Near-Edge Forbidden Reflections in Resonant Diffraction by Modulated Crystals

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High sensitivity of the atomic tensor factor near absorption edges to the displacements of both resonant and neighbouring atoms can provide additional reflections in resonant X-ray diffraction by incommensurately modulated crystals. In the presence of modulation the local symmetry of each resonant atom becomes lower than in the basic structure, hence additional tensor elements can appear. In this report, some calculations of the structure factors are presented for the Co-åkermanite taking into account what already known [1] about its two-dimensional modulation. Co atoms, in the corresponding basic structure, are in the (2a) sites with $\overline{4}m$ symmetry of the $P \overline{4}2_1m$ space group, which make it impossible to obtain any forbidden reflections near Co K-edge in the dipole-dipole approximation. However, the main reflections h00, h=2n+1 corresponding to the basic structure can appear near Co K-edge owing to the dipole-quadrupole contribution. We showed that the displacement terms in the anisotropic tensor factor could mainly contribute to the first order satellites, providing the forbidden reflections satellites near the Co K-edge with hhlm0, m=2n+1 or $h00m \ m, \ h=2n+1$.

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[1] Hagiya K., Kusaka K., Masaaki O., Iishi K., *Acta Cryst.*, 2001, **B57**, 271. Keywords: x-ray anisotropy, incommensurate crystals, satellites