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Observation of the orbital fluctuation in $Y_{1-x}Ca_xTiO_3$ by using soft x-ray linear dichroism

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We have performed measurements of linear dichroism in x-ray absorption (XLD) at Ti $L_{2,3}$ edges of a Mott-insulating ferromagnet $YTiO_3$ [1], where orbital ordering occurs in the triply degenerate Ti $3d$ t_{2g} states. The crystal structure is of a distorted perovskite one (orthorhombic $GdFeO_3$-type, space group: $Pbnm$), which is very similar to the skutterdite structure. Dichroic spectra and their integrated intensities have been obtained for the incident electric field with polarizations parallel to a, b, and c axes. The observed fine structures in the XLD spectra for $YTiO_3$ originate from the orbital polarization at each Ti-site. The comparison of the spectra with atomic multiplet calculations on the basis of the Mizokawa-Fujimori scheme [2] removes the ambiguity about the orbital polarization, i.e., the relative weights of $|xy\rangle$, $|yz\rangle$, and $|zx\rangle$ orbits, which are crucial for the origin of ferromagnetism. The observed spectra at the Ti $L_{2,3}$ are well reproduced by using the wave functions $0.8|zx\rangle - 0.6|yz\rangle$ and $0.8|zx\rangle + 0.6|yz\rangle$, which are alternately arranged in the Ti sites 1, 2 and 3, 4, respectively. These coefficients of the wave functions were determined by the '*trichroism*' method, that is, comparison between the calculation and the experimental spectra for the three planes. These results are consistent with those proposed by the nuclear magnetic resonance measurement [3] in the ferromagnetic state of $YTiO_3$. Furthermore we have studied Ca-substitution effect on the orbital polarizations in $YTiO_3$. In the range of $0 \leqq x \leqq 0.2$ of $Y_{1-x}Ca_xTiO_3$, the energy dependence of their dichroic spectra do not change but their integrated intensities gradually weaken and seems to vanish toward x=0.4, where insulator-to-metal transition occurs. This behavior means that the orbital fluctuation grows with increase of x and vanishment of orbital order may coincide with metal-insulator transition. Similar x dependence of orbital fluctuation was also observed in the resonant x-ray scattering [4]. In conclusion, since the XLD method by using synchrotron radiation is applicable to the paramagnetic system without applying a magnetic field, it is a promising technique to determine the orbital order in various $3d$-transitional metal oxides as well as some kinds of f-electron compounds which show quadrupole ordering.

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