# Orbital Ordering in $YVO_3$

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## Introduction

A neutron scattering study reveals that $YVO_3$ has two magnetic ordering phases. Below the first Neel temperature $T_{N1}$=118 K, the magnetic structure is antiferromagnetic in the ab plane and ferromagnetic along the c axis (so-called C type). In the low-temperature phase below $T_{N2}$~77 K, however, the $V^{3+}$ spins are anti-ferromagnetically arranged both in the ab plane and along the c axis (so-called G-type magnetic structure). The change in magnetic structure should be caused by a sign reversal in the super-exchange interaction between neighboring $V^{3+}$ ions along the c axis. It is well established that such a sign reversal can be led for different orbital occupations in a material with orbital ordering.[1]

## Experimental

Resonant x-ray diffraction experiments were performed at the beamline 4C of the Photon Factory, Japan. We have tuned the incident energy near the $V^{3+}$ K-edge by double Si(111) crystals. The typical energy resolution was 2 eV. The beam with the electric field perpendicular to the scattering plane ($\sigma$ polarization) was focused on a single-domain $YVO_3$ crystal by a bent cylindrical mirror. The sample was mounted in a closed-cycle He refrigerator on a four-axis diffractometer.

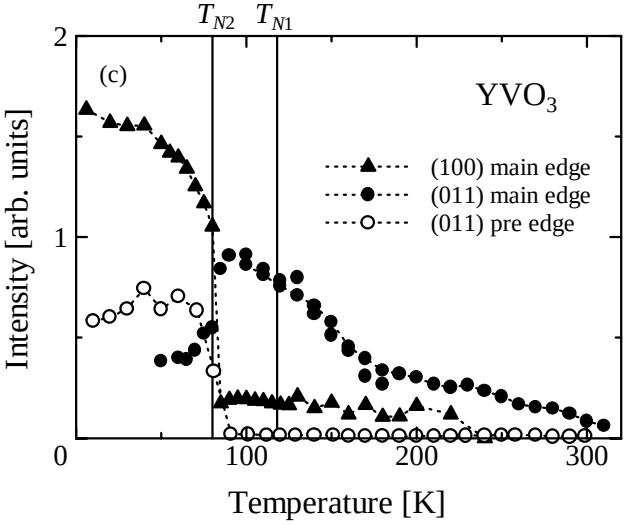


Fig. 1 Temperature dependence of the intensities of superlattice reflections.

## Results

Temperature dependence of the integrated intensity of the superlattice scattering at the main edge in a warming run is displayed in Fig. 1. Here the (011) intensity at the pre-edge is also plotted. The (100) reflection at the main edge suddenly reduces intensity as increasing temperature beyond $T_{N2}$. On the contrary, the (011) reflection at the main edge becomes stronger with a small jump as heating beyond $T_{N2}$. The (011) reflection below $T_{N2}$ might be due to the C-type orbital ordering in the distorted perovskite structure as indicated by azimuthal-angle dependence. The temperature dependence of the x-ray reflections around $T_{N2}$ is opposite of that of neutron magnetic scattering with the same indices.[2]

The (011) reflection at the pre-edge is similar in temperature dependence to the (100) reflection at the main edge. Further theoretical studies are necessary to interpret the present data. The mechanism of the x-ray resonant reflection at the 1s-3d absorption edge is not clear yet except for the cases with no inversion symmetry. The process of the pre-edge resonance would possibly be enhanced by the elongation of the $VO_6$ octahedra.

The results of the resonant scattering at the main edge strongly demonstrate a change in orbital ordering from C-type to G-type at $T_{N2}$ in the manner of a first-order transition. The C-type orbital ordering in the low-temperature phase well corresponds to the cooperative distortion of $VO_6$ octahedra below $T_{N2}$. In opposition, the G-type orbital ordering is not associated with Jahn-Teller distortion, because it would violate the mirror symmetry normal to the c axis of a Pbnm lattice system. The (011) intensity reaches a maximum at around 100 K and then gradually decreases with a small kink at around 180 K. One cannot see any anomaly at $T_{N1}$. The G-type orbital ordering appears not only in the intermediate-temperature C-type AFM phase but also in the high-temperature paramagnetic phase.

## References

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