

[s7.m7.p1] Application of D.A.N.E.S. studies to highly Absorbing Powdered Samples. S. Bos, H. Renevier, Y. Joly, V. Favre-Nicolin, E. Lorenzo, J.F. Berar, J.L. Hodeau. *Lab. de Cristallographie C.N.R.S. Grenoble-F.* V. Cajipe, P. Leone, C. Gueho, *I.M.N., Nantes-F.* G. Vaughan, *E.S.R.F. Grenoble-F.*
Keywords: DAFS, powder diffraction, anomalous scattering.

In Diffraction Anomalous Near Edge Spectroscopy, the long range structural information contained in the diffraction peaks is combined with the chemical selectivity of X-ray Absorption. Pioneering D.A.N.E.S. works on powders performed by Pickering *et al.* at the N.S.L.S. and Vacinova *et al.* at the E.S.R.F. have shown the possibility, but also the intrinsic limits, of such method applied to powders (low count rate, sampling problems and fluorescence scattering). To surpass these difficulties and to improve the anomalous data collection process on powders, on BM2 beamline at the E.S.R.F., we have performed D.A.N.E.S. studies on $\text{La}_4\text{Mn}_5\text{Si}_4\text{O}_{22}$ a mixed valence manganese oxide. This absorbing compound (absorption length of $\sim 8 \mu\text{m}$ below the absorption edge) contains three valence states of manganese Mn^{4+} , Mn^{3+} and Mn^{2+} , distributed over three crystallographic sites.

Diffacted intensities have been collected around the K absorption edge of manganese ($E = 6539 \text{ eV}$). Regarding data quality, energy scans at fixed Q positions of selected reflections is preferred to the collection of complete powder patterns at a 20-30 discrete energies. With an adequate sample spinning and a large acceptance analyser, we have obtained very good intensity versus energy spectra of different reflections. Absorption coefficient was extracted from the fluorescence spectra collected simultaneously to the diffracted intensities. D.A.N.E.S. analysis was performed by using eight reflections containing crossed combinations of the three manganese sites. After normalisation of the calculated intensities far from the edge to the observed ones using theoretical f and f' values, a refinement of the anomalous scattering factors for the three different manganese sites of this structure give three different edge positions, shifted one relatively to the other by 3 eV and 4 eV and related to the presence of three different oxidation states in the three non equivalent sites. This study shows that valence states and D.A.N.E.S. studies can be performed on samples like powders even if they are extremely absorbing.

[s7.m7.p2] Determination of Resonant Atomic Scattering Factors and observation of DAFS in the Soft X-Ray Range using Bragg Diffraction from Multilayers. H. Grimmer¹, U. Staub¹, O. Zaharko¹, H.-Ch. Mertins², ¹Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, ²BESSY GmbH, Albert-Einstein-Str. 15, D-12489 Berlin, Germany.
Keywords: resonant scattering, atomic scattering factor, DAFS.

Bragg diffraction of synchrotron radiation from Co/C, V/Ni and Ti/Ni multilayers has been used to determine the real and imaginary parts of the atomic scattering factor $f=f'+if''$ around the K edge of carbon and the $L_{2,3}$ edges of Ti, V, Co and Ni. The independent measurements of f' and f'' have been tested for coherency using the Kramers-Kronig relation.

DAFS has been observed in multilayers above the $L_{2,3}$ edges of Fe, Co, Ti and V¹.

[1] Staub U., Grimmer H. and Mertins H.-Ch. "Soft x-ray diffraction anomalous fine structure on Ni/V multilayers.", *J. Phys.: Condens. Matter*, (1999), 11: 5691 - 5697.