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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 $10 \times 10 \times 1$ mm³ wafers in (001), (110) and (111) orientation and Ψ -scans were measured for the reflections 001, 220, 110 and 111. Ti occupies Wyckoff site $2a$, 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 T_c 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 scattering (RXS). A layered manganite La_{0.5}Sr_{1.5}MnO₄ 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}O₄ has almost the same intensity as that in the pure compound La_{0.5}Sr_{1.5}MnO₄. 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}O₄. 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}O₄ 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}O₄ become strong by the substitution. We have