EXAFS Spectrum near the Ta-K Edge of $KTaO_3$

Yasuo NISHIHATA[1], Osamu KAMISHIMA[1], Hironobu MAEDA[1], Tadao ISHII[2] and Shuichi EMURA[3]

1) Faculty of Science, Okayama University, Okayama 700, Japan
2) Faculty of Engineering, Okayama University, Okayama 700, Japan
3) The Institute of Scientific and Industrial Research, Ibaraki, Osaka 567, Japan

The radiation spectrum from a bending magnet in the SPring-8 Storage Ring shows the high photon density even at as high as 100 keV. This advantage enables us to measure XAFS (X-ray Absorption Fine Structure) spectra near the K-edge of almost all elements. In general, it is easy to prepare a uniform specimen, which is required in detailed analysis, including heavy elements for the XAFS measurements in transmission mode. The finite lifetime of the core hole will smear out the EXAFS (Extended X-ray Absorption Fine Structure) signal [1], and it is serious for K-edges of elements with $Z > 40$. We have tried to detect the EXAFS signal just above the Ta-K edge (~ 67 keV) of potassium tantalate, $KTaO_3$. Here, we show a preliminary result and some problems with high energy XAFS.

$KTaO_3$ has the cubic perovskite structure and is regarded as a quantum paraelectric. EXAFS measurements near the Ta-L_{III} edge (~ 9.9 keV) and detailed analysis of Debye-Waller factor were reported previously [2]. For the sake of comparison, x-ray absorption spectrum near the Ta-L_{III} edge at room temperature and the extracted EXAFS function $k^3\chi(k)$ are shown in Figs. 1 and 2, respectively.

The powder of $KTaO_3$ was pressed into a pellet with ~ 0.3 mm thick, which was one order of magnitude thicker than that adopted for EXAFS measurement near the Ta-L_{III} edge. X-ray absorption spectrum was measured by using an EXAFS facility installed at the beamline 14A of the 2.5 GeV storage ring of the Photon Factory in the National Laboratory of High Energy Physics (Tsukuba). The measurements were carried out in transmission mode with a Si 553 double-crystal monochromator. The incident and transmitted x-ray intensities, I_0 and I, were monitored with an ionization chamber 17 cm long with flowing Kr gas and an ionization chamber 31 cm long with flowing Xe gas, respectively.

Figure 3 shows the x-ray absorption spectrum near the Ta-K edge of $KTaO_3$ at room temperature. It seems that EXAFS signal smears and the edge jump is not so sharp as the spectrum near the Ta-L_{III} edge. The EXAFS function $\chi(k)$ was extracted from the absorption spectrum following the standard procedure.

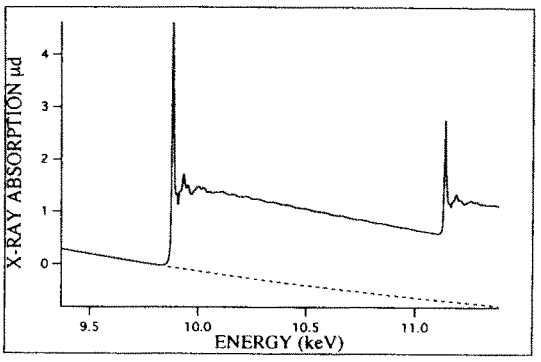

Fig. 1. X-ray absorption spectrum near the Ta-L_{III} edge of $KTaO_3$ at room temperature.

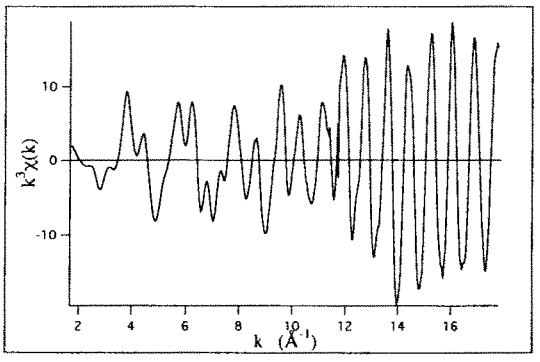

Fig. 2. EXAFS function $k^3\chi(k)$ of the Ta-L_{III} edge.

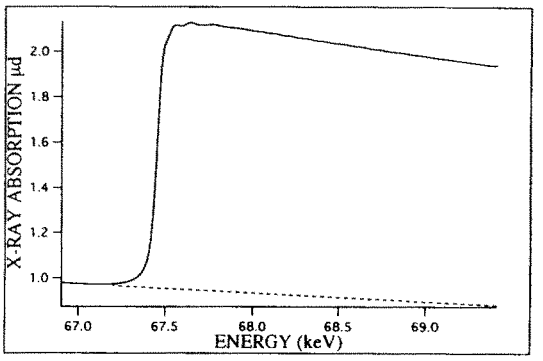

Fig. 3. X-ray absorption spectrum near the Ta-K edge of $KTaO_3$ at room temperature.

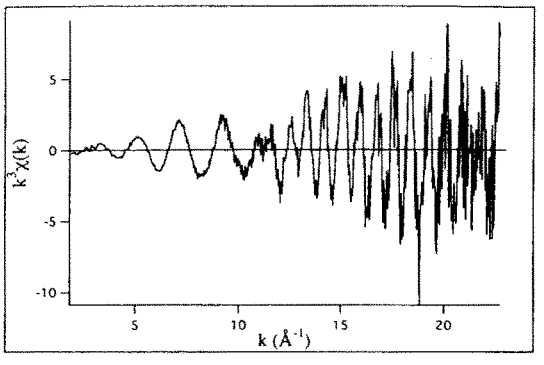

Fig. 4. EXAFS function $k^3\chi(k)$ of the Ta-K edge.

As shown in Fig. 4, a well-defined EXAFS signal is found up to k = 20 $Å^{-1}$. The energy resolution was estimated to be ~ 30 eV from the rocking curve of the monochromator crystal. The x-ray intensities, I_0 and I, were corrected by deconvoluting with the resolution function of an isosceles triangle in the further analysis. However, there is still uncertainty in the EXAFS signal due to the deconvolution process. In order to determine the local structure parameters, the programs XAFS93 and MBF93 were employed in the data analysis. Since the Ta atom is located at the center of the O octahedron, the coordination number of O atom was fixed to 6. Local structure parameters for harmonic vibration model were obtained and are given in Table 1. Local structrure parameters calculated from the spectra of the Ta-L_{III} edge are also tabulated [2]. In the analysis, the mean free path of the photoelectron λ was considered to depend on wave vector k: $\lambda = k/\eta$. EXAFS signal is generally reduced due to the short lifetime of the K hole. This smearing effect behaves in a similar manner to the mean free path term [1], and can effectively be taken together into η in the EXAFS function. Thus, the Debye-Waller factor $\sigma^{(2)}$ was evaluated rather small compared with that evaluated from the Ta-L_{III} edge. We found that the local structure parameters depended on the range of the curve fitting in k space.

Table 1. Local structure parameters of the O shell around the Ta atom for the harmonic vibration model.

Edge	N	R_{Ta-O}(Å)	$\sigma^{(2)}$($Å^2$)	η($Å^{-2}$)
K	6	1.99(1)	0.0047(7)	3.0(2)
L_{III}	6	2.005(2)	0.0070(2)	0.69(3)

References

[1] D. G. Stearns, Philos. Mag., 49, 541 (1984).
[2] Y. Nishihata, O. Kamishima, K. Ojima, A. Swada, H. Maeda and H. Terauchi, J. Phys.: Condens. Matter, 6, 9317 (1994).