Materials Science

Orbital Ordering in RVO₃ Studied by a Resonant X-ray Scattering

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Introduction

Perovskite-type vanadium oxides, RVO₃ (R: rare earth or Y), have two 3d electrons on the V^{3+} ions, which have the orbital degree of freedom of t_{2g} electron. As a result, RVO₃ shows various physical properties coupled with the orbital and spin states depending on *R*-ions [1]. Recently, the pressure effect on the orbital ordering in RVO_3 has been systematically investigated by high-pressure and low-temperature x-ray diffraction experiment [2]. They indicated that the pressure generally stabilizes the C-type orbital ordering (C-OO) phase, and proposed that the covalency among the *R*-ion d, the oxygen 2p, and the vanadium 3d orbitals is a key parameter for the stabilization of C-OO phase. However, the orbital state under the high pressure is not clear so far. The resonant xray scattering (RXS) is one of the techniques for measuring the order-parameter of the orbital ordering and determining the wave function of the ordered orbitals. Using the RXS technique we have therefore investigated the orbital state in YVO₃ at ambient pressure preparatory to high-pressure RXS experiment.

Experiments

The high quality single crystal of YVO_3 was grown by a floating-zone technique. The (0 0 1) surface was cut and polished with fine emery paper. The RXS experiments were performed by four-circle diffractometer at beam lines 4C and 3A in the Photon Factory. The incident beam was monochromatized by a pair of Si(111) crystals, giving an energy resolution about 2 eV, and focused by a bend cylindrical mirror. The x-ray energy near the V *K*edge (~5.48 keV) was utilized for measuring the RXS signal. Polarization analysis was performed using a PG(004) analyzer crystal. For low temperature experiment, the sample was mounted in a closed cycle He cryostat.

<u>Results</u>

YVO₃ shows two successive phase transition at $T_{\rm OO1}$ ~200K and at $T_{\rm OO2}$ ~80K: the transition from the orbital disordered (OD) state to the G-type orbital ordering (G-OO) is observed at $T_{\rm OO1}$, and the G-OO transforms to the C-OO at $T_{\rm OO2}$ (< $T_{\rm OO1}$). The orbital ordering in the G-OO phase was estimated by the azimuthal angle dependence of the RXS at (0 1 1) [3]. However, the result was not clear. Here we found new

RXS signal of σ -> σ ' scattering component at (0 0 1) which resonates near the V *K*-edge energy shown in Fig. (a). The temperature dependence of the RXS intensity was also observed at *E*=5.48keV as shown in Fig. (b). As a result, the signal is only observed in the G-OO phase, and completely disappears in the C-OO and OD phases. We therefore expect to be able to estimate the order parameter of the G-OO phase using the RXS signal. This signal will be important to determine orbital states under high pressure.

References[1] S. Miyasaka et al., Phys. Rev. B **68** (2003) 1000406. [2] D. Bizen et al., Phys. Rev. B 78 (2008) 224104. [3] M. Noguchi et al., Phys. Rev. B **62** (2000) 9271. * hironori.nakao@kek.jp

