

## Pressure-induced phase transition in anatase TiO<sub>2</sub>

Takao Sekiya<sup>1\*</sup> (7970), Mika Okumura<sup>1</sup> (7971), Nozomu Hamaya<sup>2</sup> (1229), Ayako Ohmura<sup>2</sup> (4719), Hiromi Yamazaki<sup>2</sup> (6164) and Miyuki Ishizuka<sup>2</sup> (8364)

<sup>1)</sup> Graduate School of Technology, Yokohama National Univ., Yokohama 240-8501, Japan

<sup>2)</sup> Graduate School of Humanities and Sciences, Ochanomizu Univ., Tokyo 112-8610 Japan

There are many studies for the pressure-induced structural phase transition of anatase to columbite-type having isostructure with  $\alpha$ -PbO<sub>2</sub> (TiO<sub>2</sub>-II). The results, however, throw us into confusion because the data is so scattered. This is very likely to come from the properties of the starting materials, single crystal or powder. Our Raman spectroscopy reveals that anatase single crystal shows sharp pressure-induced phase transition in the range of 4.3-4.6 GPa, while the transition of powdered anatase is observed in the higher pressure. In this study, we investigate structural properties of anatase single crystal and its powdered samples under high pressure using X-ray diffraction.

Anatase single crystals were grown by chemical vapor transport method. We used a single crystal having about 120×100×60 μm<sup>3</sup> in size. Our powdered samples were prepared by crushing and grinding anatase single crystals in an alumina mortar and separated into two by sedimentation in alcohol. The Powder 2 is smaller than the Powder 1 in particle size. High pressures were obtained by a diamond anvil cell (DAC) with 4:1 mixture of methanol and ethanol as pressure medium.

Anatase single crystal at pressures less than 4.1 GPa gave some X-ray diffraction spots assigned to anatase reflections. When the pressure reaches to 4.4 GPa, no reflection spots were observed and whole or large part of the crystal instantly lost its transparency. The powdered samples initially contain a trace of columbite-type phase, which are likely to be formed in the crushing and grinding process. For the Powder 1, the reflection lines due to

columbite-type phase increase in intensity at 5.9 GPa. For the Powder 2, which is composed mainly of smaller particles than the Powder 1, new reflection lines due to columbite-type phase can be observed at about 7.9 GPa. After the compression of the Powders 1 and 2 to 6.8 and 9.7 GPa, a trace of the diffraction lines due to anatase can be observed. This indicates the transition is not completed at the pressures. Figure shows change of lattice constants of anatase depending on pressure. The pressure-dependence of powdered samples gives linear plots within uncertainties of our experiment. Little difference is observed between the powdered samples, while a slight difference can be also observed between single crystal and powder.

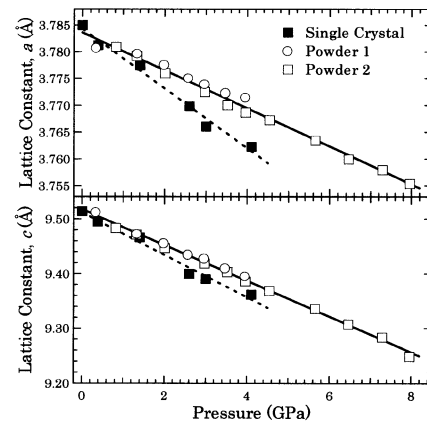


Figure Pressure-dependence of lattice constants of anatase.

## Structure and physical properties in the pressure-induced insulator-metal transition of layered Mn compound

Akiyuki MATSUSHITA<sup>\*1)</sup> 5654, Yuh YAMADA<sup>2)</sup> 5191, Tomohiro SHIBATA<sup>2)</sup> 6068, Hiroaki HAMADA<sup>2)</sup> 8003, Yuichiro MASUDA<sup>2)</sup> 8004, Kazuki FUKUDA<sup>2)</sup> 8005, Hiroki TAKAHASHI<sup>3)</sup> 8069, Jun SHIBATA<sup>3)</sup> 8087

1) National Institute for Materials Science

2) Interdisciplinary Faculty of Science and Engineering, Shimane University

3) College of Humanities and Sciences, Nihon University

Ba<sub>2</sub>MnZn<sub>2</sub>As<sub>2</sub>O<sub>2</sub> crystallizes in the Sr<sub>2</sub>Mn<sub>3</sub>As<sub>2</sub>O<sub>2</sub> structure type (I4/mmm) in which Mn<sub>2</sub>As<sub>2</sub><sup>2-</sup> layers and MnO<sub>2</sub><sup>2-</sup> layers are alternatively stacked along c-axis separated by Ba<sup>2+</sup> cations. This compound is a semiconductor at ambient pressure with an activation energy  $T_0$  of 1070K. Interestingly  $T_0$  shows a strong pressure dependence and finally this compound exhibits insulator-metal transition around 5 GPa (Fig.1). We have pursued powder X-ray diffraction measurement under high pressure and low temperature using diamond anvil cell. Figure 2 shows the normalized lattice parameters  $a/a_0$  and  $c/c_0$  as a function of pressure, where  $a_0$  and  $c_0$  are those at 300 K. The pressure coefficient of  $c/c_0$  is about 2.4 times larger than that of  $a/a_0$  and is considerably large comparing other layered compounds such as High-Tc superconductors. We may attribute the large pressure dependence of the electrical resistivity to this large pressure coefficient of  $c/c_0$ . In Figure 3 we show the temperature dependence of the normalized lattice constants at 5.4 GPa. We can clearly observe a change in temperature coefficients of the lattice constants around 200K which is attributable to the metal-insulator transition.

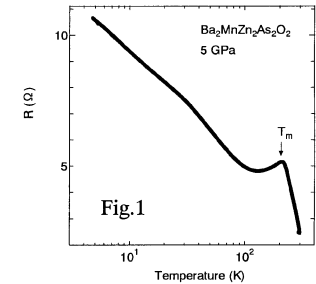


Fig.1

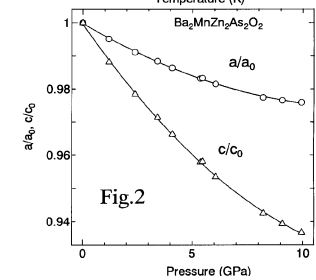


Fig.2

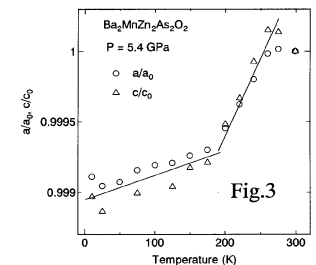


Fig.3