High-pressure torsion of TiO₂-ZnO composites: phase transformations, vacancy formation and changes in optical and photocatalytic properties

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 TiO_2 and ZnO are two semiconductors with promising optical properties, considered as potential candidates for solar and photocatalytic applications. Although chemical methods have been primarily used to enhance the optical properties of these oxides, the current authors recently reported enhanced photocatalytic activity of pure TiO_2 and ZnO by plastic straining due to the formation of high-pressure phases and oxygen vacancies.

In this study, to improve the optical properties further, large fractions of ZnO/TiO₂ interphase boundaries are also introduced by the application of high-pressure torsion (HPT) straining to a mixture of anatase-TiO₂ and wurtzite-ZnO powders. It was found that the concentration of oxygen vacancies and the fraction of nanograined high-pressure TiO₂-II and rocksalt-ZnO phases increase with increasing plastic strain. Moreover, due to the plastic strain effect, the rutile-TiO₂ phase is formed at room temperature, which is at least 600 K below the reported anatase-to-rutile transition temperature. These structural features, together with the formation of large fraction of interphase boundaries, lead to electron spin resonance, optical bandgap narrowing, diminishing of the band-to-band photoluminescence and thus, enhancement of photocatalytic hydrogen production. Despite improvements in the photocatalytic activity of TiO₂-ZnO composites after large straining, photocatalytic activity becomes poor by processing at ultra-large strains due to the significant reduction in crystallinity.