Ti K-edge EXAFS on the local structural change of PbTiO$_3$

Takafumi MIYANAGA$^{1*}$, Kei SATO$^1$, Shigenobu MATSUDA$^1$, Djibril DIOP$^2$

$^1$Faculty of Science and Technology, Hirosaki University, Hirosaki, Aomori 036-8561, Japan
$^2$Department of Physics, Faculty of Science and Technology, Anta Cheikh Diop University of Dakar, Dakar, Senegal

**Introduction**

Structural change in perovskite materials have been long studied using by X-ray diffraction and neutron diffraction [1]. On the other hand, X-ray absorption fine structure (XAFS) is a technique to study the local structure of the materials and considered as a complementary technique to the former two methods. During the last two decade, much evidence accumulated indicating that local distortion in perovskite compounds also exist above the phase transition temperature. Sicon et al. extensively studied for PbTiO$_3$ EXAFS at wide temperature range [2].

In this report we study the local structural change around Ti atom. We found the discontinuous change of the longest Ti-O(3) distance through the transition temperature as shown in Pb-O(3)[3].

**Experimental**

Powder sample of PbTiO$_3$ was purchased and sample verification was performed by X-ray powder diffraction method. X-ray absorption spectra of Ti K-edges (4.9 keV) were measured at BL9A of Photon Factory (KEK) with transmission mode. Si(111) double crystal monochromator was used. EXAFS data analyses were performed by XANADU code [4]. In the least-square curve-fitting procedure, the theoretical EXAFS parameters calculated from FEFF6 code [5] were used.

**Results and Discussion**

Figure 1 shows the EXAFS $\tilde{\chi}(k)$ spectra for Ti K-edge at various temperatures. Up to 10 Å$^{-1}$, satisfactory quality data were obtained.

![EXAFS spectra](image)

**Fig. 1** EXAFS $\tilde{\chi}(k)$ spectra of Ti-K edge EXAFS for PbTiO$_3$ at various temperatures.

Using the non-linear least-square-fitting method, we can determine the structural parameters. Figure 2 shows the variations of three kinds of Ti-O interatomic distances with temperature. The interatomic distance of Ti-O(2) is almost constant in whole temperature range. That of Ti-O(3) decreases gradually as temperature increases up to $T_c$ and does not change with temperature over $T_c$. As for Ti-O(1), we find complex behavior between Ti-O(2) and Ti-O(3). These phenomenon is quite similar to the result of Pb-O(1,2,3) obtained from Pb L$_{\text{III}}$-edge EXAFS study [3]. That is: the longest Ti-O(3) shows the typical “displacive” behavior as well as Pb-O(3) and Ti distortion remains at temperature over $T_c$.

![Temperature dependence](image)

**Fig. 2** Temperature dependence of the Ti-O(1,2,3) interatomic distances obtained from EXAFS.

**References**


* takaf@cc.hirosaki-u.ac.jp