ESRF	**Experiment** title: Resonant inelastic X-ray scattering from the Cu- valence band	**Experiment number:** HE-116
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Report:

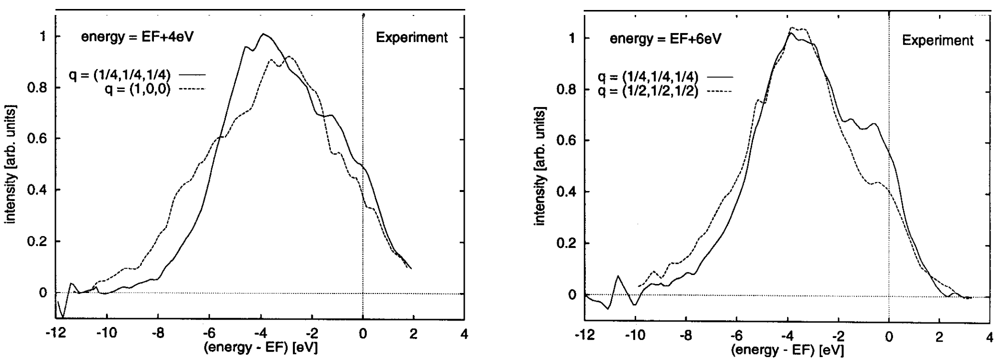
X-ray absorption and emission, if considered as two coherently coupled processes when the conditions for resonant Raman scattering are fulfilled, are linked by a law of momentum conservation, connecting wave vectors of the incident and the emitted photon wave, the momentum transfer $\vec{q}$ caused by the scattering process and the Bloch-$\vec{k}$-vectors of the involved electronic states of the transition. It is therefore possible to investigate valence and conduction bands of solids in a Bloch-$\vec{k}$-selective manner /1/, allowing to exploit the advantages of X-ray spectroscopy (element-, symmetry and bulk-sensitivity). It was our goal to prove the connection of prominent features of the electronic band structure to the shape of resonantly excited valence fluorescence spectra. From preliminary calculations we saw that this goal could better be achieved using a Cu sample, rather than using the earlier proposed Ge-sample.
Therefore, we performed measurements of the valence emission of Cu for excitation energies around the Cu K edge. We scanned the primary energy within the range of E_K to $E_K + 10\ eV$ and observed the shape of the Cu-K_{β_5} line using the Raman spectrometer at beamline ID 16. An overall energy resolution of 0.9 eV was achieved. Emission spectra were measured for three different $\vec{q}$-values: $\vec{q} \parallel (111)$ with $|\vec{q}| = 0.4 a.u.$ and $0.8 a.u.$ and $\vec{q} \parallel (100)$ with $|\vec{q}|=0.9$ a.u.
The experimental spectra obtained were confronted with calculations of valence emission spectra based on a LAPW calculation /2/ of the electronic band structure of Cu. The calculation of the valence emission spectra is performed along this line:

- For a given excitation energy, the possible Bloch-$\vec{k}$-vectors within the first Brillouin zone to which a Is-electron can be excited, are deduced from the band structure of unoccupied states.
- The law of momentum conservation for the coherently coupled absorption and emission process is used to calculate those Bloch-$\vec{k}$-points from where reemission from the valence band is allowed, simply by adding $\vec{q}$ and backfolding into the first Brillouin zone)

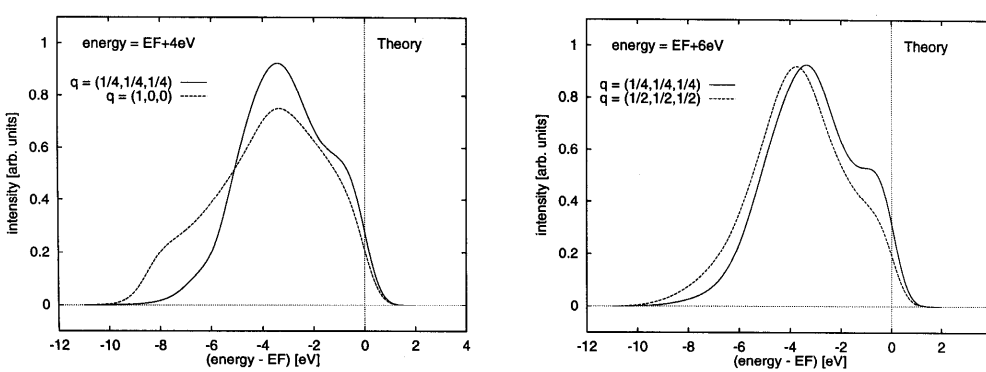
- For all these z-points, emission contributions are summed up, weighted according to symmetry character and density of states of the contributing bands.

The Figures show a comparison of theoretically and experimentally obtained spectra, which are in general in a very good agreement. It must be noted, that in contrary to theoretical predictions by Carra et al. /3/, no contribution from disturbing core-exciton-processes had to be taken into account to achieve this good agreement. This can be attributed to the large screening of the core-hole-state at higher energies.
We therefore state that the measurement of resonantly excited valence spectra is a promising tool to investigate the properties of electronic band structures. In a next step, this method will be applied in a way that will allow to determine the electronic band structure in an ARPES-like manner by measuring for a series of {and so chasing the signatures of certain bands and their dispersion.

Experimental spectra for $\vec{q}\,\|(111)$, $q = 0.4a.u.$ and $\vec{q}\,\|$ (100), q = 0.9a.u. for $E_{in} = E_K + 4eV$ (left) and for $\vec{q}\,\|(111)$, $q = 0.4a.u.$ and $\vec{q}\,\|(111)$, $q = 0.8a.u.$ for $E_{in} = E_K + 6eV$ (right)



Theoretical spectra for $\vec{q}\,\|(111), q = 0.4a.u.$ and $\vec{q}\,\|$ (100), $q = 0.9a.u.$ for $E_{in} = E_K + 4eV$ (left) and for $\vec{q}\,\|(111)$, $q = 0.4a.u.$ and $\vec{q}\,\|(111)$, $q = 0.8a.u.$ for $E_{in} = E_K + 6eV$ (right)



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/3/ P. Carra et al., Phys. Rev. Lett 43, 68 (1997), ESRF-newsletter 29, 20 (1997)