ESRF	**Experiment title:** New way of band mapping of NiO using resonant inelastic x-ray scattering	**Experiment number:** HE-3310
Beamline: ID16	**Date of experiment:** from: 27-Jan-2010 to: 02-Feb-2010	**Date of report:** 21-Sep-2010
Shifts: 18	**Local contact(s):** Simo Huotari	*Received at ESRF:*

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Report:

The aim of the experiment was to study the crystal field excitation spectra of NiO using high-resolution RIXS at the Ni K edge, as a function of transferred crystal momentum. The idea was to confirm **k**-dependence of the RIXS cross section and its use as a novel tool as a unoccupied-band mapping.

The experiment was done at the beamline ID16. The incident beam from three consecutive undulators was monochromatised by a combination of a cryogenically cooled double-crystal Si(111) premonochromator and a Si(444) channel-cut postmonochromator; the resulting incident bandwidth was 80 meV. The beam was focused into a spot size of 35×100 μm (V×H) on the sample, which was a cuboid-shaped single crystal of NiO. The spectrometer was based on a vertical Rowland circle with a spherically shaped but diced Si(551), curvature radius $R = 1$ m. The photon energy was 8.3 keV, corresponding to the Ni K edge.

The experimental technique was resonant inelastic x-ray scattering (RIXS), in which the energy-loss (energy transfer value denoted as E) spectra of valence-electron excitations are measured as a function of incident-photon energy E_1. Thus the spectra depend on both E_1 and E, represented in two-dimensional RIXS plane.

The purpose of this experiment was to study the reduced-wave-vector (**k**) dependence of the RIXS plane in NiO. The possibility for this Bloch wave vector dependent RIXS [1] in NiO is offered by the very localized and well-separated nature of different excitation channels that probe different final states, which in turn depend on the band structure. The measurements were done by tuning the incident-photon energy E_1 around the nearly-quadrupolar pre-edge (around 8.332 eV) of the Ni K absorption edge, shown in Fig. 1a. We used the $\mathbf{G} = [3\ 0\ 0]$ reciprocal space vector as the zone center. This allowed us to work close to 90° scattering angle, minimizing nonresonant quasielastic scattering. The RIXS maps of NiO in the d-d excitation region have typically three discernible peaks, which we label A,B, and C, at $E = 1$ eV, 1.6 eV, and 3 eV, respectively. In NiO in the $D4h$ symmetry the possible intermediate states with $3d^9$ configuration are of a_1 and b_1 symmetries. We have noted [2] that it is more probable for the peak A to be originated from the a_1 state, and for peak B from the b_1 state. By observing the E_1-dependence of the peaks A and B, it becomes possible to infer the relative splitting of the unoccupied a_1 and b_1 states as a function of **k** (Fig.1 right panel). Further analysis and theoretical calculations are currently being done, and a manuscript is under preparation.

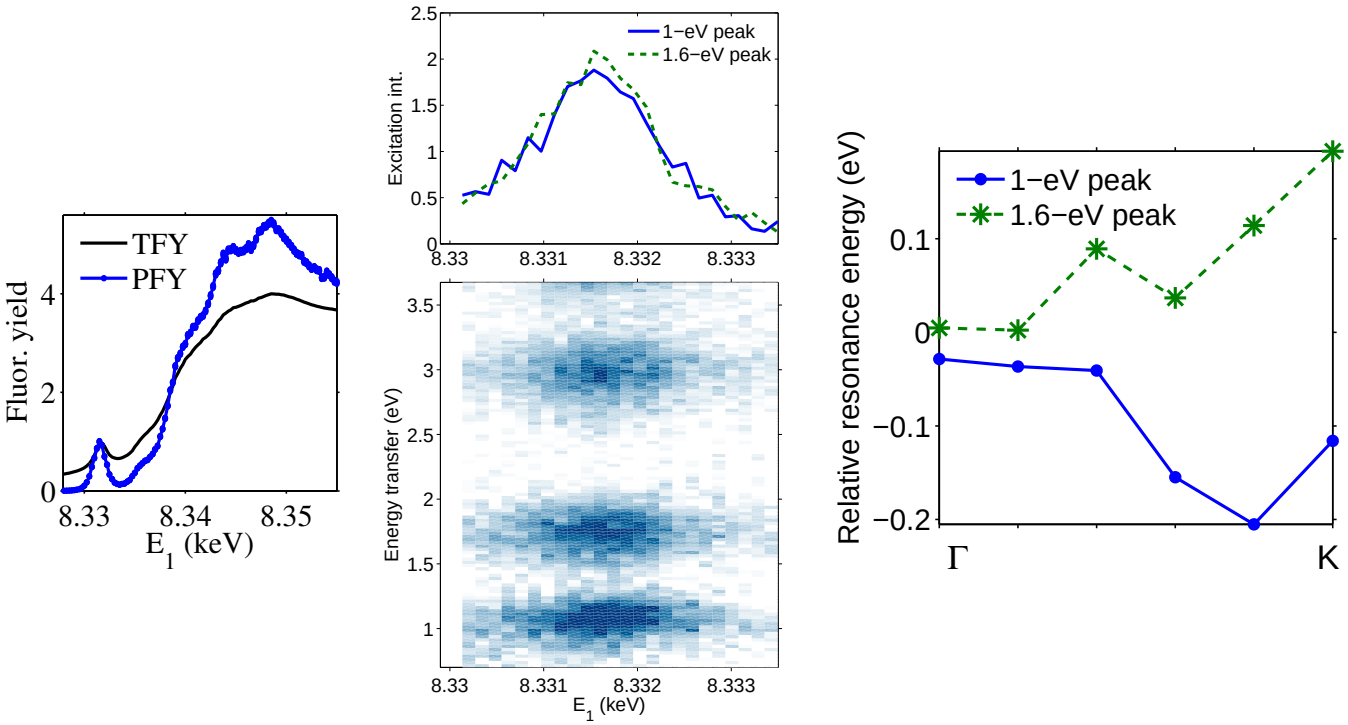

Figure 1. Left: X-ray absorption spectra of NiO measured with two techniques, total fluorescence yield (TFY) and partial fluorescence yield (PFY). The experiment concentrates on the prepeak at 8.332 keV. Middle: The RIXS map at the Γ point with the incident-energy dependence of the three d-d excitations. Right: relative peak resonances of the 1-eV and 1.6-eV peaks.

[1] H. Enkisch *et al.*, Phys. Rev. B 60, 8624 (1999)

[2] S. Huotari *et al.*, *Orbital energies of NiO in high pressure to up 55 GPa*, manuscript in preparation; ESRF experiment HE-2878.