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Structure of TiO_2 rutile synthesized under strong gravity field

Akira YOSHIASA[1], Rabaya BAGUM [1], Kazumasa SUGIYAMA[2], Yuta OGATA[1],Tomotaka NAKATANI[1], Maki OKUBE[3] and Tsutomu MASHIMO[1]
[1] Graduate School of Sciences, Kumamoto Univ. Kumamoto 860-8555, Japan
[2] Institute of Material Science, Tohoku *University, Sendai 226-8503, Japan*
[3] Tokyo Institute of Technology, Nagatsuta, Yokohama 226-8503, Japan.

Introduction

Materials research using strong gravitational field (1-10 x10^5 G, 1G =9.8 m/s^2) is still an unexploited area, even though materials science research utilizing microgravity fields is now active. To study sedimentation of atoms or crystal instability in solids under strong gravitational fields, we developed a high temperature ultracentrifuge apparatus that can generate a long duration acceleration field in excess of 10^6 G at elevated temperatures [1]. Titanium oxide-based materials attracted great interest and have been under intensive investigation due to their interesting optical, dielectric, catalytic, thermal and mechanical properties. Ultracentrifuge experiments were performed on single crystals of TiO2 rutile in the solid-state phase to examine changes in structure to produce new gravitationally induced phases at comparatively lower temperatures, below the melting point of the initial material. The crystal structure was investigated by X-ray diffraction analysis.

Experimental

We created this structure by applying a strong gravitational field (0.4×106 G) along the c-axis direction during heat treatment at 400°C.The rotor could be heated by radiation from a hot carbon, hollow cylinder that is heated by a high frequency heating system. Compositions of the single crystals were determined by EPMA.

Single-crystal X-ray diffraction measurements were carried out with a four-circle diffractometer at the BL-10A beam line of the Photon Factory, Tsukuba, Japan, using monochromatized synchrotron X-ray (λ = 0.70006 Å) radiation. Structute refinements were performed using full matrix least squires program RFINE2 (Table 1). Our refinement yields full occupancies for all sites.

Results and Discussion

A portion of crystallographic data for samples is summarized in Tables 1. Ambient rutile-type TiO2 consists of edge-sharing TiO6 octahedral groups. The Ti ions form a tetragonal lattice which are expanded along a, when we apply gravity along with c-axis direction and the octahedra are distorted small. The small changes in the crystal structure induce drastic changes in electronic properties. The anisotropy (c/a ratio) of the tetragonal phase changed, as the TiO6 octahedral unit in the structure became more anisotropic. The ratio of the shared and unshared edges has decreased than standard sample. These changes occurred well below the melting point of rutile, indicating that strong gravity method can control structures with developing properties. Strong gravitational fields has practical means of producing new phase materials. This is totally different from usual rutile. We open a new area in strong gravity-induced material science research.

Table 1. TiO_2 Experimental data

This study

Crystal data	Starting sample	Gravity sample
Space group	$P4_2/mnm$	$P4_2/mnm$
a(Å)	4.5973(4)	4.6189(4)
c(Å)	2.9538(4)	2.9357 (4)
c/a	0.643(3)	0.635(3)
V (Å^3)	62.42(3)	62.635(3)
Z	2	2
Wavelength (Å)	0.71069	0.70006

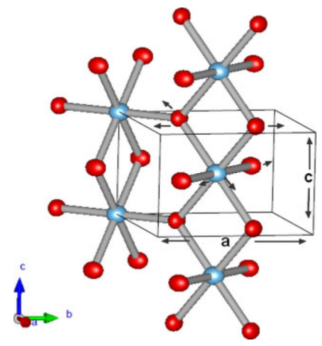

Figure 5. Crystal structure of gravity sample with indicating gravity effect.

References

[1] Rabaya Bagum, Akira Yoshiasa, Satoru Okayasu, Yusuke Iguchi, Masao Ono, Maki Okube, Tsutomu Mashimo, JOURNAL OF APPLIED PHYSICS (2010) 108 053517 7pp

* yoshiasa@sci.kumamoto-u.ac.jp