ESRF	**Experiment title:** Resonant inelastic x-ray scattering (RIXS) from NiAl at the Ni-K-edge	**Experiment number:** HE 459
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Report:

Recent studies /1/ have shown that in the case of resonantly excited fluorescence emission from valence electrons the two-step model of absorption followed by emission breaks down. In this case the absorption and emission of a photon has to be treated as one single resonant inelastic scattering process, giving rise to a law of Bloch $\vec{k}$-momentum conservation which couples the processes of absorption and emission of a photon. As a result the shape of resonantly excited valence fluorescence spectra strongly depends on both the excitation energy and the momentum transfer $\vec{q}$ allowing one to investigate the electronic band structure of the valence electrons Bloch $\vec{k}$-selectively. Moreover, due to the resonant excitation, this technique is element specific and symmetry selective giving the possibility to trace bands of a certain character that belong to a certain element.
Contrary to soft x-rays, the momenta of hard x-ray photons are no longer negligible but are of the same order as the dimensions of the first Brillouin zone. Thus, the momentum transfer $\vec{q}$ can be varied by changing the scattering angle to probe the whole Brillouin zone Bloch $\vec{k}$-selectively.
It was our goal to show the selectivity of RIXS to Bloch $\vec{k}$-momentum, element, and symmetry in the hard x-ray regime. As for previous experiments on Copper, the effect of Bloch $\vec{k}$-selectivity on the RIXS spectra of Ni in NiAl was calculated, showing an even stronger effect than for Copper/2/.
Resonantly excited fluorescence spectra were measured at beamline ID28 using the Raman specrometer, achieving an overall experimental resolution of 1.0 eV. A set of spectra was measured with four $\vec{q}$-values parallel to the 110 axis and 5 different primary energies $\hbar\omega_1$ for each $\vec{q}$. The experimentally choosen absolute values of $\vec{q}$ were 0.1, 0.25, 0.4, and 0.5 in units of $|\langle 110\rangle| \cdot 2\pi/a$, a being the lattice constant, whereas the excitation energies $\hbar\omega_1$ for each $\vec{q}$ were set to 0.6, 1.1, 1.7, 2.4, and 5.5 eV above the 1s binding energy of Ni. One series for fixed $\vec{q}$ and two series for fixed $\hbar\omega_1$ are shown in the figure.
Together with the measured spectra (dashed lines) we show calculated resonant fluorescence spectra (solid lines). These are based on a LAPW band structure calculation using the WIEN97 package /3/.

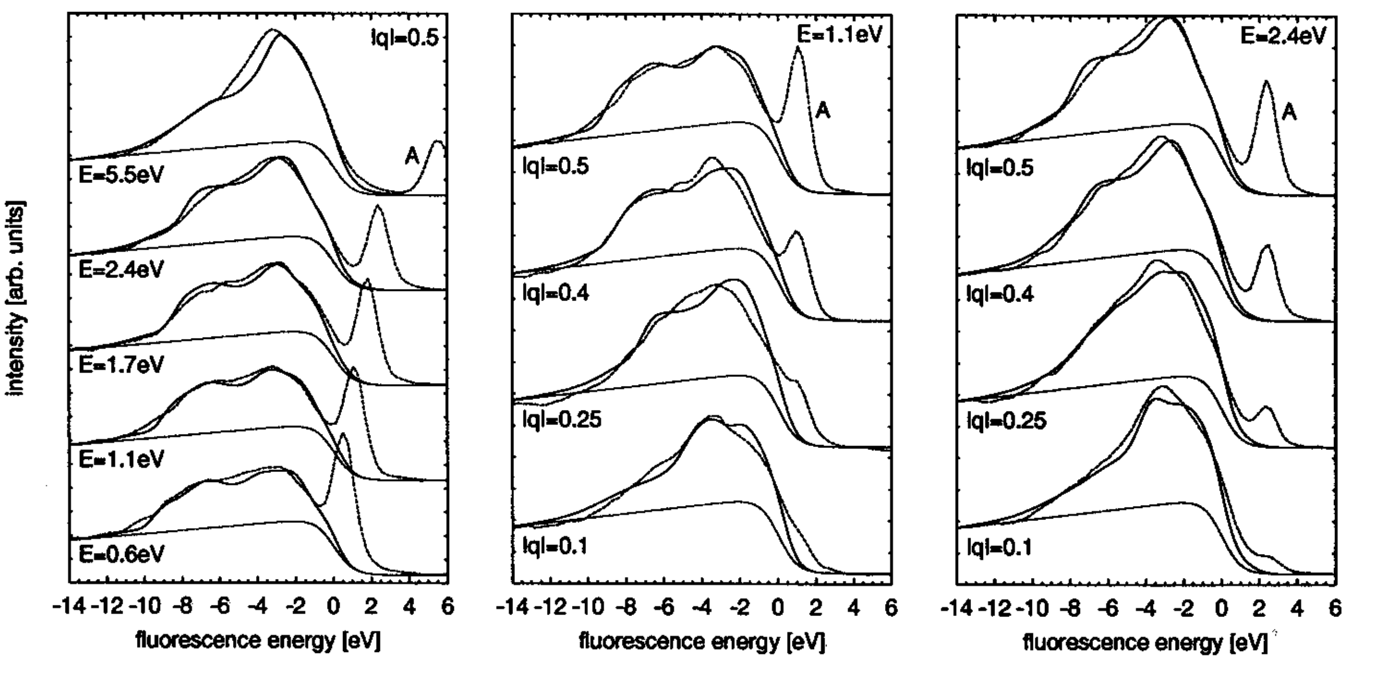
The energy eigenvalues and the partial charges at 9139 $\vec{k}$-points in the irreducible wedge of the first Brillouin zone have been taken into account. As a result of the element specificity and the dipole selection rule mainly Ni 4-p states contribute to the emission spectra. Further on we have accounted for the resolution of the monochromator (0.85 eV) and the spectrometer (0.5 eV) together with the energy width of the core hole due to the finite life time of the intermediate state (1.5 eV) in the calculation.

The dotted lines denote the so-called shake-off satellite on top of which the fluorescence line rests. This satellite originates from the excitation of a second valence electron into the conduction band during the emission process, sometimes referred to as a radiative Auger effect /4/. The satellite line shown does only mimic its general behavior because to our knowledge there exists up to now no calculation in this energy region. To make the calculated spectra comparable to the experiment we show the sum of the calculated spectra and the estimated satellite.

As can clearly be seen, there is in general a very good agreement between measured and calculated spectra. Differences are most likely to originate from the satellite whose fine structure is not known so far. Dispersive features are present in both constant $\vec{q}$ and constant $\hbar\omega_1$ series, definitively prooving the validity of the mechanism of Bloch $\vec{k}$-selectivity. We have to emphasize that, contrary to soft x-ray RIXS, in this case there is no so-called incoherent contribution originating from interactions of the intermediate state with phonons and excitons that leads to a breakdown of the $\vec{k}$-selectivity.

The short life time of the intermediate state, ruling out such effects, and the large photon wave vectors allowing one to scan the whole Brillouin zone without changing the primary energy are clear advantages of the use of hard x-ray for RIXS.

Figures: Measured (dashed lines) and calculated (solid lines) spectra together with the estimated shake-off satellite (dotted line): for constant momentum transfer (left pannel), for constant primary energy (middle and right pannel). The primary energy $E = \hbar\omega_1$ and the fluorescence energy $\hbar\omega_2$ are scaled to be Zero at the Ni 1s binding energy (8333 eV). $|\vec{q}|$ is given in units of $|\langle 110\rangle|\frac{2\pi}{a}$. The narrow peaks labeled with A are due to quasielastic scattering and define the experimental resolution function.



/1/ See for example J. A. Carlisle *et al.*, Phys. Rev. B **74**, 1234 (1995) and references therein.

/2/ ESRF report to experiment HE-116, also H. Enkisch *et al.*, submitted to Phys. Rev. B.

/3/ P. Blaha, K. Schwarz and J. Luitz, **WIEN97**, Vienna University of Technology, Vienna 1997, updated version of P. Blaha, K. Schwarz, P. Sorantin, and S.B. Trickey, Comp. Phys. Commun. **59**, 399, (1990).

/4/ T. Åberg, Phys. Rev. A **4**, 1735 (1971).