



	Experiment title: Resonant Inelastic X-ray Scattering Study of NaV ₂ O ₅	Experiment number: HE-1372
Beamline: ID16	Date of experiment: from: 03 Apr 2003 to: 10 April 2003	Date of report: 25 Feb 2004
Shifts: 18	Local contact(s): Dr. G. Vanko	<i>Received at ESRF:</i>
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Report:

NaV₂O₅ is a highly correlated, low dimensional ladder system, which has been in the focus of intensive theoretical and experimental interest in the past few years after the discovery of a spin- and charge-ordering phase transition at $T_C = 34$ K. Above T_C the V atoms are in $V^{4.5+}$ state with one electron per V-O-V rung, giving rise to an antiferromagnetic spin- $\frac{1}{2}$ chains along the ladders. Below T_C the spin system goes to nonmagnetic spin-singlet state, opening a magnetic excitation gap. This is accompanied by a lattice dimerization. The exact nature of the charge disproportionation below T_C is still controversial. Coupled spin-charge dynamics arising from the antiferroelectric charge ordering (the system is a Mott insulator above and below T_C) in the ladder system is speculated to be responsible for opening up the spin gap. As in many Mott systems the strong electron correlation effects are evidenced by a charge-gap around the Fermi energy. The singly occupied d_{xy} band is split into two Hubbard subbands d_{xy} and d_{xy}^* opening the charge gap around the Fermi surface.

The aim of the experiment was to use resonant inelastic x-ray scattering at the V K -edge in single crystal NaV₂O₅ to probe the evolution of the empty Hubbard bands across T_C . The relatively low energy of the V K -edge at 5.4 keV was an experimental challenge and pioneering effort to exploit the low energy limits of RIXS technique at ESRF beamline ID16 was made at the course of this work. This included e.g. manufacturing of a novel Ge bend analyser crystal in ESRF, which was a major undertaking as previously only Si wafers had been tested.

The excitation associated with the upper Hubbard bands proved to have too low cross section to be measurable with the achieved intensity. Especially the novel Ge analyzer crystal throughput was not yet at the desired level. We believe that after some further effort with the Ge analyzer crystals, the upper Hubbard band excitations in NaV₂O₅ are achievable at ID16.

During the experiment we measured the polarized resonant inelastic scattering spectra at different crystallographic orientations using the V $1\bar{z} \rightarrow 3p$ decay channel. This way we could probe the spatial symmetry of the involved empty $3d$ states hybridized with the empty p symmetry states. The results, shown

in figure 1. for the scans where the scattered photon intensity is analyzed at fixed energy, show a considerable spatial asymmetry of the empty states near the fermi energy. Effort is currently on the way to model the spectra using computational approaches based on multiple scattering formalism and density-functional theory.

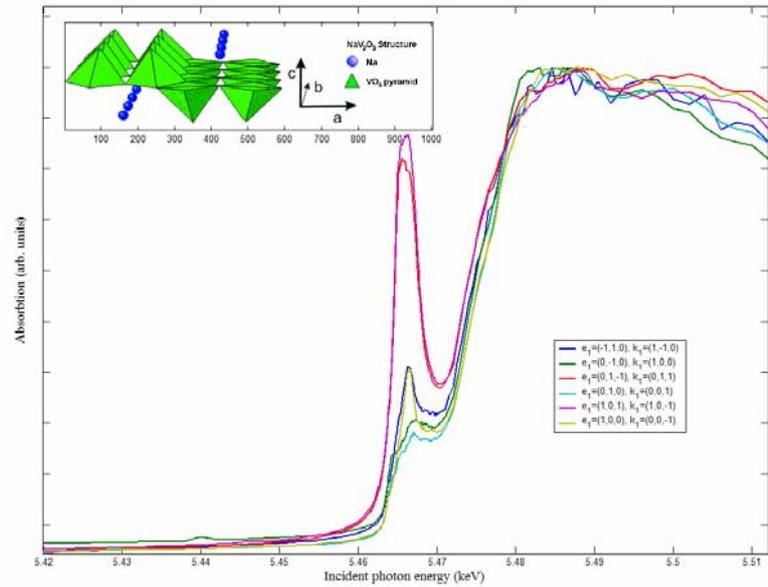


Figure 1. Resonant inelastic x-ray scattering at the V *K*-edge in NaV₂O₅.

