Magnetic X-ray scattering and orbital ordering study of YVO_3 single crystal (ESRF: HE-607, ID20, April 14-20, 1999)

(Main proposer: Prof. Dr. G.A. Sawatzky, Univ. of Groningen)

We have recently reported on a peculiar magnetic property of YVO_3 single crystal: below the Neél temperature $T_N = 116$ K the magnetization in a small magnetic field first quickly increases with decreasing temperature and then starts decreasing and changes sign at 95 K, followed by a sudden 2nd sign reversal at 77 K[1]. We found that a first order phase transition occurs at 77 K, associated with a magnetic phase transition from a C-type antiferromagnetic ordering to a G-type one. There is also strong evidence for a crystal phase transition at 200 K, which we think is due to a change in orbital ordering[2].

Our measurements in last run at ID20, ESRF showed very interesting results. YVO_3 has $Pbnm$ orthorhombic symmetry at room temperature. In our experiment, reflections (201) and (300) which are forbidden by $Pbnm$ symmetry show a clear resonance at the V K-edge in the temperature region of 200 – 77 K as displayed in Fig. 1. The resonance occurs only in the $\sigma - \pi$ polarization geometry, not in $\sigma - \sigma$. The resonance signal for (201) is much stronger than for (300). A weak pre-edge resonance of reflection (300) was also noticed. Below 77 K, reflection (201) again showed strong resonance behaviour. However, we could not detect the (300) reflection below 77 K. It is not sure if the absence of (300) below 77 K was due to the fact that the crystal partly shattered on going through the first order phase transition. (After the measurements, it was found a half of the crystal used in the experiment was crashed.) We definitely need to re-study this below 77 K using a thin crystal which we know will stay in tact.

The intensity of the resonance peak increases with decreasing temperature as shown in Fig. 2. There is little anomaly on crossing the Neél temperature at 116 K. Attempt to measure the magnetic scattering using different polarization geometries did not succeed. This is most probably due to the fact that magnetic reflections might be coincident with reflections of orbital ordering below the Neél temperature.

To verify if the crystal structure changed below 200, reflection (201) which is forbidden by $Pbnm$ symmetry was measured at an off-resonant energy as a function of temperature as shown in Fig. 3. From this one can see that the crystal structure is further distorted below 200 K from the $Pbnm$ symmetry due to orbital ordering.

It is clear at this point that it is very crucial to perform azimuthal scans of the resonant reflections both below and above 77 K, in order to verify the above results and to give a detailed picture of the kind of possible orbital ordering.

---

[1] Y. Ren, T.T.M. Palstra, D.I. Khomskii, E. Pellegrin, A.A. Nugroho, A.A. Menovsky & G.A. Sawatzky. Nature, **396**, 441-444 (1998).

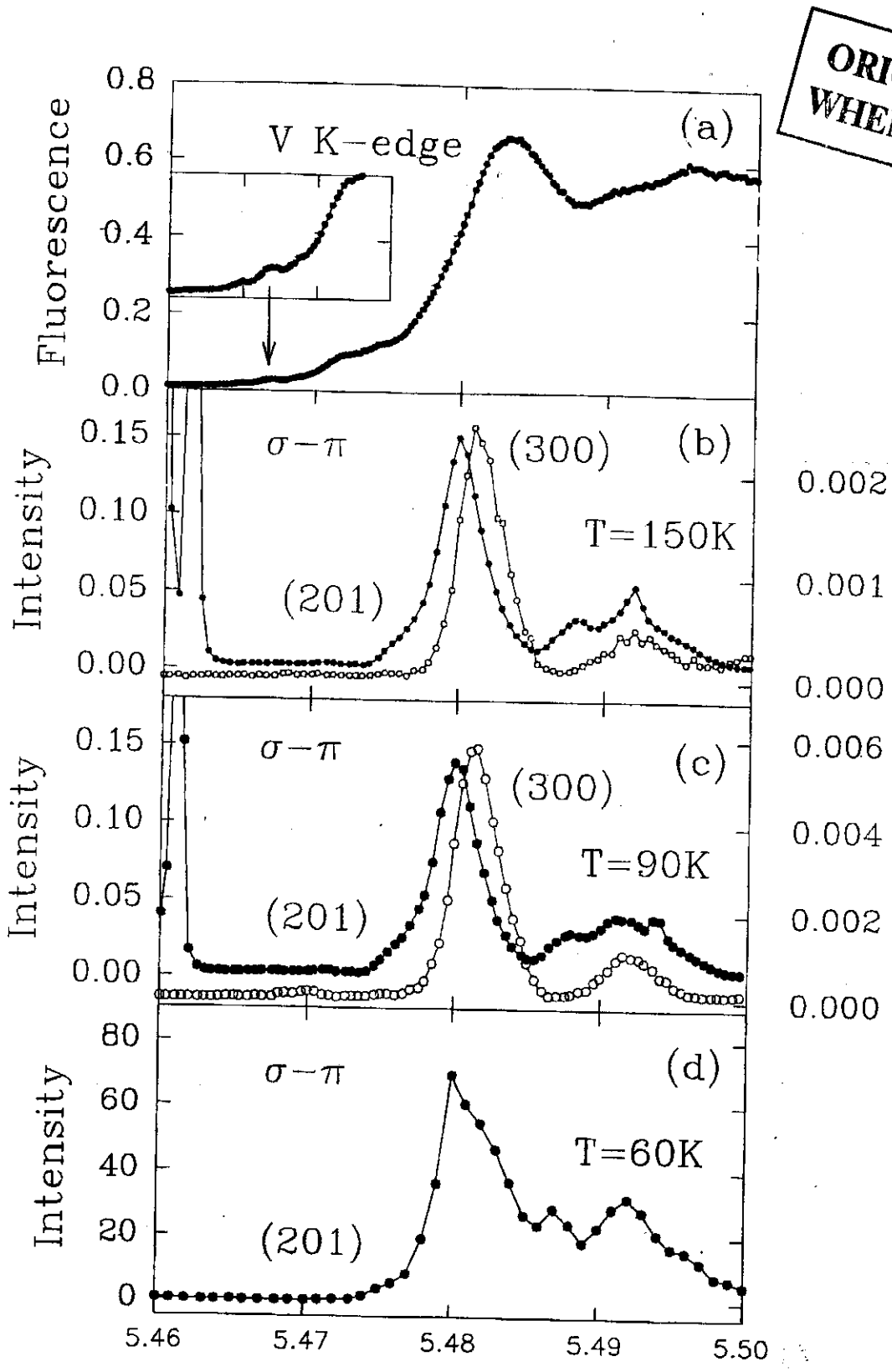
[2] Y. Ren, T.T.M. Palstra, D.I. Khomskii, A.A. Nugrohu, A.A. Menovsky & G.A. Sawatzky, submitted to Phys. Rev. B.

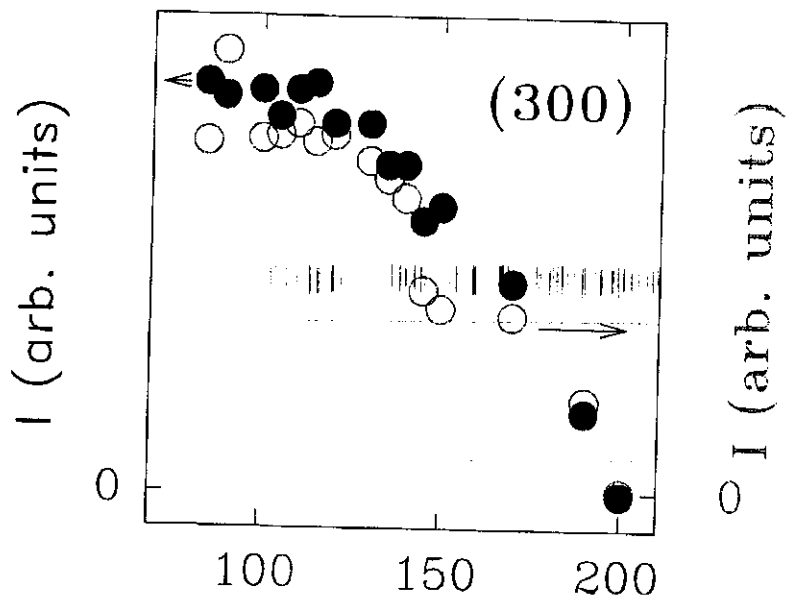
Figure captions

Fig. 1 : (a) V K-edge fluorescence spectrum. Energy-dependent resonance of the "forbidden" reflections (201) (filled circles) and (300) (open circles) in $\sigma - pi$ polarization geometry at (b) 150 K, (c) 90 K and (d) 60 K.

Fig. 2 : Resonant peak intensities of the (300) reflection at the V K-edge (filled circles) and at the pre-edge (open circles) as a function of temperature.

FIg. 3 : Intensity of reflection (201), forbidden in $Pbnm$, as a function of temperature near 200 K, measured in an off-resonant energy.


ORIGINAL WHEN RED
Fluorescence
V K-edge
(a)
0.8
0.6
0.4
0.2
0.0
Intensity
σ−π
(300)
(b)
T=150K
(201)
0.15
0.10
0.05
0.00
0.002
0.001
0.000
σ−π
(300)
(c)
T=90K
(201)
0.15
0.10
0.05
0.00
0.006
0.004
0.002
0.000
Intensity
σ−π
(d)
T=60K
(201)
80
60
40
20
0
Intensity
5.46
5.47
5.48
5.49
5.50



ORIGINAL WHEN RED

Fig. 2

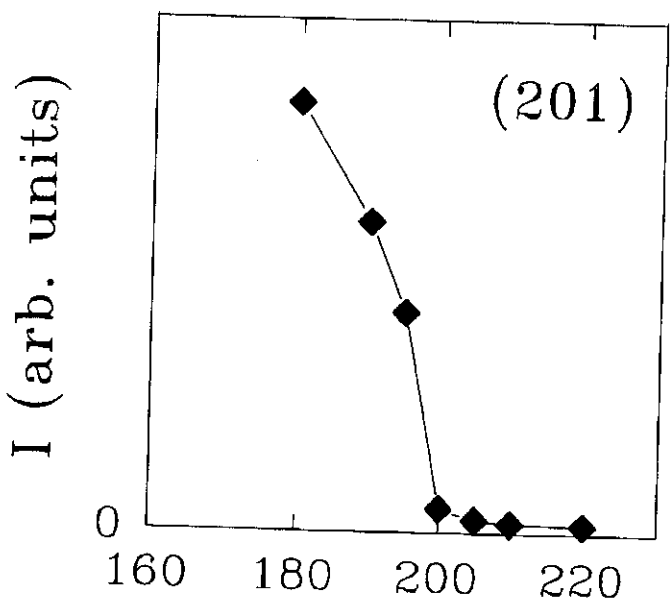


Fig. 3