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Synchrotron x-ray single-crystal structure analysis of a spinel oxide FeV_2O_4 with spin and orbital degrees of freedom YOICHI NII, HAJIME SAGAYAMA, TAKA-HISA ARIMA, IMRAM, Tohoku University , RIU SAKAI, SHINOBU AOYAGI, EIJI NISHIBORI, HIROSHI SAWA, Department of Applied Physics, Nagoya University, KUNIHISA SUGIMOTO, SPring-8/JASRI, HIROYUKI OHSUMI, MASAKI TAKATA, RIKEN SPring-8 Center — It has been reported that FeV_2O_4, which has orbital and spin degrees of freedom both in tetrahedral $Fe^{2+}(d^6)$ sites and octahedral $V^{3+}(d^2)$ sites, exhibits successive structural phase transitions, accompanying a ferrimagnetic transition. The origin of the phase transitions is supposed to be a cooperation and/or competition between the orbital and spin degrees of freedom both in Fe^{2+} and V^{3+}. By a synchrotron x-ray single-crystal structure analysis, we determined the space group and atomic coordinate of each phase (cubic- HT-tetra.- HT-ortho.- LT-tetra.). The results suggest that the HT-tetra. (a>c) and HT-ortho. phases should be ascribed to the FeO_4 local compression, whereas VO_6 elongation should be responsible for the LT-tetra. (c>a) phase. We also discuss the orbital ordering (OO) pattern assuming strong electron-lattice coupling. A conceivable OO pattern of V^{3+} at the LT-tetra. (c>a) is *ferroic* one with *yz* and *zx* orbitals occupied, which is unique among spinel-type vanadates.

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