



	Experiment title: Orbital and spin ordering of GdVO ₃	Experiment number: HE 2300
Beamline: BM28	Date of experiment: from: 22 nd November 2006 to: 28 th November 2006	Date of report: 28/02/2007
Shifts: 18	Local contact(s): L. Bouchenoire	<i>Received at ESRF:</i>
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Report:

The perovskite orthovanadates RVO₃ (R = rare earth) provide an ideal environment to study the orbital degree of freedom and its interplay with the spin, charge and lattice. There are two t_{2g} electrons in V³⁺, and these adopt the high-spin configuration $S = 1$ due to Hund's-rule coupling. One electron always occupies the d_{xy} orbital due to the orthorhombic distortion, and the other electron occupies one of two possible states, d_{yz} or d_{zx} . The low temperature magnetic structure of GdVO₃ is C-type, with spins arranged ferromagnetically along the c direction and antiferromagnetically in the ab plane [1]. According to the Goodenough-Kanamori rules, this should lead to G-type orbital ordering (OO) with alternating occupation of orbitals in all three directions [2].

We have studied the OO in zero field by resonant x-ray scattering using BM28 at the ESRF. G-type OO was found at $Q=(011)$, and the observed resonant energy line shape in the σ - π channel is shown in Fig. 1. The agreement with *ab-initio* calculations of the orbital signal at the V K edge [4,5] shows that we are detecting the orbital ordering. The observed azimuthal dependence of the resonant x-ray scattering intensity shown in Fig. 2 agrees with the calculations for the proposed G-type OO model. Finally, the order parameter in Fig. 3 indicates an onset temperature $T_{OO} = 200$ K, in agreement with heat capacity measurements.

[1] L.D. Tung, *Phys. Rev. B*, **73**, 024428 (2006).

[2] J.B. Goodenough, *Magnetism and chemical bond*. Interscience: New York, (1963).

[3] Y. Joly, *Phys. Rev. B* **63**, 125120 (2001).

[4] Y. Joly, S. Di Matteo and C.R. Natoli, *Phys. Rev. B* **69**, 224401 (2004).

Fig. 1. The energy lineshape of the resonant x-ray signal with Q fixed at (011). The two large peaks at the $4p$ edge are the signature of orbital ordering [4].

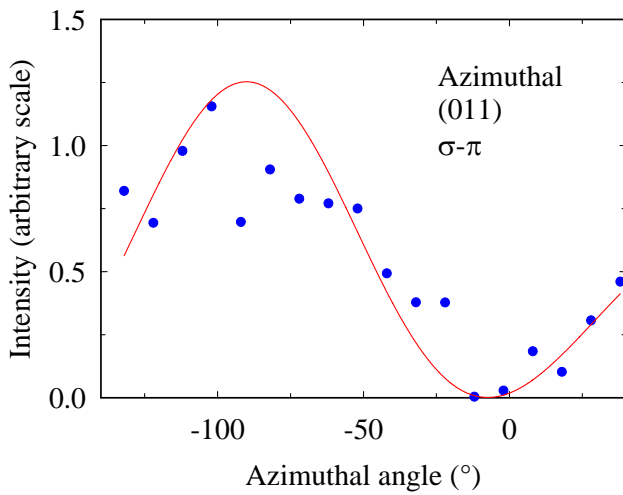
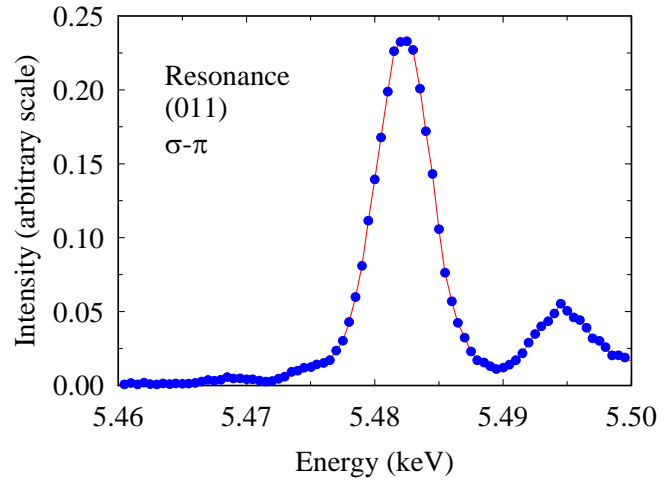


Fig. 2. The integrated intensity of the (011) reflection as a function of azimuthal angle. The solid line shows the calculated dependence for G-type orbital ordering.

Fig. 3. The integrated intensity of the (011) reflection as a function of temperature. The onset temperature $T_{OO}=200\text{K}$ agrees with the observed peak in the heat capacity for GdVO_3 .

