# Ti K-edge EXAFS on the local structural change of $PbTiO_3$

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## 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. Sicron *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 monochrometer 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 $k^2\chi(k)$ spectra for Ti *K*-edge at various temperatures. Up to 10 $Å^{-1}$, satisfactory quality data were obtained.

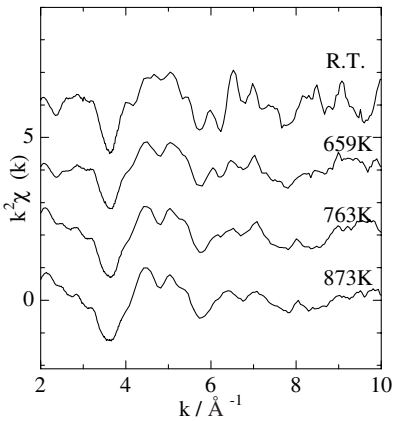


**Fig. 1** EXAFS $k^2\chi(k)$ spectra of Ti-*K* edge EXAFS for $PbTiO_3$ at various temperatures.

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 $L_{III}$-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 $T_c$.

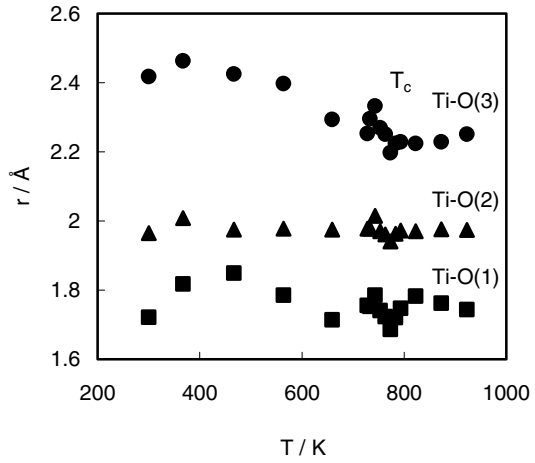


**Fig. 2** Temperature dependence of the Ti-O(1,2,3) interatomic distances obtained from EXAFS.

## References

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