ESRF

Experiment title: Resonant inelastic X-ray scattering from Cu and Ge valence bands

Experiment number: HC-312

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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 conservation of momentum relation, connecting wave vectors of the incident and the emitted wave, the momentum transfer $\vec{q}$ caused by the scattering process and the Bloch-k-vectors of the involved electronic states of the transition. It is therefore possible to investigate valence and conduction bands of solids in an Bloch-$\vec{k}$-selective manner /1/, allowing to exploit the advantages of X-ray spectroscopy (element- and bulk-sensitivity). It was our goal to extend this usefull technique to the hard X-ray region,

Therefore, we performed measurements of the resonantly excited fluorescent emission from the Ge-valence band using a single-crystalline sample. We scanned the primary energy within the range of E_o = 11,088 *eV* to E_o = 11.112 *eV* and observed the shape of the **Ge-K**$_{\beta_2}$-line using the medium energy resolution setup of beamline BL 21 and the installed Raman spectrometer. For this energy range together with the monochromator crystal installed at the beamline (Si (111)-reflection), an energy width of the primary beam of 2.5 *eV* could be achieved. This type of scan was performed for three different $\vec{q}$-values: $\vec{q} \parallel [111]$, $\vec{q} \parallel [110]$ with $|\vec{q}| = 0.5$ a.u. and $\vec{q} \parallel [111]$ with $|\vec{q}| = 4.1$ au.

The fig. shows some of the obtained fluorescence spectra for primary energies below the Ge absorption edge (E_{Ge_K} = *11.103 eV)* exhibiting the following features:

- contributions of the Ge-plasmon (marked **A**). This feature vanishes a) for large $|\vec{q}|$ and b) when E_o reaches E_{Ge_K} due to absorption within the sample. Note, that this plasmonic excitation does not show any resonant behaviour.
- the Ge K_{β_5}-line (marked **B**) due to transitions from M_{IV}, M_V to K

- a broadening of the flourescence excitation for $E_o = 11.099,5\,eV$ and $\vec{q} \parallel [111]$ in comparison to the spectra for $\vec{q} \parallel [110]$ that can be understood as follows: Excitation from the Is-core-level to the lowest conduction bands will end up around the X- and the Γ-point (see Fig.). Adding a momentum transfer of [111]-type and the correct magnitude of 0.5 au. shows, that emission will take place mainly from states around the L-point where there is a high DOS /2/. This does not hold for $\vec{q} \parallel [110]$, in this case emission takes place merely from states between Γ and X. This effect demonstrates the **validity of momentum conservation for emission and absorption,** when excitation takes place resonantly.

/1/ Ma et al., Phys. Rev B48, 2109 (1993)

/2/ Papaconstantopoulos: Handbook of band structures, Plenum, N. Y.