ESRF	**Experiment title:** Element specific and symmetry selective determination of the electronic band structure of solids by resonant inelastic scattering spectroscopy RIXS: A Model Experiment	**Experiment number:** HE-683
Beamline: ID16	**Date of Experiment:** from: 25-Aug-99 to: 31-Aug-99	**Date of Report:** 25-Feb-00
Shifts: 18	**Local contact(s):** J.-P. Rueff, A. Shukla	*Received at ESRF:* 11 - MAR 2000

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Report:

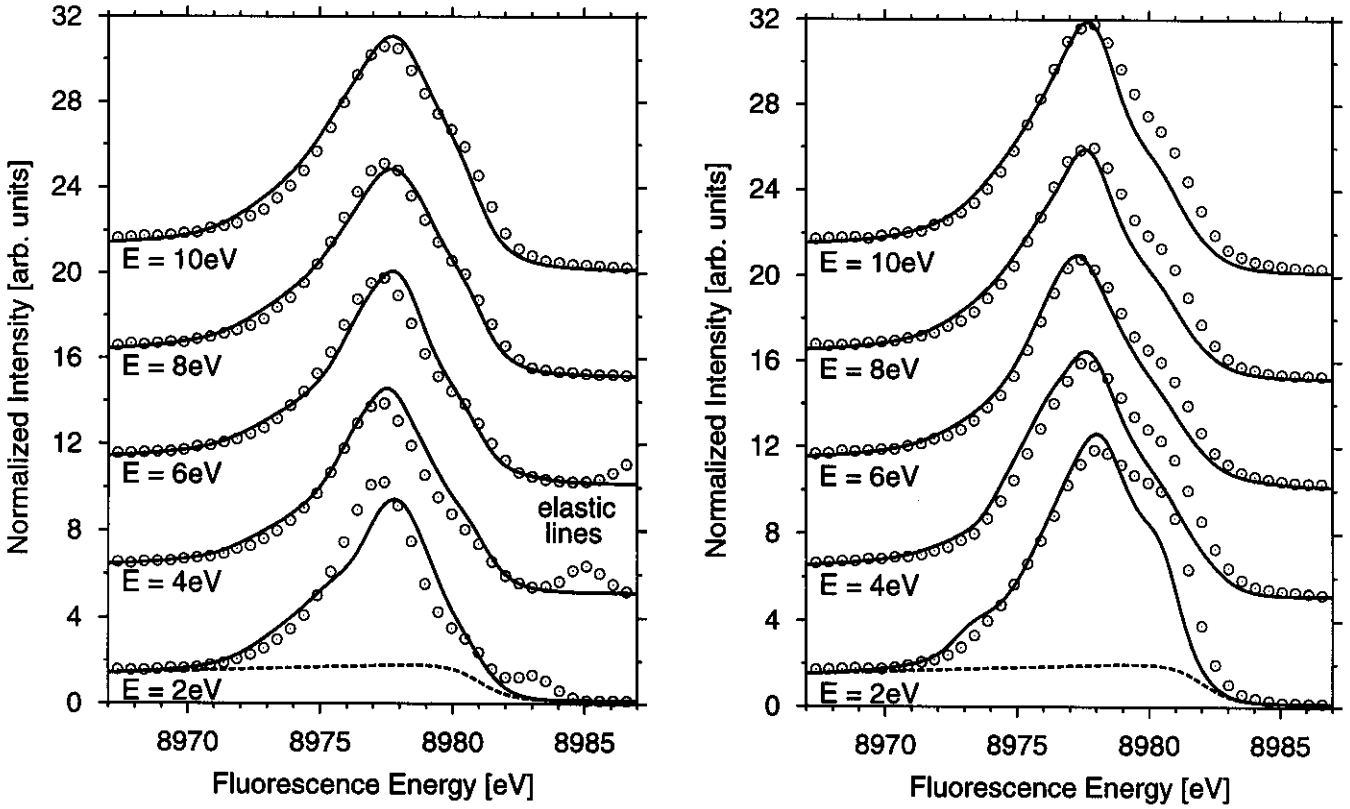
It has been shown recently, that the shape of resonantly excited fluorescence spectra from valence bands even for hard x-rays is determined by the properties of the electronic band structure via the Bloch $\vec{k}$-selectivity of the absorption and emission process/1,2/. The shape of the fluorescence spectrum changes if either the energy of the incident photon E_i or the momentum $\vec{q}$ transfered during the inelastic scattering process is changed. This effect can in reverse be exploited to probe the band structure element specifically and symmetry selectively. Thus, after having measured resonantly excited fluorescence spectra for a variety of $\vec{q}$ and incident energies E_{in}, one can extract the information about the band structure (not only energy position of the bands, but also their symmetry element-specifically), that is contained redundantly in these spectra. This so-called "ill-posed inverse problem" can be solved using appropriate well-established methods as maximum entropy/3/.

The aim of this experiment was to collect a set of RIXS spectra that is appropriate for the above mentioned reconstruction. Since its properties seemed to make it well suited as a model substance in this experiment, we had proposed GaAs as the sample. But as we found out in a test run during inhouse research time (see attached report), semiconductors and insulators are no appropriate samples to measure RIXS spectra since the presence of a core exciton destroyes the Bloch $\vec{k}$-momentum conservation which is essential for this kind of experiment. We therefore decided to use Copper instead of GaAs as the sample. Like GaAs, Copper has a simple and well understood band structure and was successfully used in a previous experiment of similar kind /4/.

Thus we have investigated 8 different values of the momentum transfer $\vec{q}$ and 5 different values of the incident energy E_{in} for each $\vec{q}$. The values of $\vec{q}$, reduced by some reciprocal lattic vector $\vec{G}$, were choosen to be uniformly distributed within the first Brillouin zone, comprising the 5 high symmetry points Δ, X, W, Σ, and L of the fcc Brilluoin zone. The values of the incident energy were 2, 4, 6, 8, and 10 eV above the Cu K edge (E_K = 8980 eV). For two values of $\vec{q}$ the results are shown below.

The strong dependence of the shape of the valence fluorescence spectra on both the incident energy E_{in} and the momentum transfer $\vec{q}$ is clearly visible. The essential features of the measured spectra (circles) are resembled in the calculation (solid line).
The intense low energy tail of the valence line is due to the so-called 'shakeoff satellite'. This satellite, sometimes referred to as 'radiative Auger effect' /5/, originates from the excitation of a second valence electron into the conduction band during the relaxation of a valence electron into the core hole while emitting the fluorescence photon. Therefore the energy of the emitted photon is reduced by the energy that is necessary to excite the second valence electron. The minimum energy loss the photon can suffer is close to zero whereas the maximum energy loss is in principle unlimited. Since the transition probability for large losses is smaller than for small losses the shakeoff satellite shows a slowly decreasing tail on its low energy side and a steep drop on its high energy side, that is coincident with the high energy tail of its mother line, thereby obscuring the fine structure of the valence line as can be seen in the figures.
Thus, before the acquired fluorescence spectra can be used in the reconstruction of the band structure, the shakeoff satellite must be accounted for. Until now we have tried to approximate the satellite by a linearly rising line multiplied by a Fermi function that is centered at the high energy side of the valence line /1/ (dashed line in the figures), but most likely this arbitrary approximation will introduce errors into the reconstruction procedure. The shakeoff satellite can not be measured independently from its mother line but it can be calculated as the convolution of an energy loss function with the energy distribution of the mother line /6/. Therein the loss function contains all information about the shakeoff process that is: 1. the DOS of the electrons that can be excited into the unoccupied states, 2. the unoccupied DOS, and 3. the transition probability between those two states.
Before this calculation procedure for the shakeoff satellite can be used in the reconstruction, its validity must be checked which requires further investigation (see new proposal).

Figures: RIXS from Cu, $\vec{q} = W$ (left) and $\vec{q} = L$ (right) .



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