Structure of thin film TiO_2 grown by magnetron sputtering analyzed by ion, electron, and X-ray scattering

K. A. Janik[1], B. Seger [2], M. B. Sillassen[3], C. D. Damsgaard [1,2], I. Chorkendorff [2],
J. B. Wagner [1]

[1] *Center for Electron Nanoscopy, Technical University of Denmark, 2800 Kongens Lyngby, Denmark*
[2] *Department of Physics, Technical University of Denmark, 2800 Kongens Lyngby, Denmark*
[3] *Interdisciplinary Nanoscience Center and the Department of Physics, Aarhus University, 8000 Aarhus, Denmark*

Titanium dioxide (TiO_2) receives a lot of attention in the context of hydrogen production by photocatalytic water splitting, where TiO_2 can be used as a layer protecting silicon photocathodes. For this application, the TiO_2 material is synthesized by the physical vapor deposition (PVD) in form of thin films. The overall structural quality of the TiO_2 films, and thereby their properties, depends on the PVD processing conditions. Hence, our study focuses on getting a clear insight into films' structure by comprehensive description of compositional, morphological, and crystallographic aspects of such deposits. A set of techniques that employ ion, electron and X-ray scattering is used for this purpose.

This work presents an example of structural characterization of a TiO_x deposit grown on Si <001> by reactive DC magnetron sputtering from a metal titanium (Ti) target in an Ar/O_2 gas mixture. Rutherford backscattering spectrometry (RBS) indicates that the TiO_x film is close to the stoichiometric compound, i.e. TiO_2. X-ray diffraction performed in the symmetric (θ-2θ) and asymmetric (ω-2θ) scans shows that the film is polycrystalline and composed of two crystallographic phases, i.e. rutile and anatase. As revealed by scanning electron microscopy (SEM), the deposit is characterized by columnar grains. The crystallinity and morphology of the deposit is further studied by electron diffraction (ED) and transmission electron microscopy (TEM). TEM and ED measurements are performed on thin focused ion beam (FIB) milled lamellas prepared in the direction parallel and perpendicular to the direction of the TiO_2 film growth.

Keywords: titanium dioxide, Rutherford backscattering, electron diffraction, X-ray diffraction, grazing incidence X-ray diffraction