ESRF

Experiment title: Moment urn Transfer Dependence of Inelastic X-ray Scattering from the Li K-edge

Experiment number: HC397

Beamline:	**Date of Experiment:**		**Date of Report:**
ID16/BL21	from: 29.5.96	to: 07.06.96	01.10.96

Shifts:	**Local contact (s):**	*Received at ESRF:*
21	M. Krisch	

Names and affiliations of applicants (*indicates experimentalists):

M. Krisch, F. Sette, C. Masciovecchio, and R. Verbeni
Inelastic Scattering Group, ESRF

Report:

Inelastic x-ray scattering (IXS) with 80 *meV* energy resolution from the Li K-edge was measured at 8.7 nm^{-1} and 97 rim-l momentum transfer, q, in lithium metal at 30 K. The transition from dipolar $1s \rightarrow p$ excitations at small q, to monopolar $1s \rightarrow s$ excitations at large q, - predicted theoretically by Doniach et al. [1] -, could be demonstrated by spectral changes reflecting either the p or s partial empty density of states above the Li Fermi level. The possibility of switching the symmetry of the final state in the scattering process by simply changing the momentum transfer to the sample, allowed to determine the exponents α_0 and α_1 of the Mahan, Nozières, and De Dominicis [2,3] (MND) threshold theory. The MND theory casts the spectral shape near an x-ray absorption threshold into an analytical form, in which many-body- effects, due to the reaction of the conduction electron cloud on the creation of the core-hole, are contained in the threshold exponents α_l, where l is the angular momentum quantum number of the conduction-state wave function of the photoelectron. A complete and satisfying explanation of the Li K-edge was still missing, due to the incompatibility of the experimentally determined values of the singularity index α (from photoemission) and α_1 (from soft x-ray absorption) with two sum rules of the MND theory. From a careful analysis of the threshold line shape we obtain $\alpha_1 = +0.05$ and $\alpha_0 = -0.13$. The value of α_1 close to zero confirms earlier results. Moreover, both values are in good agreement with calculations of Girvin and Hopfield [4], who included exchange effects in the many-body interactions. It is therefore tempting to conclude that the present determination of α_1 and α_0 shows experimentally the importance of exchange effects between the ls core-hole and the lithium valence electrons, and thus finally provides a satisfying explanation of the many-body effects at the Li K-edge.

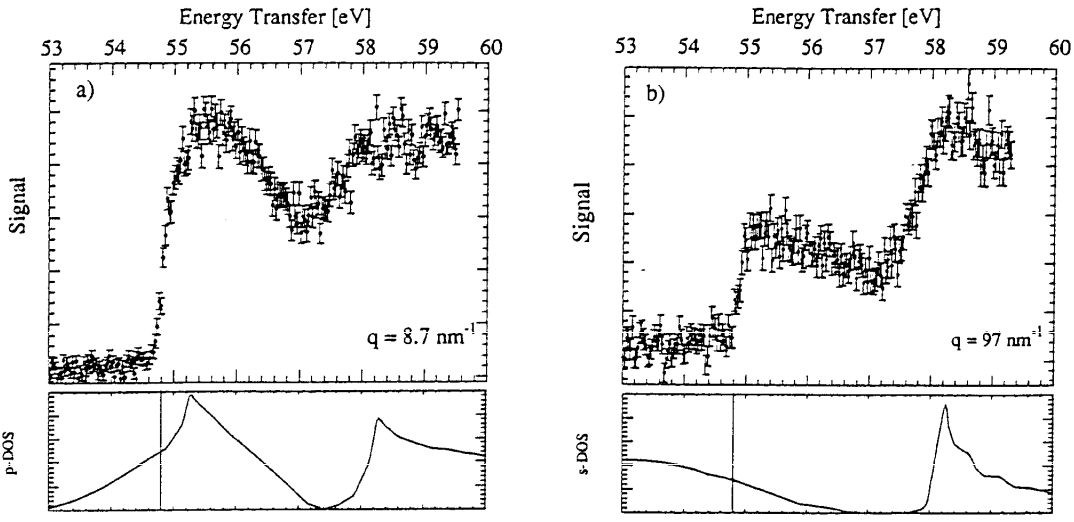

FIG. 1 -Inelastic scattering spectra from the Li K-edge at an incident photon energy of $\hbar\omega_1$=10 keV and momentum transfers q=8.7 rim-1 (a) and 97 nm^{-1} (b) as a function of energy transfer $\hbar\omega_1$-$\hbar\omega_2$. The data are shown with their error bars. The bottom panels show the p-(a) and s-(b) partial density of states [5]; the Fermi level is indicated by the vertical line.

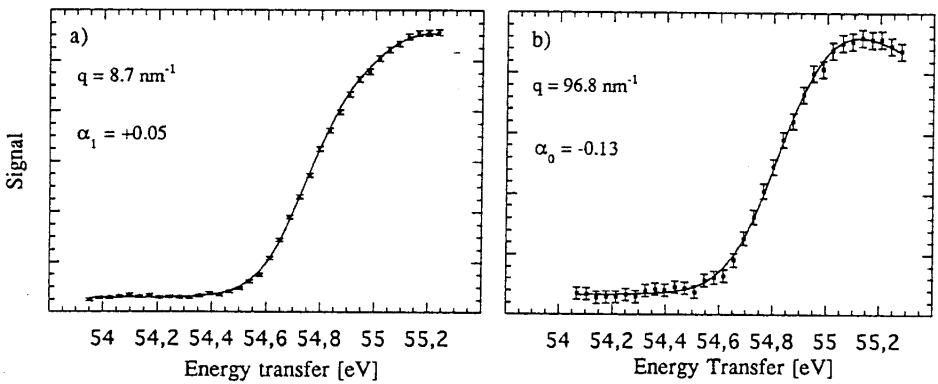

FIG. 2- Inelastic scattering spectra in the immediate vicinity of the Li K-edge at q=8.7 nm^{-1} *(a)* and 97 rim-l (b) as a function of energy transfer. The threshold exponents α_0 and α_1 are obtained by a χ^2 minimization of the experimental data (shown with their error bars) with the MND threshold function, multiplied with the corresponding empty density of states, and convoluted by phonon broadening, lifetime, and experimental resolution broadening functions (solid line).

[1] S. Doniach, P.M. Platzman, and J.T. Yue, Phys. Rev. **B** **4,3345** (1971).
[2] G.D. Mahan, Phys. Rev. 163,612 (1967).
[3] P. Nozières and C.T. De Dominicis, Phys. Rev. 178,1097 (1969).
[4] S.M. Girvin and J.J. Hopfield, Phys. Rev. Lett. 37,1091 (1976).
[5] D.A. Papaconstantopoulos, Handbook of the band structure of elemental solids, Plenum Press, New York and London, (1986).