

ATS Scattering from Cuprite, Cu_2O

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Introduction

Using ATS scattering,[1] we can obtain local information about anisotropic environment for a specific atom. Though the scattering is very weak compared with Thomson scattering, we can obtain only an anisotropic factor by measuring a “forbidden” reflection because the isotropic part is excluded from the reflection.

Cuprite, Cu_2O , belongs to a cubic system, $Pn\bar{3}m$, and the copper atom of the site symmetry $\bar{3}m$ is placed at the middle point of two oxygen atoms. The “forbidden” reflection of cuprite was first studied by Kirfel et al. near the Cu K-absorption edge.[2] They measured the energy dependence of the forbidden 005 reflection and observed two peaks just near the edge and at about 20 eV below the edge. Their measurements of azimuthal dependence were in good agreement with the calculation based on the dipole approximation. In other materials, the polarization analysis and azimuthal dependence revealed that most of the scattering are caused by dipole transition.[3, 4] In some cases, however, multi-pole effects were observed especially below the edge.[5, 6] Therefore, in the present report, we investigate the details of energy and azimuthal dependence of the “forbidden” reflections of cuprite.

Experimental

The sample crystal with a (001) surface was prepared from a natural crystal from Zaire. A powder sample was also prepared for absorption measurement. The synchrotron experiments were carried out at BL3A using a four-circle diffractometer. The polarization state of incident X-rays was σ -polarized. In order to obtain the energy and azimuthal dependence, integrated intensity was measured for the 001 and 003 “forbidden” reflections. Energy spectra of the ATS reflections were measured from 8.941 keV to 9.023 keV.

Results and Discussion

Figure 1 shows energy dependence of the intensity for the 001 and 003 reflections of cuprite. The continuous curve represents the observed absorption spectrum of the powder sample. As shown in this figure, the spectra are distributed in very wide range, over 50 eV, but there is no peak below the edge contrary to the observation by Kirfel et al. The shapes of the energy spectra for the 001 and 003 reflections are essentially the same. This result indicates that these ATS scattering are caused by dipole transition process. In fact the observed azimuthal dependence at 8.982 keV and 8.998 keV agrees with the curves calculated from atomic scattering tensors of second rank. (see, Fig. 2) The magnitude of an off-diagonal element of the scattering tensor for one copper atom is 1.9 electrons for the main peak at 8.982 keV. This

value is very large compared with that for one iron atom in iron pyrite and magnetite, 0.2 and 0.3 electrons, respectively.[6,7] We presume that this large anisotropic term is due to the anisotropic environment of the copper atom with a strong linear coupling between oxygen atoms.

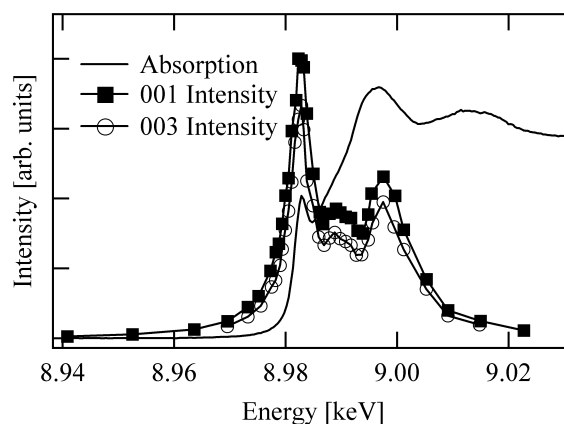


Fig. 1 Energy spectra of the 001 and 003 reflections.

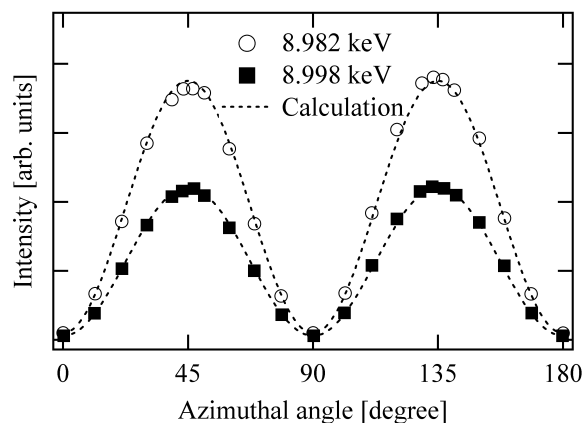


Fig. 2 Azimuthal dependence of the 001 reflection at 8.982 keV and 8.998 keV.

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