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Anisotropic resonant x-ray scattering in rutile, TiO_2

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Introduction

A polarization-dependent phenomenon in x-rays can be observed near absorption edge using synchrotron radiation. This phenomenon is explained by anisotropic tensor of susceptibility (ATS), which is attributed to anisotropic environment of the absorbing atom. In general ATS scattering based on this anisotropy is very weak, but we can measure the intensity using a forbidden reflection because the anisotropic tensors violate the conventional extinction rule for the Bragg reflection.

The dipole approximation is usually applied on the ATS (anomalous) scattering factor. Many of experimental results observed up to now on the ATS scattering are explained by electronic dipole transition. ATS scattering from rutile, TiO_2, near the Ti K-absorption edge was first reported by Kirfel et al. and they concluded that this scattering was caused by dipole transition.[1]

However, in the pre-edge region of transition metals we have observed the quadrupole effect for some samples.[2, 3] In this case ATS scattering depends on the x-ray wave vectors as well as its polarization, and reflects the details of local electronic states of the atom in the crystal. In the present work we investigated the detailed properties of energy spectrum and azimuthal angle dependence of the ATS scattering from rutile near the Ti K-edge.

Experimental Results

The experiment was carried out with four-circle diffractometers at BL3A and 4C, where the incident beam was polarized horizontally and the scattering plane was perpendicular to it, i.e. σ-polarized setting. We first measured absorption spectrum of the powder sample near the Ti K-edge. In order to obtain the ATS property the integrated intensity was measured for the 100 and 001 forbidden reflections at different x-ray energies or azimuthal angles around the scattering vector.

Figure 1 shows the absorption spectrum and energy dependence of the 100 reflection intensity. The inset in the Fig. 1 shows the close-up view in the pre-edge region. As shown in this figure there are the main peak and middle peak near the edge, two peaks in the higher energy region and three peaks in the pre-edge region.

In the higher energy region the shape of energy spectra of the 100 and 001 reflection is almost the same. This indicates that the ATS scattering is caused by electronic dipole transition. In the pre-edge region, however, the 100 spectrum shows the different shape from the 001 reflection. This indicates that the ATS scattering is dependent on the wave vector, i.e. contribution of the quadrupole effect.

Figure 2 shows the azimuthal angle dependence of the 100 reflection at the main peak, 4.9759 keV, and the lowest energy peak, 4.9594 keV, where these intensities are depicted in different scales. The observation at the main peak (open squares) is in good agreement with the fitting curves based on the dipole approximation (dashed line). On the contrary the profile at the lowest energy peak (dots) shows quite different shape. This property can be explained by interference between dipole transition term and quadrupole one (solid line). Similar results are obtained for other tow peaks in the pre-edge region. Therefore we conclude that the pre-edge peaks relates with the quadrupole transition from 1s to 3d state in Titanium.

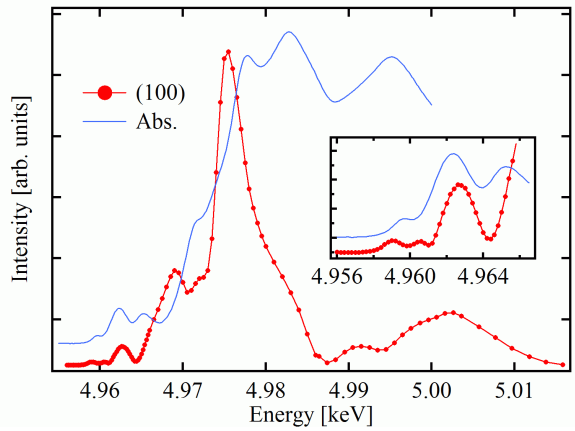

Fig. 1 Energy spectrum of 100 reflection intensity and absorption curve of rutile.

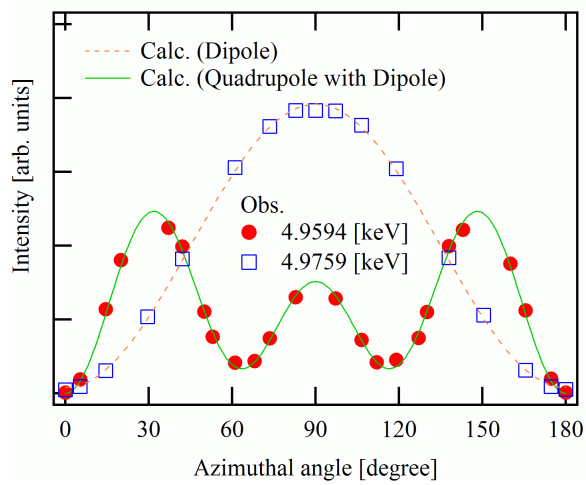

Fig. 2 Azimuthal angle dependence of 100 reflection intensity of rutile at two different energies.

References

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