

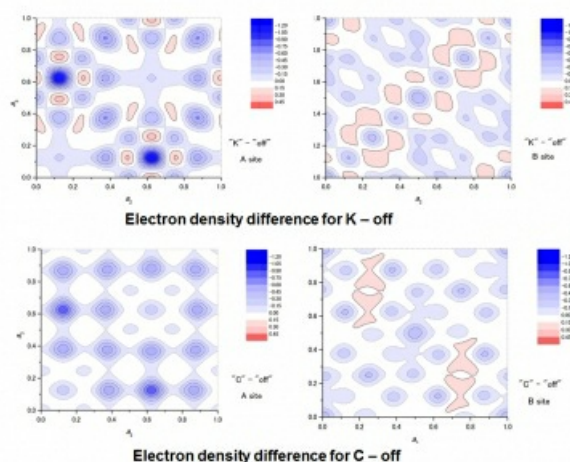
The energy state of electrons in Mn-Ferrite by XRS

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Manganese-Ferrites ($Mn_xFe_{3-x}O_4$) have been extensively studied due to their magnetic and electrical properties. The spinel structure has tetrahedral and octahedral cation sites that are referred to as A and B sites, respectively, with multiple valence states of Mn and Fe. The complicated cation distributions in $Mn_xFe_{3-x}O_4$ is of great interest to researchers since these physical properties strongly depends on it. However, due to small difference of X-ray scattering power between Mn and Fe, it is generally difficult to determine the cation distributions in $Mn_xFe_{3-x}O_4$. X-ray resonant Scattering (XRS) is a technique combining X-ray diffraction and absorption spectroscopy. Near the absorption edge, the X-ray scattering power is enhanced and it allows us to focus on selected atomic species in a crystal. The resonant process involves electronic transitions from core level into unoccupied states and analysis using the resonant effect provides information about the charge and orbital configuration of electrons. In this study, the site occupancy and the electron-density distributions of Mn in $Mn_xFe_{3-x}O_4$ were investigated by XRS. Conventional intensity measurements were made using a Rigaku AFC-5S four-circle diffractometer for Mo K α radiation. The site occupancies of Mn and Fe atoms was determined on the basis of the resonant scattering effect at the Fe K absorption edge ($\lambda = 1.7535 \text{ \AA}$), by using a vertical-type four-circle diffractometer at BL-10A of the Photon Factory, Tsukuba, Japan. The diffraction intensity data at Mn K pre-edge ($\lambda_K = 1.8978 \text{ \AA}$), threshold ($\lambda_C = 1.8944 \text{ \AA}$) and off-edge ($\lambda_{off} = 1.9019 \text{ \AA}$) was collected with an AFC-5u diffractometer at BL-6C. The difference Fourier method was used to extract the resonant effect between λ_K and λ_{off} , and λ_C and λ_{off} and determine the distribution of electrons which contribute the resonance related to the electronic transitions at λ_K and λ_C . In the presentation, energy states of 3d electrons of Mn ions and origin of the resonant effects related to electron orbits will be discussed by comparison between the electron-density distribution and DOS calculation[1].

[1]Zuo X. & Vittoria C. (2003) . IEEE Trans. Magn., Vol. 39, No. 5, (2003), pp 3133-3135.



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