	Experiment title: Charge, orbital and/or, magnetic order in $NdNiO_3$	**Experiment number**: HE 945
Beamline: ID20	**Date of experiment**: from: 7.2.01 to: 13.02.01	**Date of report**: **27.8.01** *Received at ESRF:*
Shifts: 1 2	**Local contact(s)**: L. Paolasini	

Names and affiliations of applicants (* indicates experimentalists):

U. Staub* (Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland

G. I. Meijer* IBM Research, Zurich Research Laboratory, Rueschlikon, Switzerland

F. Fauth* ESRF

Report:

A prototype bandwidth controlled metal-insulator transition occurs in $RNiO_3$, R being the trivalent rare-earth ions (La to Lu) or Y. $RNiO_3$ exhibit a thermally driven metal-insulator transition at T_{MI} and a further transition to long-range antiferromagnetic order at $T_N \leq T_{MI}$. Since the two fold degenerate Ni orbital e_g is singly occupied, one may expect a significant Jahn-Teller distortion and associated orbital ordering (x^2-y^2/$3z^2$-r^2 type) in the insulation state of the $RNiO_3$ compounds [1]. Such a formation of an orbital superlattice could indeed explain the unusual magnetic ordering. Recently, high-resolution synchrotron powder diffraction found that $YNiO_3$ is monoclinic indicating a charge ordered ground state, however, no indication have been found for the larger R ions (e. g. Nd)[2].

The resonant X-ray scattering experiments focused on reflections of type (0hl) and (h0l) with both h and l odd. For non charge order $NdNiO_3$, these reflections have no contribution from the Ni site. Fig. 1a shows the energy dependence of the (105) and (015) reflections with σ–σ polarization in the insulating state at 20K. The spectra of the (105) show a strong maximum (minimum for (015)) at 8344 eV, approximately 10 eV above the Ni K-edge (8333 eV). This behavior is a clear evidence that these reflections contain a significant

contribution from the electronic states of the Ni ions. The observed scattering is not due to Templeton & Templeton scattering because we probe a diagonal element in the scattering tensor for σ–σ polarization. The resonant scattering of the (105) reflection is shown in Fig. 1b for different temperatures. The non resonant X-ray intensities as well as the energy dependence decrease for increasing temperatures. Above T_{MI} the scattering is independent of the energy with no longer a resonant contribution from Ni. This shows that there is a single electronic configuration of the Ni ions in the metallic phase. These experiments are direct proof for charge order at the metal-insulator transition of $NdNiO_3$, even though no monoclinic distortion can be observed with high-resolution powder diffraction.

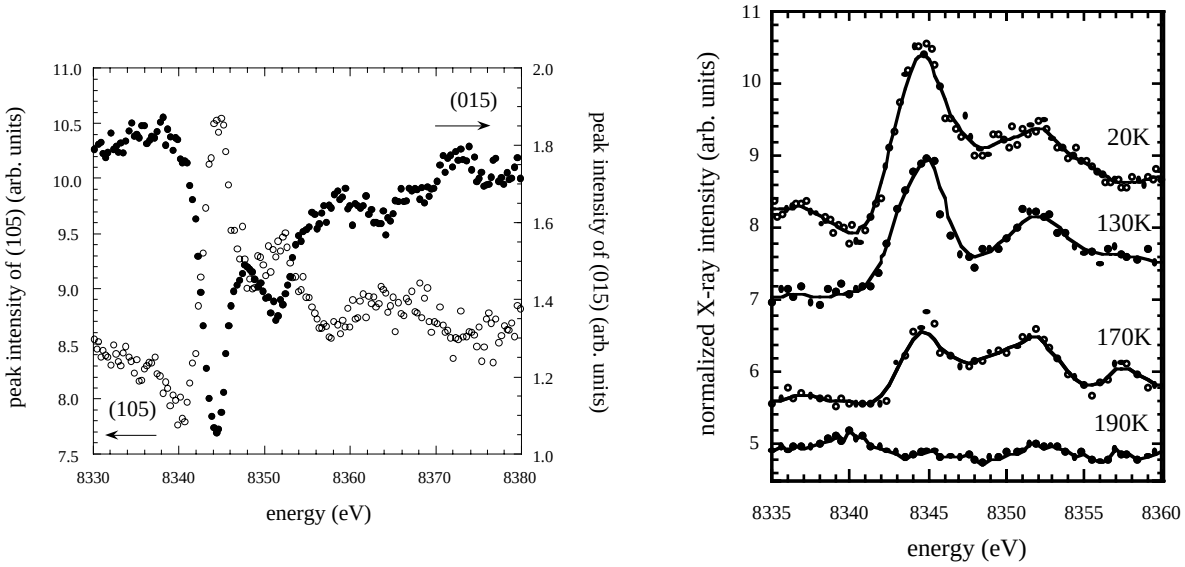

Fig. 1a Left: Energy dependent X-ray intensity of the (015) and (105) reflections taken at 20K with σ-σ polarization, which are sensitive to the charge order. The lines are guides to the eye. (filled circles (105); open circles (015)). 1b Right: Energy dependent X-ray intensity of the (105) reflection for selected temperatures. The lines are guides to the eye.

[1]J. Rodríguez-Carvajal, S. Rosenkranz, M. Medarde, P. Lacorre, M. T. Fernández-Díaz, F. Fauth and V. Trounov, Phys. Rev. B **57,** 456 (1998).
[2]J. A. Alonso, J. L. García-Muñoz , M. T. Fernández-Díaz, M. A. G. Aranda, M. J. Martínez-Lope and M. T. Casais, Phys. Rev. Lett. **82,** 3871 (1999).