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Quantitative evaluation of quadrupole transition effect in ATS scattering from 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 the absorption edge. This scattering is sensitive to the electronic states in anisotropic environment, especially to the direction of the electronic orbital. We have studied the ATS scattering in iron pyrite (FeS_2), magnetite (Fe_3O_4) and so on.[1] These experimental results above the edge are in good agreement with the calculation based on the electric dipole transition. Below the edge, however, the effects of quadrupole transition have been observed.

Magnetite 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. (For the B site the d-q scattering is not allowed.) We previously studied the energy and azimuthal angle dependence of the 002 and 006 forbidden reflections.[2] We observed two resonant peaks in energy spectrum near the Fe K-absorption edge. The main resonant peak is just above the edge and the second peak in the pre-edge region. From the difference of the two reflection intensities we concluded that the main peak was mainly caused by d-d scattering from the B site and the pre-edge peak by d-q scattering from the A site. However, we did not quantitatively evaluate each contribution because the azimuth dependence is completely same in both scattering. In the present report we investigated the 046 forbidden reflection in order to estimate the quantitative contribution from the A and B sites.

Experimental Results

The experiment was carried out with a four-circle diffractometer at BL4C, where the incident beam was σ-polarized. The integrated intensity was measured for the 046 forbidden reflection at different X-ray energies or azimuthal angles near the Fe K-absorption edge.

We observed the main and pre-edge resonant peaks similar to those in the previous experiment. The figures 1 and 2 show the azimuth dependence of the reflection at the main and pre-edge resonant energies, respectively. In these figures the circles denote the observations and the dashed line the calculation from the d-d or d-q scattering only. As shown in these figures the observation at pre-edge resonance almost agrees with the d-q calculation, while at the main resonance there is a little difference between the observation and the d-d calculation. The solid line is the result of curve fitting considering the interference between the d-d and d-q scattering, where we used three parameters, absolute values of the anisotropic tensorial element for the d-d and d-q scattering factors, f(dd) and f(dq), and the phase difference of these factors. From the results we determined the ATS scattering factors; the f(dd) is 0.36 and the f(dq) is 0.22 electrons/atom at the main resonance, the f(dd) is 0.06 and the f(dq) is 0.21 electrons/atom at the pre-edge resonance. Thus we have found that the d-q scattering from the A site has relatively large effect on the both resonance.

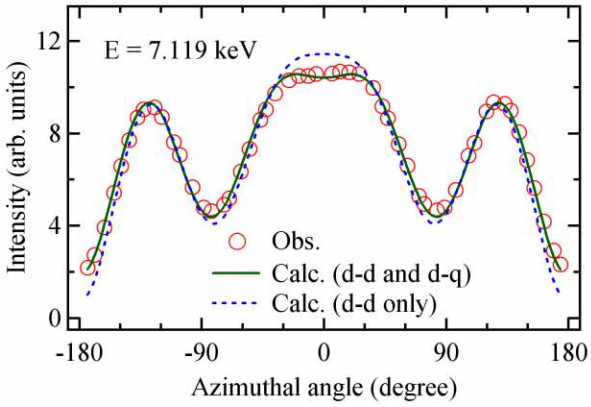

Fig. 1 Azimuthal angle dependence of the 046 forbidden reflection at the main resonant energy, 7.119 keV.

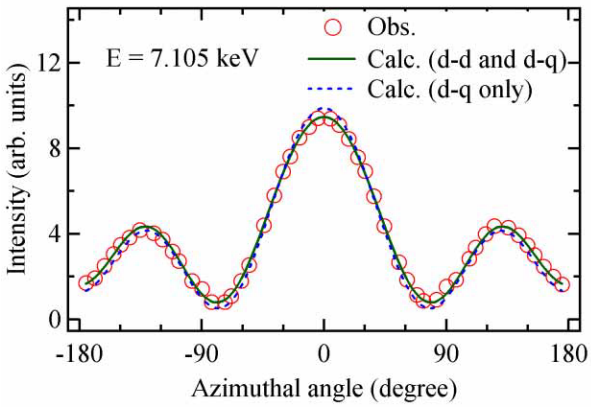

Fig. 2 Azimuthal angle dependence of the 046 forbidden reflection at the pre-edge resonant energy, 7.105 keV.

References

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[2] M. Kanazawa et al.: J. Phys. Soc. Jpn. **71** (2002) 1765.

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