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# Structure determination of TiO 2 crystal surfaces using total-reflection high-energy positron diffraction (TRHEPD)

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Single-crystal TiO 2 surfaces have been studied extensively as a testing ground for metal-,molecule-, and nanoparticle adsorptions [1, 2], providing opportunities to understand thecatalytic reactions on an atomic level. Knowledge on their topmost- and subsurface structures,where catalytic processes occur, is critical factor in the understanding of the fundamentals andthe reaction mechanisms of solid catalysts.

We investigated the structures of a rutile-$TiO_2$ (110) (1×2) [3] and of an anatase-$TiO_2$(001) (1×4) surfaces by means of a newly developed total-reflection high-energy positron diffraction (TRHEPD) apparatus [4, 5] at Slow Positron Facility, KEK, Japan. TRHEPD [6], the positron counterpart of reflection high-energy electron diffraction (RHEED), provides an exceedingly surface-sensitive tool for the structural determination [7]. The rutile-$TiO_2$ (110) (1×2) surface was as yet undetermined and widely discussed over the past 30 years. Our TRHEPD analysis [3] showed that the outermost atomic arrangement is explained by relaxing a basic structure of $Ti_2O_3$ composition [8] into an asymmetric configuration. This conclusion agreed well with a recent theoretical model [9] determined by a global optimization varying both composition and arrangement of the surface.

Successful formation of a single-crystal, vacancy-less anatase-$TiO_2$ (001)-(1×4) surface on a $SrTiO_3$ (001) crystal substrate was recently reported [10]. Several models have been proposed for this structure [2], based on surface-science techniques and/or theoretical calculations, but the rigorous atomic arrangement is yet to be settled. We report that the result of the TRHEPD experiment best matches that of the structural calculation assuming the “Ad-molecule model” [11] with some modifications of the atomic positions.

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