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The dynamical interaction in a simultaneous twenty-four beam diffraction in a two-plate silicon cavity assembly for 14.4388 keV X-rays is studied, where the diffracted X-rays are reflected back and forth between the two crystal plates via the (12 4 0) reflection. The dynamical theory of X-ray diffraction with a Cartesian coordinate system is employed to calculate the interference pattern due to Fabry-Perot type resonance. The calculated intensity distribution of the transmitted beam is in good agreement with the measured one. The dispersion surface, linear absorption coefficients, wavefield intensities, and excitations of mode are also calculated. The formation of standing waves and phase change under the cavity resonance condition will be discussed.

Keywords: twenty-four beam diffraction, X-ray cavity, dynamical interaction

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Site-selective determination of coordination symmetries by anisotropic anomalous X-ray scattering

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Based on an experiment of *Kirfel* and *Petcov* on rutile (136) $P4_2/mnm$, which verified anisotropic anomalous scattering (AAS) by measuring 'Forbidden Reflection near Edge Diffraction' (FRED), we aimed to extend the results with allowed reflections to extract more tensor symmetries of the Ti scattering factor tensor f_{ij} by fitting the model of AAS to the experimental data. Results from DFT calculations will also be presented. Furthermore we intended to study possible restrictions for atomic site occupation of unknown structures in an identified space group due to these local symmetry relations exemplary for this model structure. Experiments were carried out at DESY/HASYLAB BL C using a Si (111) double crystal monochromator tuned to an energy of 4985 eV. An automated optimization and Ψ-scan routine for a sample setup with rotating degree of freedom assured AAS measurements at the reflection maxima. The rutile samples investigated were 10x10x1 mm^3 wafers in (001), (110) and (111) orientation and Ψ-scans were measured for the reflections 001, 220, 110 and 111. Ti occupies Wyckoff site 2*a*, its tensor symmetry must follow the local symmetry *m.mm* leaving 3 complex elements f_{11}, f_{12}, f_{33}. Simulations showed dependencies: 001 to f_{12}, 220 to f_{11}-f_{33}, 110 to f_{11}-f_{33}, 111 to f_{12}. For the 001 reflection intensity real and imaginary part correlate, but the 111 intensity displays asymmetric influence so the ambiguity is separable. The measured data show clear evidence of AAS and the 001 FRED and 111 intensities could be fitted: $f'_{Ti}\, d'_{12}$ = -5.44 * 0.5(8) $f''_{Ti}\, d''_{12}$ = 3.98 * 1.4(2) Since f_{13} and f_{23} were refined to zero, the positioning of Ti within the unit cell would by inverse symmetry arguments with respect to site symmetry only be consistent on Wyckoff sites *a*, *b*, *e*, *f*, *g* (out of *k*).

Keywords: anisotropic anomalous dispersion, X-ray resonant scattering, anomalous scattering methods

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Resonant X-ray diffraction study of low temperature magnetite

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Magnetite was one of the first magnetic materials discovered, and has historically been cited as the model charge ordered system. However, the low temperature structure is yet to be fully resolved, complicating our understanding of the nature of the superstructural ordering. We have conducted resonant x-ray scattering, examining the pre- and post sample polarisation dependence at the iron K-edge in order to probe the (0 0 odd)$_C$ and forbidden (0 0 half integer)$_C$ reflections.

Keywords: resonant scattering, anomalous diffraction, X-ray charge-density analysis

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Orbital ordering and the impurity effect in layered manganites

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The charge, spin, and orbital ordering states in perovskite-type transition metal oxides and the doped compounds have attracted much interest because of their intriguing phenomena such as high Tc superconductivity, colossal magnetoresistance effect, magnetoelectric effect and so on. Impurity ions substituted for the transition metal ions in these compounds effect a change in the local electronic state. In this study we have investigated the impurity effect on the charge/orbital ordering of layered manganites by using resonant x-ray scatting (RXS). A layered manganite $La_{0.5}Sr_{1.5}MnO_4$ shows charge and orbital ordering below about 220 K. We have studied how the ordering state is changed by the substitution of Cr, Fe, Ga ions for Mn ions by using RXS at absorption edge energy (EA) of Cr, Fe, Ga as well as Mn. The RXS at Mn EA in $La_{0.5}Sr_{1.5}Mn_{0.97}Cr_{0.03}O_4$ has almost the same intensity as that in the pure compound $La_{0.5}Sr_{1.5}MnO_4$. In contrast, we could not observe any RXS intensity at Mn EA in $La_{0.5}Sr_{1.5}Mn_{0.97}Fe_{0.03}O_4$. These results indicate that the charge and orbital ordering state is not changed by the substitution of Cr but the orderings collapse by the substitution of Fe. Moreover, the most interesting result is the Ga substitution effect. The RXS at Mn EA in $La_{0.5}Sr_{1.5}Mn_{0.97}Ga_{0.03}O_4$ has four times larger intensity than that of the pure compound: The orderings in $La_{0.5}Sr_{1.5}Mn_{0.97}Ga_{0.03}O_4$ become strong by the substitution. We have

tried to get the RXS at Ga EA but could not detect the signal within our experimental error. This means the local orbital state at Ga site is quite isotropic in the ab-plane of the compound.

Keywords: orbital ordering, impurity effect, resonant X-ray scattering

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Flipping ratio in circularly polarized X-ray diffraction

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The flipping ratio in circularly polarized x-ray diffraction has been expected to be complementary technique to that in polarized neutron diffraction which is known as a powerful technique to investigate magnetization density distribution in atomic scale. However, the establishment of this technique has been prevented by extremely small flipping ratio. The purpose of the present study is to make this promising technique practicable by applying the helicity modulation technique which has been used in highly accurate x-ray magnetic circular dichroism measurements at BL39XU/SPring-8. This experiment was performed on the synchrotron radiation facility SPring-8. Linearly polarized x-ray from an undulator was transformed into circularly polarized one by a diamond x-ray phase retarder. The Flipping ratio in diffraction intensity was measured by modulating photon-helicity at a certain frequency and detecting synchronized response of diffraction intensity through lock-in amplifier. Charge scattering ought to cancel out in this technique. The result of the first experiment revealed two fatal problems on lock-in amplifier output; an extremely large background and alteration of output on time. The cause of these problems was supposed to be residual charge scattering arising from counter error in degree of circular polarization between right and left handed one, which was induced by shift in incident angle of x-ray beam into a phase retarder. Therefore it became clear that the feedback system for optimizing the incident angle into a phase retarder is essential to eliminate these problems. We have recently invited a feedback system and succeeded in solving the technical problems on measuring flipping ratio in circularly polarized x-ray diffraction by using this feedback system.

Keywords: X-ray diffraction technique, X-ray polarization, magnetic X-ray scattering

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Development of a polarization rotator for X-ray magnetic diffraction

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X-ray magnetic diffraction is a promising method to directly determine not only electronic spin and orbital angular momentum density distributions in materials but also the chirality of higher-order magnetic structure. Moreover the combination of X-ray magnetic diffraction with microbeam technologies will make it possible to investigate magnetic structures in mesoscopic system. However experimental techniques of X-ray magnetic diffraction have remained almost unchanged for two decades. In order to take advantage of high-performance of the third generation synchrotron radiation source, we have developed a polarization rotator for the experimental separation of spin and orbital contribution to magnetization (LS separation). The polarization rotator was assembled from a pair of diamond X-ray phase retarders functioning as quarter-wave plate (QWP). The first QWP transformed linear polarization into circular one and the second QWP did inversely. Inclination angle of the polarization plane of transmitted X-ray is controlled by rotating an optic axis of the second QWP around the traveling direction of transmitted X-ray. The performance of the polarization rotator was evaluated at an X-ray undulator beamline, BL29XUL of the SPring-8. We have confirmed that polarization of transmitted X-ray is manipulated as expected. The performance of the polarization rotator can be designed so as to give priority to degree of polarization or photon flux, which facilitates X-ray magnetic diffraction experiments. We have conducted an LS separation study on holmium using the polarization rotator. The results were well explained by theoretical value of L(K)/S(K)=9.7 within experimental error. This polarization rotator significantly improved measurement precision.

Keywords: X-ray magnetic diffraction, X-ray polarization, polarization rotator

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Multiple-wave X-ray resonant diffraction using iterative Born approximation

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Multiple-wave X-ray diffraction, a phase-sensitive scattering process, is a useful tool for studies in crystallography and solid state physics. According to the dynamical theory, the asymmetry of a three-wave intensity distribution is closely related to x-ray phase, scattering factor, structure factor and charge distribution. Based on this, recently we have successfully connected the information of anomalous fine structure function with the variation of three-wave intensity profiles in the vicinity of an absorption edge. Moreover, by measuring the multiple-wave intensity profiles near absorption edges (at resonance), one can easily obtain the EXAFS/DAFS-like local structure information either by the dynamical theory or iterative Born approximation. However, the iterative Born approximation, not like the dynamical theory, is simpler and easier to handle, which can be applied to diffraction from epitaxial thin films. In this paper, we will report on the iterative Born approximation method and illustrate how it works for the analysis of multiple-wave X-ray resonant diffraction.

Keywords: multiple-wave diffraction, resonant diffraction, iterative Born Approximation