Crystal structural analysis of rutile-type titania

Yong Phat, Masatomo Yashima, Takahiro Wakita, Takafumi Komatsu
Department of Materials Science and Engineering, Interdisciplinary Graduate School of Science, Tokyo Institute of Technology

Titanium dioxide (titania) is a technologically important material with applications in photocatalysis, paints, gas sensors, electrochromic devices, lithium ion batteries, and dye-sensitized solar cells. TiO2 crystallizes most commonly in either the rutile (space group P42/mmm) or anataze-type structure. For bulk titania crystals at ambient conditions, rutile is more stable than anatase and has therefore been more widely studied. In contrast to the extensive studies on its crystal structure, however structural properties of the rutile structure in high temperature have not been studied in detail and not well understood. In this study, we investigated the crystal structure of rutile-type titania at high temperatures by using neutron powder diffraction method.

Rutile-type titania powders were pressed into pellets. These pellets were used for high-temperature neutron diffraction measurements. Neutron diffraction measurements were performed in air with a 150-detector system, HERMES [1], installed at the JRR-3M reactor in Japan Atomic Energy Agency, Tokai, Japan. Neutrons with wavelength 1.8143 were obtained by the (331) reflection of a Ge monochromator. Diffraction data were collected in air from room temperature to high temperatures. A furnace with MoSi2 heaters [2] was placed on the sample table, and used for neutron diffraction measurements at high temperatures. The experimental data were analyzed by a combination of Rietveld analysis, the maximum-entropy method (MEM) and MEM-based pattern fitting (MPF). Computer programs RIETAN-FP, PRIMA and VESTA were utilized for the Rietveld and MPF analyses, MEM calculation and visualization of crystal structure and nuclear-density distribution, respectively. The data analysis is now in progress.

Reference

[1] K. Ohoyama et al., Jpn. J. Appl. Phys. 37 (1998) 3319.
[2] M. Yashima, J. Am. Ceram. Soc. 85 (2002) 2925.