figure 1: Schematic illustration of the in-situ photocatalytic BCDI experiment. (a) Au/TiO_2 heterostructure was placed in the in-situ BCDI liquid cell and the excitation wavelength was controlled using a xenon lamp. This setup allowed us to systematically irradiate the green (532 nm), UV (365 nm), and green/UV (532 nm and 365 nm) to the Au/TiO_2 heterostructure during BCDI measurements. The incident focused X-ray beam interacts with the single AuNP inside the reaction liquid cell. Diffraction patterns from the single AuNP were collected at the off-specular (111) Bragg angles. (b) Schematic illustration of the photocatalytic degradation mechanism of MB by Au/TiO_2 heterostructure under green and UV light irradiation.

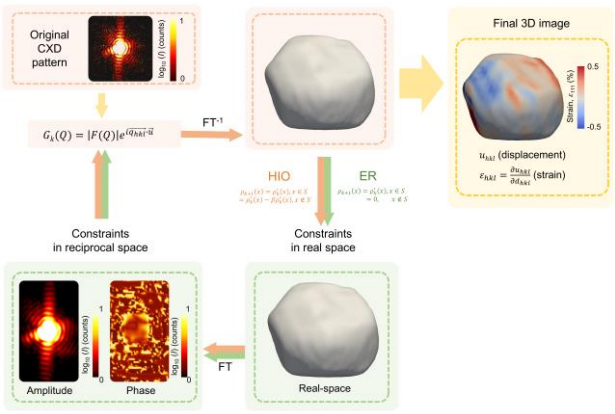

Figure 2 Schematic diagram of phase retrieval algorithm combined with Error reduction (ER) and Hybrid input-output (HIO) using coherent diffraction pattern.