Poster Presentation

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Orbital Order and Structural Phase Transitions in Vanadium Spinel FeV_2O_4

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Orbital degrees of freedom plays an important role in condensed matter physics because it is strongly related with phase transitions and induces the fascinating physical properties. A spinel oxide FeV_2O_4 is one of the peculiar examples because this compound has double orbital degrees of freedom at both Fe^{2+} and V^{3+} ions. Furthermore, this material represents exotic physical properties [1,2], i.e.; multiferroic, large magnetostriction, and successive structural transitions with decreasing temperature: cubic - tetragonal ($c < a$: tetraHT, 138K) - orthorhombic (orthoHT, 108 K) - tetragonal ($c > a$: tetraLT, 68 K). However, the origin of structural transitions and physical properties is controversial until now. In order to clarify the origin, we have performed synchrotron x-ray diffraction experiments at low temperatures at beamline BL02B2 (for the powder samples) in SPring-8 and BL-4C (for the single crystal) of the Photon Factory, KEK. Furthermore, we have carried out the magnetization and the specific heat measurements using polycrystalline samples and single crystal of FeV_2O_4. We have firstly found another orthorhombic phase (orthoLT) below 30 K in the polycrystalline sample of FeV_2O_4, shown in figure 1. The Rietveld analysis was performed, and the overall qualities of fittings were fairly good. In order to investigate the details of the orbital state of Fe^{2+} and V^{3+} in FeV_2O_4, we have performed the normal mode analysis, which is based on static displacements of the tetrahedron of FeO_4 and octahedron of VO_6. In the orthoLT phase, we found the orbital order of Fe^{2+} ions, which is mixture of $3z^2$-r^2 and y^2-z^2 orbitals, without change of orbital order of V^{3+} ions. This result indicates that the origin of the orthoLT phase is derived from the competition between cooperative Jahn-Teller effect and relativistic spin-orbit coupling of Fe^{2+} ions. We also discuss the origins of the other phase transitions considering the orbital state of V^{3+} and Fe^{2+} ions, and then the orbital dilution effect, where the structural and magnetic properties are investigated by using powder samples substituted for Fe^{2+} and V^{3+} ions by other ions (Mn^{2+} and Fe^{3+}) with no orbital degrees of freedom.

[1] *T. Katsufuji et al. J. Phys. Soc. Jpn., 77, 053708 (2008),* ***[2]*** *Y. Nii et al., Phys. Rev. B, 86, 125142 (2012)*

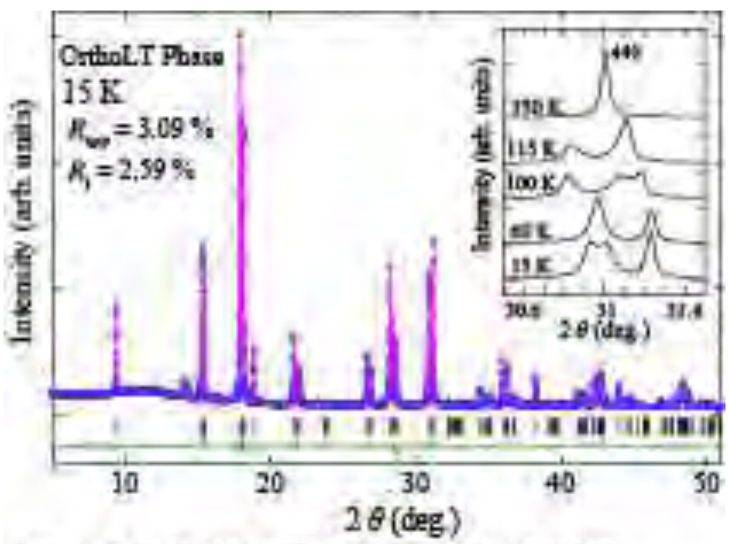

Figure 1. Results of Rietveld analysis for FeV_2O_4 at 15K. The inset shows the temperature dependence of the synchrotron powder diffraction around the 440 cubic Bragg reflection.

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