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Energy spectrum of ATS scattering with dipole-quadrupole transition process in magnetite, Fe_3O_4

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Introduction

ATS (anisotropic tensor of the susceptibility) scattering can be observed in the forbidden Bragg reflections near absorption edge. The scattering is dependent on the x-ray polarization (and wave vector) so that the scattering is sensitive to the anisotropy of the electronic state in the absorbing atom, e.g. to the direction of the electronic orbital. Magnetite (Fe_3O_4) has a spinel structure, in which the Fe atoms occupy the tetrahedral A site and the octahedral B site. The ATS scattering with dipole-dipole (d-d) transition process is allowed for the B site but not allowed for the A site because of the site symmetry. For the A site, therefore, we must consider more higher approximation, dipole-quadrupole (d-q) term. From the physical point of view the mixed dipole-quadrupole transitions are very interesting because they provide us with a method to study the hybridization of electronic orbitals with different parity.

We previously measured the energy dependence of the 002 and 006 forbidden reflections near the Fe K-edge (Fig. 1).[1] In this figure the main resonant peak is just above the edge and the second peak in the pre-edge region, but the width of the main peak is different between two reflections. It is seemed that there may be other overlapping peak in the lower energy side of the 002 main peak. However, we did not distinguish two different scatterings from A and B site because the 00*l* forbidden reflections have the same azimuth dependence and x-ray polarization property. Therefore, we measured separately each energy spectrum of the d-d or d-q scattering by utilizing the x-ray polarization property of the 046 forbidden reflection.

Experimental Results

The experiment was carried out with a four-circle diffractometer at BL4C, where the incident beam was σ-polarized. For polarization analysis an analyzer system was set on the 2θ arm, where Si (331) was used as the analyzer crystal. The integrated intensity was measured for the 046 forbidden reflection at different x-ray energies near the Fe K-absorption edge.

The circles in Fig. 2 show the energy dependence of the 046 reflection intensity at azimuthal angle $\varphi = 85.0$ degrees, where the origin of the angle φ is taken to provide maximum intensity in the azimuth dependence of the d-d scattering. At $\varphi = 85.0$ the d-d scattering from B site is dominant without polarization analyzer. The squares in Fig. 2 show energy spectrum on the condition where the d-q scattering from A site dominantly contributes to the intensity. This condition is fulfilled at $\varphi = 154.8$ and polarization angle $\varphi_A = 84.5$, which is near π polarization setting. As shown in Fig. 2 other remarkable peaks have not been observed. Therefore we conclude that the different shape of the 00*l* resonant peak in Fig. 1 is caused by the interference between the d-d and d-q scatterings. We have found that the d-q scattering gives two similar resonant peaks near the edge and the peak at higher resonant energy is rather larger. This fact agrees with the result of least-squares analysis for azimuth dependence in a previous report.[2] Thus the mixed dipole-quadrupole scattering from A site plays very important role in all region of the energy spectrum near the edge.

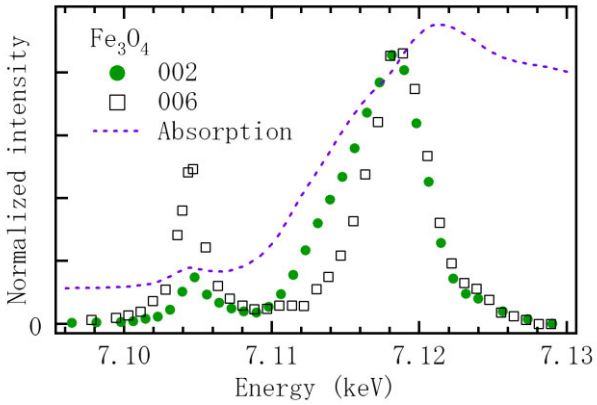

Fig. 1 Energy spectra of the 002 and 006 reflections.

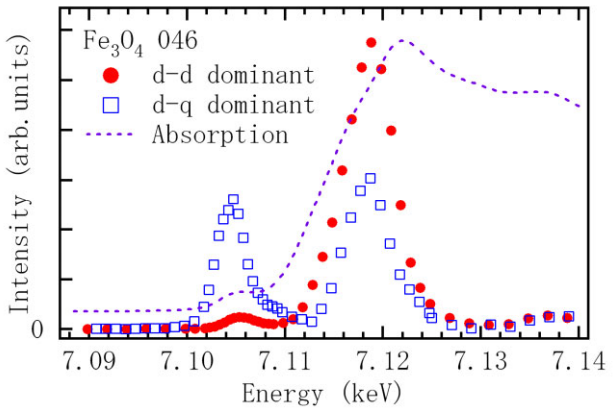

Fig. 2 Energy spectra of the 046 reflection on different conditions.

References

[1] M. Kanazawa et al.: J. Phys. Soc. Jpn. **71** (2002) 1765.
[2] J. Kokubun et al.: PF Act. Rep. 2005 #23 Part B 136.

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