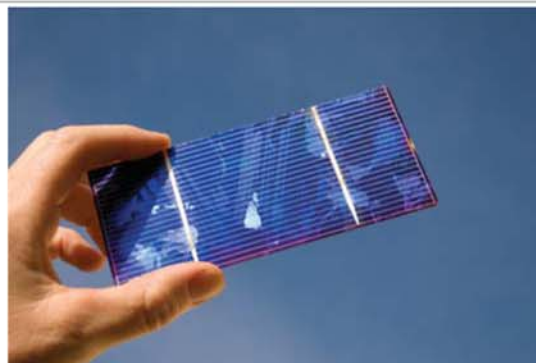


INSIDE THE STRUCTURE OF DYE-SENSITIZED SOLAR CELLS

TiO₂ nanoparticles have been utilized in a multitude of applications, photocatalysis, dye-sensitized solar cells, gas sensors, hydrogen storage etc

Dye-sensitized solar cells (DSSCs) belong to the family of thin film solar cells and are an attractive and a considerably cheaper way of producing electricity. DSSCs are designed like a traditional alkaline battery and do not require a tricky manufacturing process. They are produced by a porous titanium dioxide nano particles layer. This layer is covered with a molecular dye that can absorb sunlight, and is submerged in an electrolyte solution with a platinum-based catalyst



Dye-Sensitized Solar Cell

The challenge: nanocrystalline domains in structurally disordered wires; low X-Ray pattern quality

Solution: Automated 3D Diffraction tomography & Precession Electron Diffraction

above it. When sunlight passes through the cell and reaches the dye layer, it activates electrons, which then enter the titanium dioxide layer.

Then these electrons flow towards the transparent electrode and get collected in order to power a load. The electrons flow through the external circuit and then re-enter the cell on a metal electrode to flow into the electrolyte, which then transports them back to the dye molecules.

In order to obtain highly efficient DSSCs two counteracting requirements have to be met. First a large number of dye/ semiconductor interfaces are needed to ensure a high photocurrent (i.e. high surface area), and at the same time a high transport rate of electrons towards the front electrode is essential. By using TiO₂ nanorods as an additive to the commonly used nanoparticulate TiO₂ semiconductor, these demands can be met.

Sodium titanate nanorods represent an important intermediate product in the synthesis of TiO₂ nanorods. Despite the importance of sodium titanate nanorods as a precursor for long TiO₂ nanorods, little effort has been made to investigate the crystal structure of these nanostructures. X-ray powder diffraction crystallography failed to

resolve the structure of such nanorods due to the often low-quality of data, which renders a real phase determination very difficult.

The structure of NaTi₃O₆(OH)₂H₂O nanorods was determined using electron diffraction data collected by 3D diffraction tomography. Electron diffraction tomography is able to deliver in an automated way rich and quasi-kinematical electron diffraction data sets from single nanocrystals.

3D diffraction tomography data sets were collected from six different rods with different rate of disorder. The structure determination was performed on the basis of the more ordered data set. C2/m was chosen as the correct space group and the corresponding solution was used for further refinement. All maxima

in the electron density distribution of the obtained structure model are located on a mirror plane (y = 0.0 or 0.5). The three strongest maxima detected in the centres of the octahedra were assigned to the Ti atoms. The remaining weaker maxima were assigned to O, Na and water molecules of crystallization. The final structure consists of groups of corrugated layers of corner- and edge-sharing (TiO₆) octahedra arranged parallel to the (001) plane.

Crystal Structure

NaTi₃O₆(OH)₂H₂O

Monoclinic C2/m

a=21.53 Å

b=3.79 Å

c=11.92 Å

β=136.3°

Experimental data

tilt range: ±60° step: 1°

No ind. reflections: 628

No ind. atoms: 13

R = 35.8 %

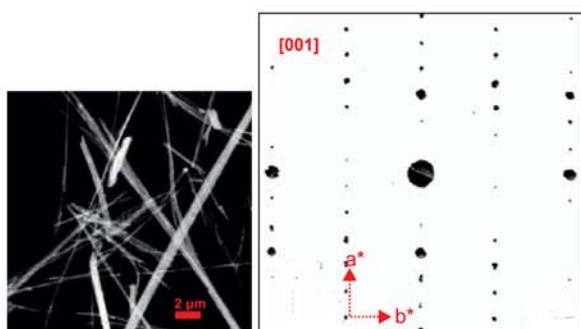


figure 1

STEM IMAGE OF NANORODS & (001) PROJECTION OF 3D RECONSTRUCTION RECIPROCAL SPACE THROUGH ADT DATA SET

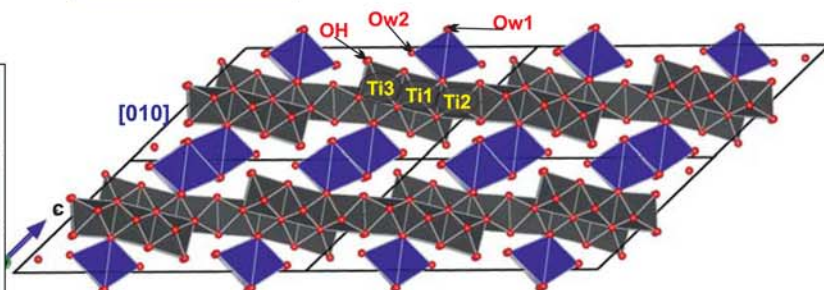


figure 2

MODEL OF NaTi₃O₆(OH)₂H₂O (VIEW IN [010]).
H ATOMS OMITTED. {NaO₆} OCTAHEDRA ARE VIEWED EDGE-ON.
HYDROGEN BONDS ARE DRAWN AS DOTTED LINE