Alignment of crystalline domains by magnetic field in spinel FeV_2O_4

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Introduction

It is now widely accepted that the orbital degrees of freedom of localized electrons play important roles in determining various properties of materials. Recently, the orbital ordering of triply degenerate t_{2g} states have been extensively studied, for example, in perovskite vanadates (LaVO₃) and spinel vanadates (ZnV₂O₄, MnV₂O₄), both having V³⁺ ions with two *d* electrons in the t_{2g} states. However, most compounds studied thus far with regard to this issue have only one site having an orbital degree of freedom; however, the manner in which the orbital degrees of freedom at different sites compete or cooperate with each other has not yet been studied.

Here, spinel oxides (AB_2O_4) with two different magnetic ions at the tetrahedral site (A site) and the octahedral site (B site), both of which have orbital degrees of freedom, are appropriate for studying this issue. In FeV₂O₄, Fe³⁺ ion in the d^6 high-spin electron configuration occupies the tetrahedral site of the spinel structure (surrounded by four oxygen ions on the corner of a tetrahedron), where there are three electrons in the doubly degenerate *e* states. On the other hand, the V³⁺ ion in the d^2 high-spin electron configuration occupies the octahedral site (surrounded by six oxygen ions on the corner of an octahedron), where there are two electrons in the triply degenerate t_{2a} states.

Experiment

Single crystals of FeV_2O_4 were grown by the floating-zone method in Ar gas flow. X-ray diffraction measurement was carried out at BL-4C (without magnetic field) with a wavelength of 1.127 Å and at BL-3A (with magnetic field) with a wavelength of 0.8856 Å.

Results

Figure 1 (a) shows the (800) peak of X-ray diffraction at various temperatures. The peak is split into two peaks (110 K); it then splits into three peaks (100 K), before merging into two peaks again (60 K) with decreasing temperature. There exists further splitting at 10 K. This indicates that the crystal structure changes from cubic, tetragonal, orthorhombic, tetragonal, and orthorhombic again with decreasing temperature. The lattice constants obtained from the position of the diffraction peak are plotted as a function of temperature in Fig. 1 (b). The *c*-axis is shorter than the other axis in the high-temperature (HT) tetragonal phase, while it is longer in the low-temperature (LT) tetragonal phase.

Figure 1 (c) shows the (800) peak at 40 K in the LT tetragonal phase at 0 T and 0.2 T. The peak at the lower

angle corresponds to the (008) peak and that at the higher angle corresponds to the (800) peak. These two peaks come from different tetragonal domains with different directions of the *c*-axis as shown in the inset. With an applied filed of 0.2 T, the (008) peak disappears but the intensity of the (800) peak increases. In this experiment, magnetic field is applied perpendicular to the scattering vector as well as along a principal axis of the cubic phase, and thus for the tetragonal domain contributing to the (008) peak, magnetic field is applied along the *a* axis. Accordingly, the disappearance of the (008) peak indicates that the *c*-axis is aligned along the magneticfield direction at 0.2 T in the LT tetragonal phase. Associated with this domain alignment, a large magnetostriction (~1%) is observed in this compound.



Fig. 1 (a) X-ray diffraction on a single crystal of FeV_2O_4 around the (800) peak at various temperatures. (b) Temperature dependence of lattice constants. (c) X-ray diffraction on a single crystal of FeV_2O_4 around the (800) peak without and with magnetic field (0.2 T). The inset shows the three domains contributing the (008) and (800) peaks.

Reference

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