Structural Analysis for Titanic Acid by XAFS

Hiroshi Ohzono*(5227), Hideaki Ohyama(6462), Yoshihisa Nagasaki[1](7630), Tomizo Matsuoka(7628), Kenji Fujiwara(5660),Yoshiaki Tsukamoto(7621), Shinji Ozaki[2](4142), Masao Takahashi[3](1285)

Matsushita Battery Industrial Co., Ltd., [1] Matsushita Electric Industrial Co., Ltd., [2] Matsushita Technoresearch Inc., [2] The Institute of Scientific and Industrial Research, Osaka University

Titanic acid has an ability to realize the novel phase and performance in the industrial field such as solid –state devices. There are three models, alpha, beta, and gamma, the structural phase of titanic acid. Alpha titanic acid is also called orthotitanic acid, and is expressed as H_4TiO_4. On the other hand, beta titanic acid is also called meta-titanic acid, and is expressed as H_2TiO_3. Although these are considered to be also the hydrate of titanium oxide, to our knowledge, structural analysis of these materials has not been performed in detail. X-ray diffraction method is applied to crystal structure analysis. However, there is no reference data in commercial base.

Then, we have attempted to apply the structural analysis by X-ray absorption fine structure (XAFS) method. XAFS method is applicable also to amorphous substance as X-ray diffraction patterns not shown.

The XAFS spectra of Ti-*K* edge were measured at room temperature in the transmission mode, at BL16B2 of SPring-8. The samples were made into the shape of 10mm phi pellet using cellulose. Measurement time was about 1 hour.

The Ti-*K* edge XANES spectra of alpha titanic acid, beta titanic acid, and anatase type TiO_2 and rutile type TiO_2 are shown in Fig. 1. When the spectra of alpha titanic acid and beta titanic acid are compared, it seems that the absorption edge of alpha titanic acid has shifted to a low energy side rather than that of beta titanic acid. Moreover, it is found that difference is in the standup form of each XANES spectrum. Although beta titanic acid has taken the form dried only one molecular from alpha titanic acid in the chemical formula, it is thought that the electronic states of titanium completely differ.

Furthermore, the spectrum form of XANES of beta titanic acid is similar to one of anatase type TiO_2. This result indicates that the structure of beta titanic acid closes to the structure of anatase type TiO_2. Further work will be required in order to analysis in EXAFS region in more detail.

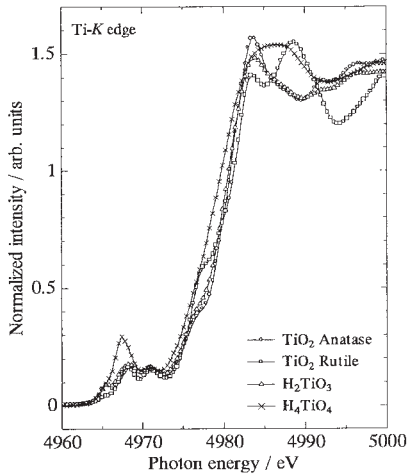

Fig. 1 Ti-*K* edge XANES spectra

Analysis of Mirco-structure and Chemical State of Hydrogen Absorbed Commercially Pure Titanium by SR-XAFS

Takenori Nakayama(0004282)[1]*, Takayuki Tsubota(0006021)[1], Takashi Watanabe(0004160)[2], Masayuki Inaba(0004163)[2], Mitsutoshi Yokomizo(0004550)[3]

[1]Materials Research Laboratory, Kobe Steel, Ltd.
[2]Kobelco Research Institute [3]Department of Chemistry, Fukuoka University

Transition metals such as titanium generally pick up a large amount of hydrogen when they are exposed to some corrosive environments. Excessive hydrogen absorption leads to precipitating hydrides in the matrix and the mechanical properties of the metals are subjected to degradation. However, their degradation mechanism has not been well clarified. Therefore, this study aims to investigate influence of hydrogen on microstructure and chemical state of commercially pure titanium by SR-XAFS to elucidate the degradation mechanism of titanium through hydrogen absorption.

The measurements of Ti K-edge XAFS spectra were done at room temperature in a transmission mode at BL16B2 station of SPring-8 to titanium without hydrogen(TH-0), titanium with TiH2(TH-2), and TiH2(TH-2).

The EXAFS spectra of these titanium samples were successfully obtained to compare radial distance function with or without hydrogen as shown in Fig.1, indicating that hydrogen extends crystal lattice of titanium. The XANES spectra were also well measured to show the change of pre-edge structure of the spectra as in Fig.2, indicating that hydrogen largely affects chemical state of titanium.

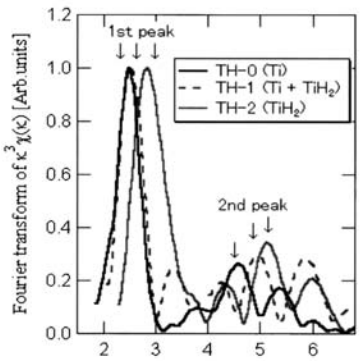

Fig.1 Ti K-edge EXAFS spectra of hydrogen absorbed commercially pure titanium.

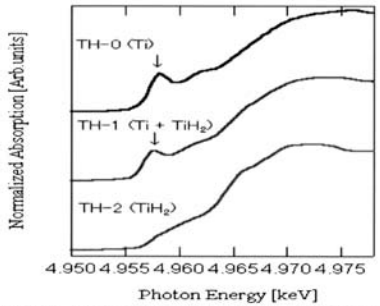

Fig.2 Ti K-edge XANES spectra of hydrogen absorbed commercially pure titanium.